wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:50 PM BST

PDB ID	:	3J3S
EMDB ID:	:	EMD-5608
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	:	11.00 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

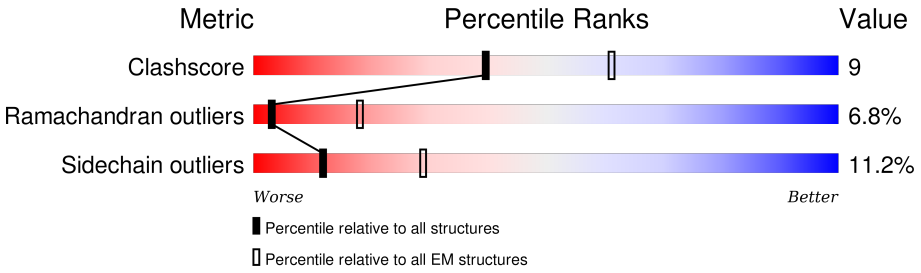
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 11.00 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	31% 9% • 57%
1	2	218	31% 10% • 57%
1	3	218	28% 12% • • 57%
1	4	218	31% 10% • 57%
1	5	218	30% 11% • 57%
1	6	218	31% 10% • 57%
2	A	810	66% 28% • ••
2	B	810	66% 26% 5% ••
2	C	810	70% 23% 5% ••

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Mol	Chain	Length	Quality of chain
2	D	810	65% 28% 5%
2	E	810	69% 22% 6%
2	F	810	68% 25%

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	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
B	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571

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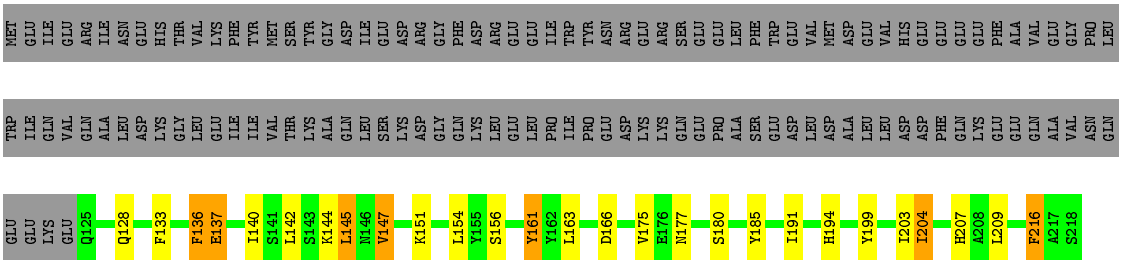
Chain	Residue	Modelled	Actual	Comment	Reference
C	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
D	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
E	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571
F	618	ALA	GLU	ENGINEERED MUTATION	UNP P37571

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.

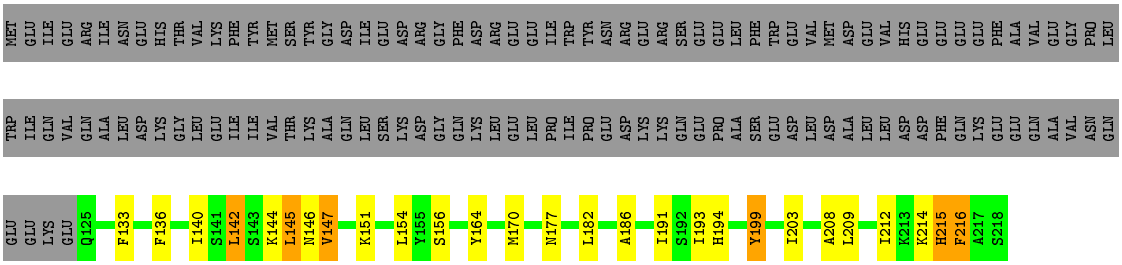
- Molecule 1: Adapter protein MecA 1

Chain 1:



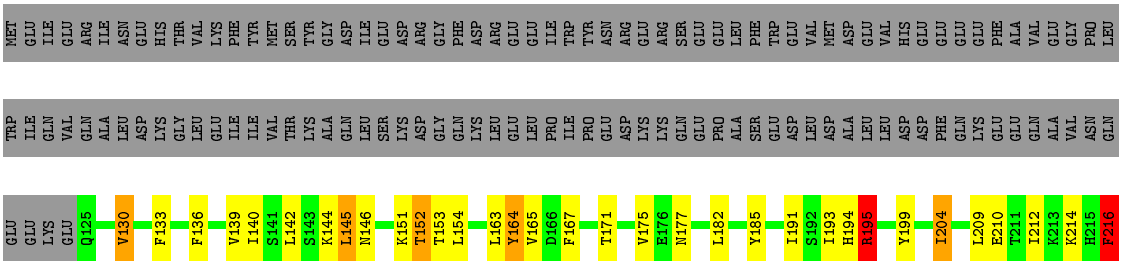
- Molecule 1: Adapter protein MecA 1

Chain 2:



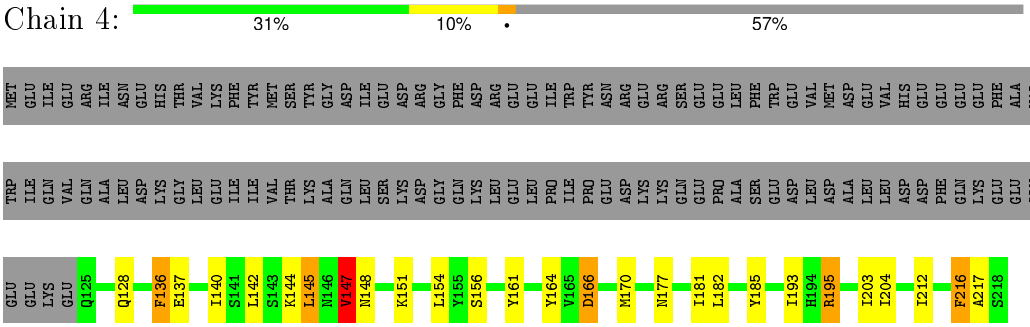
- Molecule 1: Adapter protein MecA 1

Chain 3:



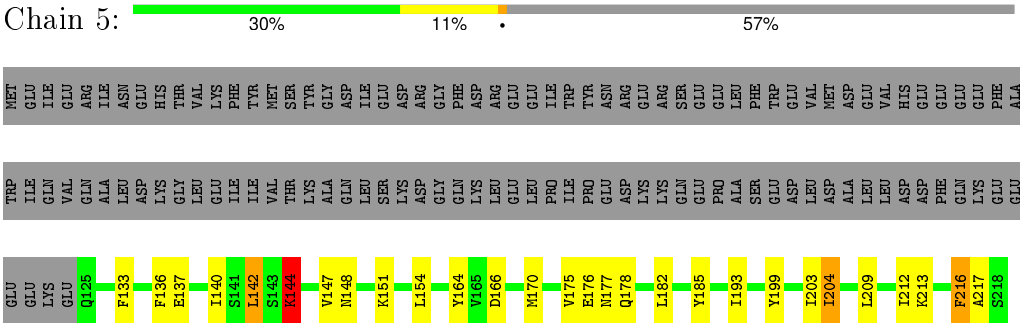
- Molecule 1: Adapter protein MecA 1

Chain 4:



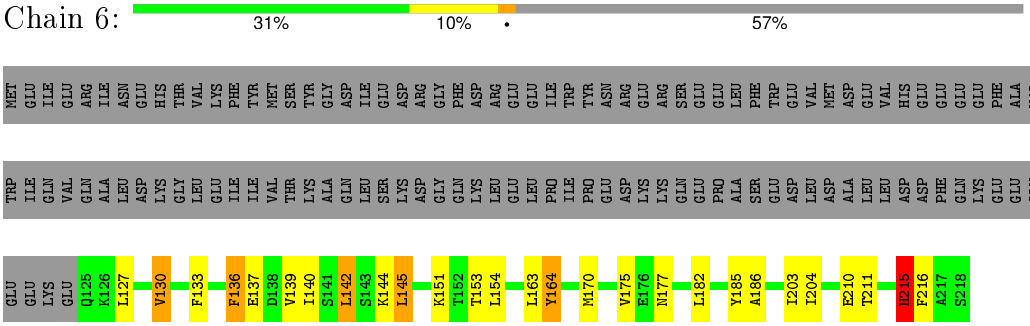
- Molecule 1: Adapter protein MecA 1

Chain 5:



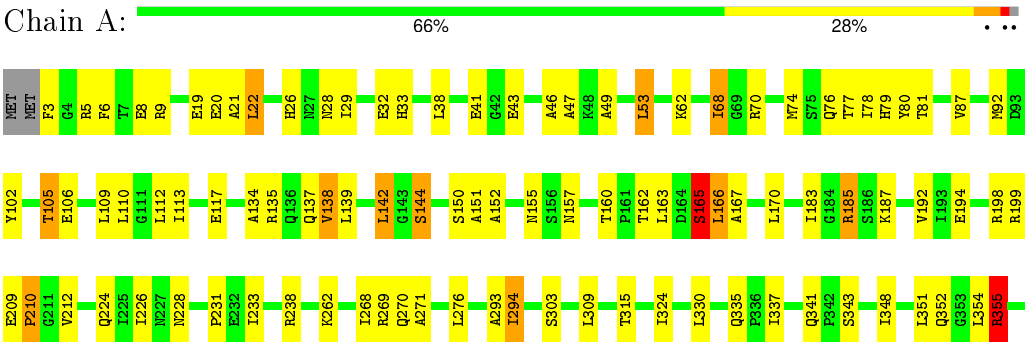
- Molecule 1: Adapter protein MecA 1

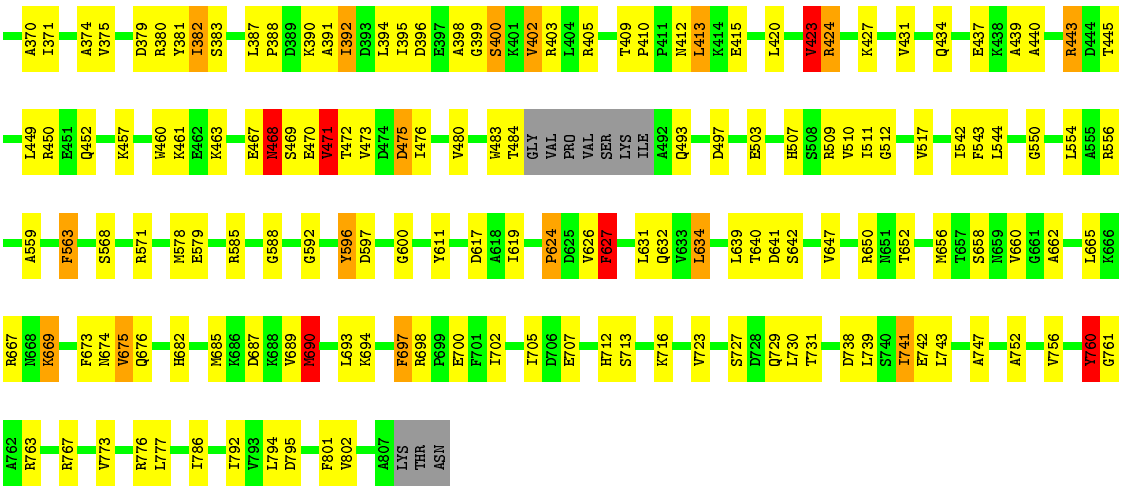
Chain 6:



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

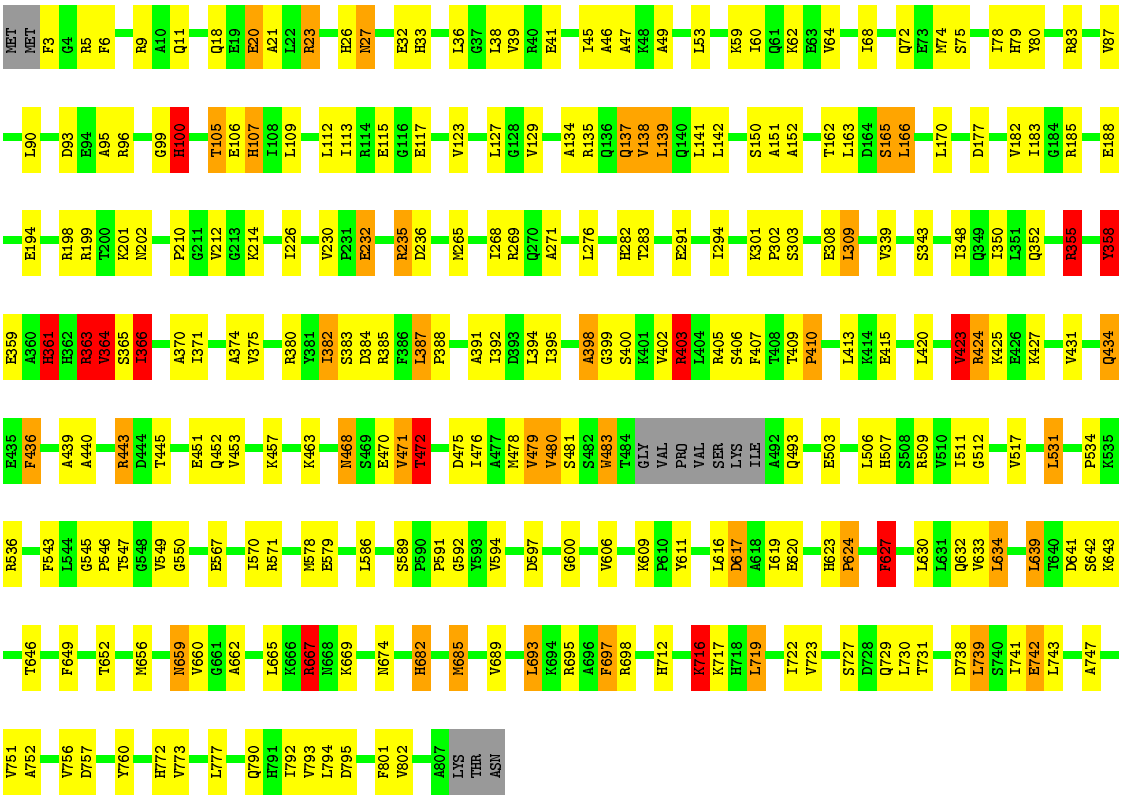
Chain A:





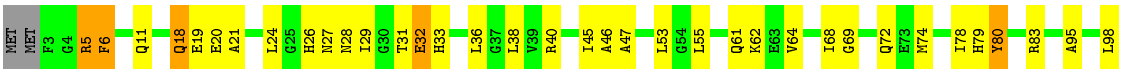
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

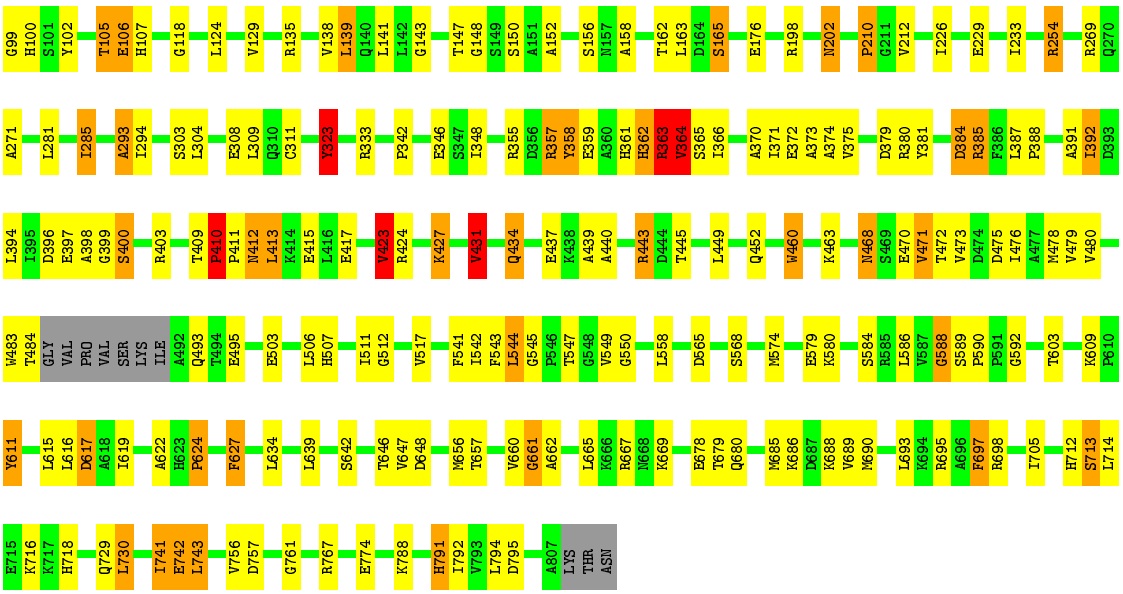
Chain B:



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

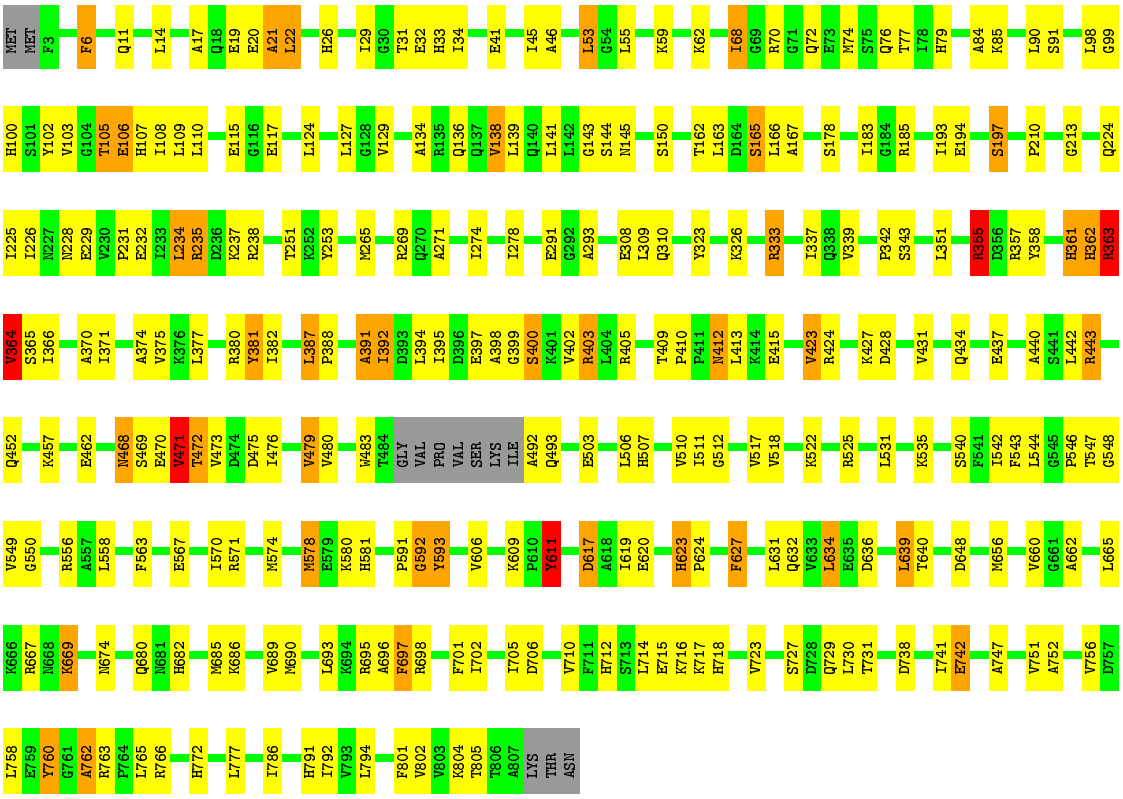
Chain C:





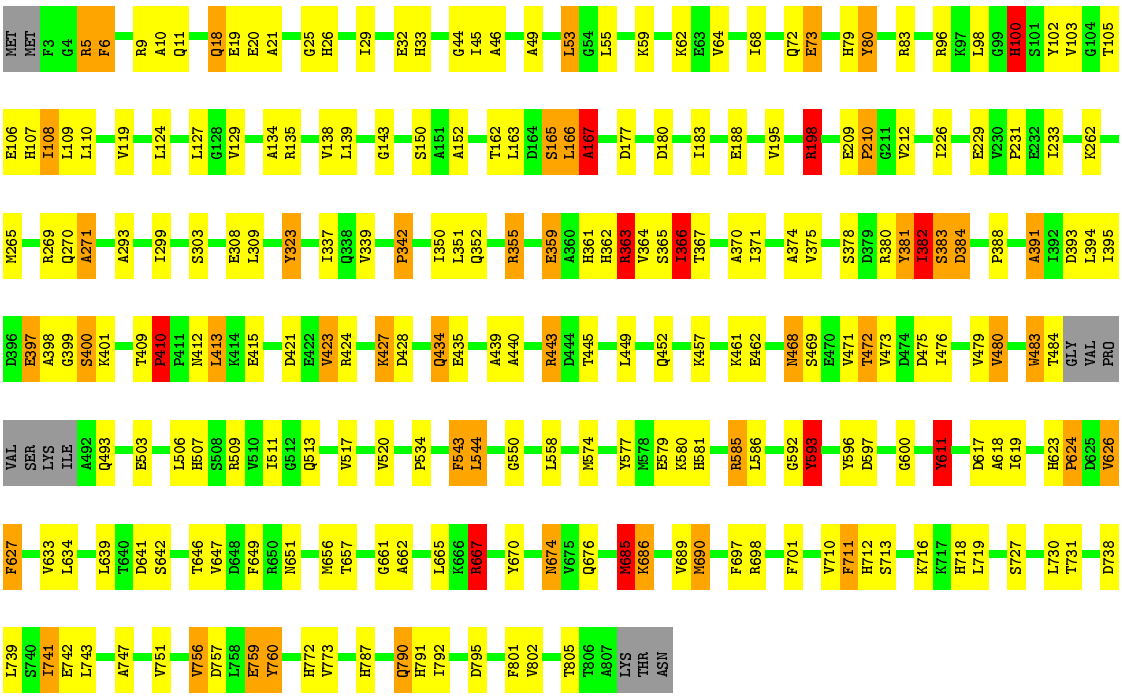
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

Chain D:



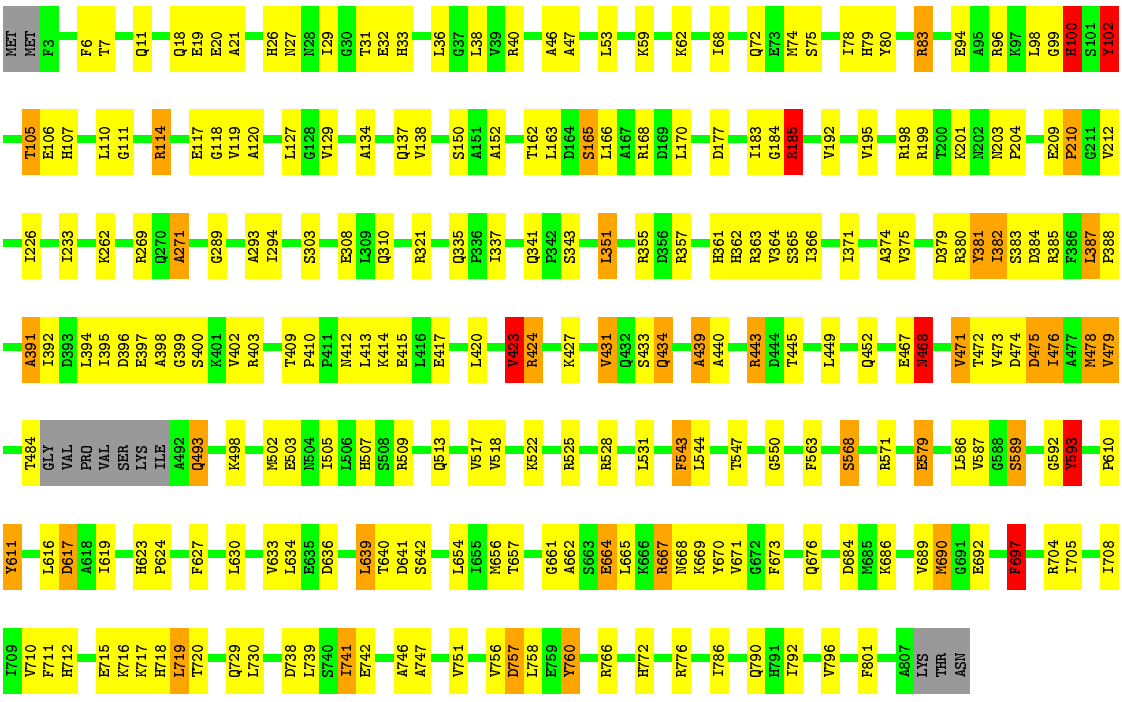
• Molecule 2: Negative regulator of genetic competence ClpC/MecB

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	41902	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)	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	0.98	0/791	1.31	4/1064 (0.4%)
1	2	0.97	0/791	1.28	3/1064 (0.3%)
1	3	0.97	0/791	1.34	5/1064 (0.5%)
1	4	0.99	0/791	1.26	3/1064 (0.3%)
1	5	0.96	0/791	1.29	4/1064 (0.4%)
1	6	0.99	0/791	1.36	5/1064 (0.5%)
2	A	1.00	0/6269	1.26	27/8441 (0.3%)
2	B	1.00	0/6269	1.30	32/8441 (0.4%)
2	C	0.99	0/6269	1.27	28/8441 (0.3%)
2	D	1.00	0/6269	1.28	29/8441 (0.3%)
2	E	0.99	0/6269	1.29	36/8441 (0.4%)
2	F	1.01	0/6269	1.28	24/8441 (0.3%)
All	All	1.00	0/42360	1.28	200/57030 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
1	2	0	1
1	3	0	4
1	4	0	1
1	5	0	1
1	6	0	2
2	A	0	19
2	B	0	20
2	C	0	12
2	D	0	17
2	E	0	15
2	F	0	14
All	All	0	107

There are no bond length outliers.

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	593	TYR	CB-CG-CD2	9.71	126.83	121.00
2	F	593	TYR	CB-CG-CD1	-8.53	115.88	121.00
2	E	167	ALA	N-CA-CB	8.31	121.74	110.10
2	C	588	GLY	N-CA-C	-8.22	92.55	113.10
2	E	611	TYR	CB-CG-CD2	-7.59	116.44	121.00
2	E	543	PHE	CB-CG-CD1	7.53	126.07	120.80
2	A	165	SER	C-N-CA	7.49	140.43	121.70
2	F	760	TYR	CB-CG-CD2	7.49	125.49	121.00
2	E	760	TYR	CB-CG-CD1	-7.40	116.56	121.00
2	F	760	TYR	CB-CG-CD1	-7.38	116.57	121.00
2	E	381	TYR	CB-CG-CD1	-7.34	116.59	121.00
1	1	136	PHE	CB-CG-CD1	7.34	125.94	120.80
2	F	543	PHE	CB-CG-CD2	-7.32	115.68	120.80
2	C	543	PHE	CB-CG-CD2	-7.14	115.80	120.80
2	B	165	SER	C-N-CA	7.08	139.40	121.70
2	E	543	PHE	CB-CG-CD2	-7.08	115.85	120.80
1	3	199	TYR	CB-CG-CD1	-7.07	116.76	121.00
2	F	165	SER	C-N-CA	7.06	139.35	121.70
2	D	253	TYR	CB-CG-CD2	7.06	125.24	121.00
2	D	165	SER	C-N-CA	6.99	139.17	121.70
2	A	627	PHE	CB-CG-CD2	-6.89	115.97	120.80
2	B	543	PHE	CB-CG-CD2	-6.89	115.98	120.80
2	D	423	VAL	CA-CB-CG1	-6.87	100.59	110.90
2	E	760	TYR	CB-CG-CD2	6.87	125.12	121.00
2	E	364	VAL	C-N-CA	6.86	138.86	121.70
2	E	6	PHE	CB-CG-CD1	-6.78	116.06	120.80
2	E	423	VAL	CA-CB-CG1	-6.78	100.74	110.90
1	6	136	PHE	CB-CG-CD1	6.76	125.54	120.80
1	6	215	HIS	CA-CB-CG	6.75	125.08	113.60
2	F	543	PHE	CB-CG-CD1	6.72	125.50	120.80
2	C	165	SER	C-N-CA	6.69	138.42	121.70
2	D	364	VAL	C-N-CA	6.68	138.41	121.70
2	E	611	TYR	CB-CG-CD1	6.67	125.00	121.00
2	B	364	VAL	C-N-CA	6.63	138.28	121.70
2	A	6	PHE	CB-CG-CD1	-6.63	116.16	120.80
2	D	611	TYR	CB-CG-CD1	-6.59	117.04	121.00
2	D	543	PHE	CB-CG-CD2	-6.56	116.21	120.80
2	F	102	TYR	CB-CG-CD2	6.53	124.92	121.00
1	3	199	TYR	CB-CG-CD2	6.51	124.91	121.00
2	E	577	TYR	CB-CG-CD2	-6.47	117.12	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	423	VAL	CA-CB-CG1	-6.45	101.22	110.90
1	6	130	VAL	N-CA-C	-6.41	93.70	111.00
2	B	543	PHE	CB-CG-CD1	6.35	125.25	120.80
1	6	216	PHE	CB-CG-CD1	-6.34	116.36	120.80
2	A	6	PHE	CB-CG-CD2	6.34	125.24	120.80
2	C	423	VAL	CA-CB-CG1	-6.33	101.41	110.90
2	E	165	SER	C-N-CA	6.31	137.49	121.70
2	B	358	TYR	CB-CG-CD2	-6.28	117.23	121.00
2	F	697	PHE	CB-CG-CD1	6.28	125.20	120.80
2	F	102	TYR	CB-CG-CD1	-6.27	117.24	121.00
2	A	543	PHE	CB-CG-CD2	-6.26	116.42	120.80
2	B	627	PHE	CB-CG-CD2	-6.21	116.45	120.80
2	C	543	PHE	CB-CG-CD1	6.21	125.15	120.80
2	A	366	ILE	C-N-CA	6.20	137.20	121.70
1	5	199	TYR	CB-CG-CD1	6.18	124.71	121.00
2	C	410	PRO	N-CA-CB	-6.15	95.83	102.60
2	D	213	GLY	N-CA-C	-6.14	97.75	113.10
2	A	669	LYS	N-CA-C	-6.13	94.44	111.00
2	C	106	GLU	N-CA-CB	6.12	121.62	110.60
2	D	543	PHE	CB-CG-CD1	6.12	125.09	120.80
2	A	402	VAL	CA-CB-CG2	-6.12	101.72	110.90
2	E	44	GLY	N-CA-C	-6.11	97.81	113.10
2	A	382	ILE	C-N-CA	6.10	136.95	121.70
2	E	366	ILE	C-N-CA	6.05	136.82	121.70
2	C	363	ARG	N-CA-CB	5.98	121.37	110.60
2	C	431	VAL	CB-CA-C	-5.97	100.05	111.40
2	D	253	TYR	CB-CG-CD1	-5.97	117.42	121.00
2	A	627	PHE	CB-CG-CD1	5.97	124.98	120.80
2	C	364	VAL	C-N-CA	5.92	136.50	121.70
2	E	6	PHE	CB-CG-CD2	5.90	124.93	120.80
2	B	6	PHE	CB-CG-CD1	-5.89	116.68	120.80
2	C	80	TYR	CA-CB-CG	-5.87	102.24	113.40
2	A	543	PHE	CB-CG-CD1	5.85	124.90	120.80
1	1	199	TYR	CB-CG-CD2	5.83	124.50	121.00
2	F	79	HIS	N-CA-C	-5.81	95.31	111.00
2	C	511	ILE	N-CA-C	-5.81	95.31	111.00
2	D	632	GLN	CB-CA-C	-5.81	98.78	110.40
2	A	423	VAL	CA-CB-CG1	-5.80	102.19	110.90
2	D	802	VAL	N-CA-C	-5.80	95.34	111.00
2	E	381	TYR	CB-CG-CD2	5.79	124.48	121.00
2	D	310	GLN	N-CA-C	-5.78	95.39	111.00
2	F	433	SER	C-N-CA	5.78	136.14	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	760	TYR	CB-CG-CD1	-5.76	117.55	121.00
2	A	690	MET	CG-SD-CE	-5.75	91.00	100.20
2	D	669	LYS	N-CA-CB	5.75	120.95	110.60
2	A	568	SER	N-CA-C	-5.75	95.48	111.00
2	E	577	TYR	CB-CG-CD1	5.70	124.42	121.00
2	F	757	ASP	N-CA-CB	5.70	120.86	110.60
1	3	195	ARG	NE-CZ-NH2	5.70	123.15	120.30
2	B	802	VAL	N-CA-C	-5.69	95.63	111.00
2	B	79	HIS	N-CA-C	-5.69	95.64	111.00
1	3	130	VAL	N-CA-C	-5.68	95.66	111.00
2	C	6	PHE	CB-CG-CD1	-5.66	116.84	120.80
2	D	611	TYR	CB-CG-CD2	5.64	124.39	121.00
2	D	805	THR	N-CA-C	-5.62	95.81	111.00
2	A	102	TYR	CB-CG-CD2	5.62	124.37	121.00
2	E	79	HIS	N-CA-C	-5.62	95.83	111.00
2	E	166	LEU	C-N-CA	5.62	135.74	121.70
2	C	358	TYR	CB-CG-CD2	-5.61	117.63	121.00
2	D	6	PHE	CB-CG-CD1	-5.59	116.88	120.80
1	5	199	TYR	CB-CG-CD2	-5.59	117.64	121.00
2	C	79	HIS	N-CA-C	-5.57	95.95	111.00
2	D	690	MET	CG-SD-CE	-5.55	91.32	100.20
1	1	156	SER	N-CA-C	-5.54	96.03	111.00
2	E	19	GLU	N-CA-CB	5.54	120.58	110.60
2	B	410	PRO	CA-C-N	5.54	132.62	117.10
2	C	743	LEU	N-CA-C	-5.51	96.13	111.00
2	F	711	PHE	N-CA-C	-5.49	96.18	111.00
2	F	440	ALA	CB-CA-C	-5.49	101.87	110.10
2	F	439	ALA	N-CA-CB	5.48	117.77	110.10
2	F	568	SER	N-CA-C	-5.47	96.23	111.00
2	C	293	ALA	N-CA-CB	5.47	117.76	110.10
2	E	742	GLU	N-CA-CB	5.46	120.43	110.60
2	A	596	TYR	CB-CG-CD1	-5.46	117.72	121.00
2	B	382	ILE	C-N-CA	5.45	135.33	121.70
1	2	199	TYR	CB-CG-CD2	5.44	124.27	121.00
2	F	478	MET	CG-SD-CE	-5.44	91.50	100.20
1	1	199	TYR	CB-CG-CD1	-5.43	117.74	121.00
2	B	398	ALA	C-N-CA	5.43	133.70	122.30
1	2	156	SER	N-CA-C	-5.43	96.35	111.00
2	D	333	ARG	N-CA-C	-5.41	96.39	111.00
1	4	216	PHE	N-CA-CB	5.40	120.31	110.60
2	A	79	HIS	N-CA-C	-5.39	96.45	111.00
1	5	217	ALA	N-CA-CB	5.38	117.64	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	6	PHE	CB-CG-CD2	5.38	124.57	120.80
2	C	176	GLU	N-CA-C	-5.36	96.53	111.00
2	F	423	VAL	CA-CB-CG1	-5.36	102.86	110.90
2	D	21	ALA	CB-CA-C	-5.36	102.07	110.10
2	D	469	SER	N-CA-CB	5.35	118.53	110.50
2	A	102	TYR	CB-CG-CD1	-5.34	117.79	121.00
2	C	358	TYR	CB-CG-CD1	5.33	124.20	121.00
2	B	611	TYR	CB-CG-CD2	-5.33	117.80	121.00
2	C	333	ARG	N-CA-C	-5.33	96.61	111.00
2	E	711	PHE	N-CA-CB	5.33	120.19	110.60
2	E	685	MET	N-CA-CB	5.32	120.18	110.60
1	3	167	PHE	CB-CG-CD1	5.31	124.52	120.80
2	A	29	ILE	N-CA-C	-5.31	96.66	111.00
2	D	403	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	C	363	ARG	N-CA-C	-5.31	96.67	111.00
2	B	6	PHE	CB-CG-CD2	5.29	124.51	120.80
2	E	323	TYR	CB-CG-CD1	-5.29	117.82	121.00
2	F	6	PHE	CB-CG-CD2	5.29	124.51	120.80
2	D	669	LYS	N-CA-C	-5.29	96.73	111.00
2	C	646	THR	N-CA-C	-5.28	96.75	111.00
2	D	6	PHE	CB-CG-CD2	5.28	124.49	120.80
2	A	802	VAL	N-CA-C	-5.26	96.80	111.00
2	B	403	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	B	358	TYR	CB-CG-CD1	5.25	124.15	121.00
2	E	382	ILE	C-N-CA	5.25	134.83	121.70
2	C	544	LEU	N-CA-C	-5.25	96.83	111.00
2	F	617	ASP	CB-CG-OD2	5.23	123.01	118.30
2	D	617	ASP	CB-CG-OD2	5.23	123.01	118.30
2	F	106	GLU	N-CA-CB	5.23	120.01	110.60
2	E	80	TYR	CA-CB-CG	-5.22	103.47	113.40
2	C	617	ASP	CB-CG-OD2	5.21	122.98	118.30
2	B	617	ASP	CB-CG-OD2	5.20	122.98	118.30
2	E	617	ASP	CB-CG-OD2	5.20	122.98	118.30
2	E	805	THR	N-CA-C	-5.20	96.97	111.00
2	B	634	LEU	CB-CG-CD1	5.19	119.83	111.00
2	C	678	GLU	CB-CA-C	-5.19	100.02	110.40
2	D	363	ARG	N-CA-CB	5.19	119.94	110.60
1	4	156	SER	N-CA-C	-5.18	97.00	111.00
2	E	198	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	B	358	TYR	CA-CB-CG	5.17	123.23	113.40
1	4	166	ASP	N-CA-C	-5.17	97.05	111.00
1	6	164	TYR	N-CA-CB	5.17	119.91	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	596	TYR	CB-CG-CD2	-5.17	117.90	121.00
2	A	617	ASP	CB-CG-OD2	5.17	122.95	118.30
2	C	143	GLY	N-CA-C	-5.17	100.19	113.10
2	B	472	THR	N-CA-CB	5.16	120.11	110.30
2	B	436	PHE	CB-CG-CD1	-5.15	117.19	120.80
2	E	383	SER	N-CA-CB	5.14	118.22	110.50
2	A	165	SER	CA-C-N	5.14	128.51	117.20
2	E	483	TRP	CB-CG-CD2	-5.14	119.92	126.60
2	F	711	PHE	N-CA-CB	5.13	119.84	110.60
2	F	440	ALA	N-CA-CB	5.13	117.28	110.10
2	B	410	PRO	N-CA-C	-5.12	98.78	112.10
2	B	685	MET	CG-SD-CE	-5.12	92.01	100.20
2	B	165	SER	CA-C-N	5.11	128.44	117.20
2	E	646	THR	N-CA-C	-5.10	97.23	111.00
1	2	199	TYR	CB-CG-CD1	-5.09	117.95	121.00
2	A	471	VAL	C-N-CA	5.08	134.41	121.70
2	C	627	PHE	CB-CG-CD1	5.08	124.36	120.80
2	E	802	VAL	N-CA-C	-5.08	97.29	111.00
2	B	646	THR	N-CA-C	-5.07	97.32	111.00
2	D	358	TYR	CB-CG-CD2	-5.06	117.96	121.00
2	B	659	ASN	N-CA-CB	5.06	119.71	110.60
2	A	166	LEU	N-CA-CB	5.06	120.52	110.40
2	B	201	LYS	N-CA-C	-5.05	97.37	111.00
2	B	471	VAL	CA-CB-CG1	-5.04	103.34	110.90
1	5	166	ASP	N-CA-C	-5.04	97.39	111.00
2	A	270	GLN	C-N-CA	5.04	134.29	121.70
2	A	742	GLU	N-CA-CB	5.03	119.65	110.60
2	B	667	ARG	N-CA-C	-5.03	97.43	111.00
2	B	361	HIS	CA-CB-CG	5.02	122.14	113.60
2	B	366	ILE	C-N-CA	5.01	134.22	121.70
2	D	627	PHE	CB-CG-CD2	-5.01	117.29	120.80
2	D	355	ARG	NE-CZ-NH2	-5.01	117.80	120.30
2	E	483	TRP	CB-CG-CD1	5.01	133.51	127.00
2	D	470	GLU	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (107) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	161	TYR	Sidechain
1	2	199	TYR	Sidechain
1	3	164	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	3	185	TYR	Sidechain
1	3	194	HIS	Sidechain
1	3	216	PHE	Sidechain
1	4	161	TYR	Sidechain
1	5	185	TYR	Sidechain
1	6	164	TYR	Sidechain
1	6	215	HIS	Sidechain
2	A	185	ARG	Sidechain
2	A	210	PRO	Peptide
2	A	355	ARG	Sidechain
2	A	363	ARG	Sidechain
2	A	409	THR	Peptide
2	A	424	ARG	Sidechain
2	A	468	ASN	Peptide
2	A	592	GLY	Peptide
2	A	596	TYR	Sidechain
2	A	627	PHE	Sidechain
2	A	667	ARG	Sidechain
2	A	697	PHE	Sidechain
2	A	716	LYS	Mainchain,Peptide
2	A	756	VAL	Peptide
2	A	760	TYR	Sidechain
2	A	767	ARG	Sidechain
2	A	776	ARG	Sidechain
2	A	80	TYR	Sidechain
2	B	107	HIS	Sidechain
2	B	199	ARG	Sidechain
2	B	210	PRO	Peptide
2	B	23	ARG	Sidechain
2	B	355	ARG	Sidechain
2	B	358	TYR	Sidechain
2	B	363	ARG	Sidechain
2	B	403	ARG	Sidechain
2	B	409	THR	Peptide
2	B	468	ASN	Peptide
2	B	536	ARG	Sidechain
2	B	592	GLY	Peptide
2	B	627	PHE	Sidechain
2	B	667	ARG	Sidechain
2	B	697	PHE	Sidechain
2	B	716	LYS	Mainchain,Peptide
2	B	756	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	B	760	TYR	Sidechain
2	B	80	TYR	Sidechain
2	C	210	PRO	Peptide
2	C	28	ASN	Mainchain
2	C	358	TYR	Sidechain
2	C	409	THR	Peptide
2	C	468	ASN	Peptide
2	C	541	PHE	Peptide
2	C	592	GLY	Peptide
2	C	697	PHE	Sidechain
2	C	716	LYS	Peptide
2	C	756	VAL	Peptide
2	C	791	HIS	Sidechain
2	C	80	TYR	Sidechain
2	D	210	PRO	Peptide
2	D	355	ARG	Sidechain
2	D	363	ARG	Sidechain
2	D	381	TYR	Sidechain
2	D	405	ARG	Sidechain
2	D	409	THR	Peptide
2	D	468	ASN	Peptide
2	D	556	ARG	Sidechain
2	D	592	GLY	Peptide
2	D	593	TYR	Sidechain
2	D	611	TYR	Sidechain
2	D	667	ARG	Sidechain
2	D	697	PHE	Sidechain
2	D	716	LYS	Mainchain,Peptide
2	D	756	VAL	Peptide
2	D	760	TYR	Sidechain
2	E	198	ARG	Sidechain
2	E	210	PRO	Peptide
2	E	381	TYR	Sidechain
2	E	409	THR	Peptide
2	E	468	ASN	Peptide
2	E	5	ARG	Sidechain
2	E	592	GLY	Peptide
2	E	593	TYR	Sidechain
2	E	627	PHE	Sidechain
2	E	667	ARG	Sidechain
2	E	716	LYS	Mainchain,Peptide
2	E	756	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	E	80	TYR	Sidechain
2	E	96	ARG	Sidechain
2	F	102	TYR	Sidechain
2	F	114	ARG	Sidechain
2	F	210	PRO	Peptide
2	F	381	TYR	Sidechain
2	F	409	THR	Peptide
2	F	424	ARG	Sidechain
2	F	468	ASN	Peptide
2	F	592	GLY	Peptide
2	F	667	ARG	Sidechain
2	F	697	PHE	Sidechain
2	F	716	LYS	Mainchain,Peptide
2	F	756	VAL	Peptide
2	F	80	TYR	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	17	0
1	2	777	0	758	15	0
1	3	777	0	758	20	0
1	4	777	0	758	13	0
1	5	777	0	758	14	0
1	6	777	0	758	12	0
2	A	6200	0	6290	116	0
2	B	6200	0	6290	133	0
2	C	6200	0	6290	110	0
2	D	6200	0	6290	137	0
2	E	6200	0	6290	116	0
2	F	6200	0	6290	119	0
All	All	41862	0	42288	771	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 (771) 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:A:619:ILE:CD1	2:A:656:MET:HB3	1.24	1.66
2:A:619:ILE:CD1	2:A:656:MET:CB	2.18	1.21
2:F:619:ILE:HD12	2:F:656:MET:HB3	1.23	1.21
2:E:619:ILE:CD1	2:E:656:MET:HB3	1.69	1.20
2:F:619:ILE:CG2	2:F:627:PHE:CZ	2.27	1.18
2:C:615:LEU:HD22	2:C:617:ASP:OD1	1.47	1.13
2:E:619:ILE:HG23	2:E:627:PHE:CZ	1.84	1.12
2:D:619:ILE:HD12	2:D:656:MET:HB3	1.15	1.11
2:F:619:ILE:HG21	2:F:627:PHE:CE1	1.85	1.11
2:A:619:ILE:HD11	2:A:656:MET:HB3	1.20	1.10
2:E:619:ILE:CG2	2:E:627:PHE:CZ	2.34	1.09
2:F:619:ILE:CG2	2:F:627:PHE:HZ	1.64	1.09
2:C:616:LEU:HB3	2:C:619:ILE:HD11	1.36	1.08
2:A:619:ILE:HD12	2:A:656:MET:CB	1.81	1.04
2:E:619:ILE:HD12	2:E:656:MET:HB3	1.10	1.04
2:B:619:ILE:CD1	2:B:656:MET:HB3	1.87	1.03
2:E:619:ILE:HG23	2:E:627:PHE:HZ	1.14	1.03
2:B:619:ILE:HD12	2:B:656:MET:HB3	1.01	1.01
2:E:619:ILE:HG21	2:E:627:PHE:CE1	1.99	0.98
2:F:619:ILE:HG22	2:F:627:PHE:HZ	1.31	0.96
2:F:619:ILE:HG21	2:F:627:PHE:HE1	1.24	0.94
2:D:619:ILE:CG2	2:D:627:PHE:HE1	1.81	0.94
2:A:619:ILE:HD12	2:A:656:MET:HB3	0.94	0.93
2:B:619:ILE:HD12	2:B:656:MET:CB	1.97	0.93
2:A:619:ILE:HD11	2:A:656:MET:CB	1.90	0.93
2:E:619:ILE:CG2	2:E:627:PHE:CE1	2.51	0.93
2:F:619:ILE:CG2	2:F:627:PHE:CE1	2.49	0.93
2:B:616:LEU:HB2	2:B:619:ILE:HD11	1.53	0.90
2:D:619:ILE:CG2	2:D:627:PHE:CE1	2.54	0.89
2:D:619:ILE:HG23	2:D:627:PHE:HE1	1.37	0.89
2:F:619:ILE:HG22	2:F:627:PHE:CZ	2.07	0.88
2:A:394:LEU:HD13	2:A:480:VAL:HG22	1.54	0.86
2:B:619:ILE:CG2	2:B:627:PHE:HE1	1.89	0.86
2:C:616:LEU:CB	2:C:619:ILE:HD11	2.05	0.85
2:C:619:ILE:O	2:C:619:ILE:HG22	1.76	0.85
2:D:619:ILE:CD1	2:D:656:MET:HB3	2.05	0.84
2:B:619:ILE:CG2	2:B:627:PHE:CE1	2.62	0.83
2:C:615:LEU:CD2	2:C:617:ASP:OD1	2.26	0.82
2:C:619:ILE:CG2	2:C:627:PHE:HE1	1.92	0.82
2:F:619:ILE:HG23	2:F:627:PHE:CZ	2.18	0.79
2:C:394:LEU:HD13	2:C:480:VAL:HG22	1.64	0.79
2:F:571:ARG:CZ	2:F:617:ASP:OD2	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:ILE:HG22	2:B:627:PHE:CE1	2.18	0.77
2:E:619:ILE:HD12	2:E:656:MET:CB	2.05	0.76
2:C:26:HIS:CD2	2:C:33:HIS:CE1	2.75	0.75
2:E:619:ILE:HG21	2:E:627:PHE:HE1	1.52	0.72
2:F:619:ILE:CD1	2:F:656:MET:HB3	2.13	0.72
2:F:513:GLN:H	2:F:718:HIS:CD2	2.08	0.72
2:D:619:ILE:HG22	2:D:627:PHE:CE1	2.25	0.72
2:E:619:ILE:HG22	2:E:619:ILE:O	1.91	0.71
2:F:26:HIS:CD2	2:F:33:HIS:CE1	2.79	0.71
2:D:619:ILE:HG22	2:D:697:PHE:HE1	1.55	0.71
2:B:21:ALA:HA	2:B:33:HIS:CE1	2.25	0.71
2:F:619:ILE:HD12	2:F:656:MET:CB	2.14	0.71
2:E:107:HIS:HA	2:E:110:LEU:HD12	1.73	0.70
2:F:619:ILE:HG22	2:F:619:ILE:O	1.90	0.70
2:D:55:LEU:HD13	2:D:124:LEU:HD22	1.74	0.69
2:C:574:MET:HG3	2:C:619:ILE:HG12	1.74	0.69
2:B:619:ILE:HG23	2:B:627:PHE:HE1	1.57	0.68
2:C:693:LEU:HD12	2:C:697:PHE:CD2	2.28	0.68
2:B:363:ARG:HH11	2:B:399:GLY:HA2	1.59	0.68
2:C:26:HIS:CG	2:C:33:HIS:CE1	2.81	0.68
2:D:363:ARG:HH11	2:D:399:GLY:HA2	1.60	0.67
2:D:363:ARG:HH12	2:D:471:VAL:HA	1.60	0.67
2:A:682:HIS:CD2	2:A:712:HIS:CE1	2.84	0.66
2:A:544:LEU:HD21	2:A:693:LEU:HD13	1.77	0.66
2:D:53:LEU:HD21	2:D:134:ALA:HA	1.77	0.66
2:D:544:LEU:HD11	2:D:693:LEU:HD13	1.77	0.66
2:D:197:SER:HA	2:D:234:LEU:HD23	1.77	0.66
2:C:619:ILE:O	2:C:619:ILE:CG2	2.43	0.66
2:E:507:HIS:CD2	2:E:517:VAL:HG11	2.32	0.65
2:F:26:HIS:CG	2:F:33:HIS:CE1	2.84	0.65
2:F:619:ILE:HG23	2:F:627:PHE:HZ	1.56	0.65
1:4:142:LEU:HD23	1:4:185:TYR:CD2	2.30	0.65
2:C:55:LEU:HD13	2:C:124:LEU:HD22	1.79	0.65
2:F:751:VAL:HG22	2:F:772:HIS:CB	2.27	0.64
2:A:21:ALA:HA	2:A:33:HIS:CE1	2.33	0.64
2:A:394:LEU:HD21	2:A:483:TRP:CE2	2.32	0.64
2:F:741:ILE:HG22	2:F:792:ILE:HD12	1.80	0.64
2:E:619:ILE:HD11	2:E:656:MET:HB3	1.77	0.64
2:C:619:ILE:HG23	2:C:622:ALA:HB3	1.80	0.64
2:C:24:LEU:HD11	2:C:61:GLN:HE22	1.62	0.63
2:C:619:ILE:CG2	2:C:627:PHE:CE1	2.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:163:LEU:HD11	1:1:209:LEU:HD21	1.79	0.63
2:F:351:LEU:HD13	2:F:391:ALA:HB1	1.79	0.63
2:B:669:LYS:H	2:B:685:MET:HE1	1.64	0.63
1:5:154:LEU:HB3	1:5:204:ILE:HD12	1.81	0.63
2:A:619:ILE:CG2	2:A:627:PHE:CE1	2.82	0.63
2:B:26:HIS:CD2	2:B:33:HIS:HE2	2.16	0.62
2:A:727:SER:O	2:A:731:THR:HG23	1.99	0.62
2:D:619:ILE:HD12	2:D:656:MET:CB	2.10	0.62
2:C:619:ILE:HG22	2:C:697:PHE:HE1	1.64	0.62
2:D:665:LEU:HD23	2:D:685:MET:HG3	1.82	0.62
2:D:682:HIS:CG	2:D:712:HIS:CE1	2.88	0.62
2:F:427:LYS:HG3	2:F:443:ARG:HA	1.81	0.62
2:C:544:LEU:HD11	2:C:693:LEU:HD13	1.80	0.62
2:A:544:LEU:HD23	2:A:658:SER:HB2	1.82	0.61
2:F:21:ALA:HA	2:F:33:HIS:CE1	2.34	0.61
2:D:21:ALA:HB2	2:D:29:ILE:CG1	2.30	0.61
2:D:26:HIS:CE1	2:D:68:ILE:HB	2.35	0.61
2:B:20:GLU:HB2	2:B:33:HIS:CD2	2.35	0.61
2:E:55:LEU:HD13	2:E:124:LEU:HD22	1.83	0.61
2:F:363:ARG:HH11	2:F:399:GLY:HA2	1.65	0.61
2:C:693:LEU:HD12	2:C:697:PHE:HD2	1.64	0.61
2:B:507:HIS:CD2	2:B:517:VAL:HG11	2.36	0.60
2:D:46:ALA:HB1	2:D:109:LEU:HB2	1.83	0.60
2:A:476:ILE:O	2:A:480:VAL:HG23	2.01	0.60
2:C:198:ARG:N	2:C:233:ILE:HG21	2.17	0.60
2:D:786:ILE:HG21	2:D:792:ILE:HG23	1.83	0.60
2:F:233:ILE:H	2:F:233:ILE:HD12	1.66	0.60
2:B:633:VAL:HG23	2:B:639:LEU:HD23	1.83	0.60
2:E:507:HIS:CG	2:E:517:VAL:HG11	2.37	0.60
2:A:363:ARG:HH12	2:A:471:VAL:HA	1.67	0.60
2:A:383:SER:H	2:A:390:LYS:HD2	1.67	0.59
2:D:685:MET:O	2:D:689:VAL:HG23	2.02	0.59
2:C:364:VAL:H	2:C:470:GLU:H	1.50	0.59
2:D:363:ARG:HH21	2:D:402:VAL:HG11	1.66	0.59
2:B:723:VAL:HG21	2:B:752:ALA:HA	1.83	0.59
2:A:395:ILE:HA	2:A:476:ILE:HD12	1.85	0.59
2:D:507:HIS:CD2	2:D:517:VAL:HG11	2.38	0.59
2:A:786:ILE:HG21	2:A:792:ILE:HG23	1.85	0.59
2:F:715:GLU:HB2	2:F:718:HIS:CD2	2.38	0.59
2:D:387:LEU:HD22	2:D:387:LEU:H	1.67	0.59
2:A:619:ILE:HG22	2:A:697:PHE:HE1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:142:LEU:HD13	1:2:209:LEU:HD21	1.85	0.58
2:E:25:GLY:HA3	2:E:73:GLU:HA	1.85	0.58
2:B:633:VAL:HG13	2:B:649:PHE:HB3	1.85	0.58
2:F:351:LEU:CD1	2:F:391:ALA:HB1	2.33	0.58
2:D:547:THR:H	2:D:763:ARG:HH21	1.51	0.58
2:E:574:MET:HG2	2:E:619:ILE:HG12	1.85	0.58
1:5:164:TYR:CG	1:5:193:ILE:HD13	2.39	0.58
2:E:633:VAL:HG13	2:E:649:PHE:HB3	1.85	0.58
2:B:106:GLU:CD	2:B:142:LEU:HD11	2.24	0.58
2:D:437:GLU:HA	2:D:440:ALA:HB3	1.84	0.58
2:B:665:LEU:HD11	2:B:689:VAL:HG11	1.86	0.58
2:E:619:ILE:CD1	2:E:656:MET:CB	2.64	0.58
2:C:21:ALA:HB2	2:C:29:ILE:HG12	1.86	0.58
2:F:747:ALA:O	2:F:751:VAL:HG23	2.03	0.58
2:F:719:LEU:HD12	2:F:720:THR:H	1.68	0.58
2:A:624:PRO:HA	2:A:627:PHE:CD2	2.39	0.58
2:F:522:LYS:HA	2:F:525:ARG:HE	1.69	0.58
2:F:289:GLY:H	2:F:321:ARG:HH12	1.49	0.57
2:B:627:PHE:HB2	2:B:698:ARG:HE	1.70	0.57
2:D:619:ILE:HG22	2:D:697:PHE:CE1	2.39	0.57
2:E:21:ALA:HA	2:E:33:HIS:CE1	2.39	0.57
2:A:723:VAL:HG21	2:A:752:ALA:HA	1.86	0.57
2:A:233:ILE:HA	2:F:361:HIS:HA	1.87	0.57
2:A:28:ASN:HB2	2:A:81:THR:HG23	1.86	0.57
2:D:548:GLY:O	2:D:762:ALA:HB3	2.04	0.57
2:A:402:VAL:HG13	2:A:405:ARG:HE	1.69	0.57
2:E:427:LYS:HG3	2:E:443:ARG:HA	1.86	0.57
2:B:616:LEU:CB	2:B:619:ILE:HD11	2.31	0.57
2:B:624:PRO:HA	2:B:627:PHE:CD2	2.40	0.57
1:3:136:PHE:CD1	2:C:431:VAL:HG11	2.40	0.57
2:A:427:LYS:HG3	2:A:443:ARG:HA	1.87	0.57
1:3:216:PHE:CZ	2:C:439:ALA:HB3	2.40	0.56
1:4:142:LEU:HD21	1:4:182:LEU:HA	1.86	0.56
2:D:399:GLY:O	2:E:233:ILE:HD13	2.05	0.56
1:2:194:HIS:CE1	2:C:141:LEU:HD22	2.40	0.56
1:3:142:LEU:O	1:3:142:LEU:HD23	2.05	0.56
2:B:276:LEU:HD23	2:B:309:LEU:HA	1.88	0.56
1:2:133:PHE:CZ	1:2:142:LEU:HD12	2.40	0.56
2:D:398:ALA:HB1	2:D:475:ASP:HB3	1.87	0.56
2:C:403:ARG:HH21	2:D:232:GLU:H	1.54	0.56
1:1:140:ILE:HD13	1:1:216:PHE:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:351:LEU:HD13	2:D:391:ALA:HB1	1.87	0.56
2:F:627:PHE:CD2	2:F:697:PHE:HA	2.40	0.56
2:E:685:MET:HG3	2:E:712:HIS:CG	2.41	0.56
2:F:26:HIS:CE1	2:F:68:ILE:HB	2.41	0.55
2:C:507:HIS:CD2	2:C:517:VAL:HG11	2.41	0.55
2:A:619:ILE:CD1	2:A:656:MET:CG	2.83	0.55
2:E:619:ILE:CG2	2:E:619:ILE:O	2.54	0.55
2:B:545:GLY:H	2:B:665:LEU:HD13	1.70	0.55
1:1:140:ILE:HD13	1:1:216:PHE:CD1	2.42	0.55
2:E:685:MET:HG3	2:E:712:HIS:CD2	2.42	0.55
1:3:130:VAL:HG22	1:3:164:TYR:CE1	2.41	0.55
2:A:484:THR:HG23	2:A:611:TYR:CE1	2.42	0.55
2:B:49:ALA:HB1	2:B:137:GLN:HB3	1.88	0.55
2:E:363:ARG:HB3	2:E:399:GLY:HA2	1.89	0.55
1:3:142:LEU:HD21	1:3:182:LEU:HD22	1.87	0.55
1:2:208:ALA:O	1:2:212:ILE:HD13	2.07	0.55
2:F:21:ALA:HB2	2:F:29:ILE:HG12	1.89	0.55
2:B:512:GLY:HA2	2:B:722:ILE:HD11	1.88	0.55
2:E:751:VAL:HG22	2:E:772:HIS:CG	2.42	0.55
2:F:633:VAL:HG11	2:F:654:LEU:HD11	1.88	0.55
2:A:542:ILE:HG13	2:A:705:ILE:HD13	1.89	0.55
2:F:776:ARG:HE	2:F:801:PHE:HB3	1.72	0.54
2:C:394:LEU:HD23	2:C:479:VAL:HG22	1.90	0.54
2:F:661:GLY:H	2:F:689:VAL:HG13	1.73	0.54
2:D:21:ALA:HB2	2:D:29:ILE:HG13	1.89	0.54
2:D:17:ALA:HB1	2:D:29:ILE:HG21	1.88	0.54
1:5:216:PHE:HA	2:E:440:ALA:HB2	1.89	0.54
2:D:394:LEU:HD13	2:D:480:VAL:HG22	1.89	0.54
2:A:26:HIS:CD2	2:A:33:HIS:CE1	2.95	0.54
2:E:351:LEU:CD1	2:E:391:ALA:HB1	2.38	0.54
2:B:741:ILE:HG21	2:B:777:LEU:HD13	1.89	0.54
2:B:90:LEU:HA	2:C:156:SER:H	1.73	0.54
1:5:142:LEU:HD13	1:5:209:LEU:HD21	1.89	0.54
2:A:387:LEU:HD12	2:A:387:LEU:H	1.72	0.54
2:F:616:LEU:HB2	2:F:619:ILE:HD11	1.88	0.53
1:1:137:GLU:HA	1:1:140:ILE:HD12	1.89	0.53
2:A:437:GLU:HA	2:A:440:ALA:HB3	1.90	0.53
2:E:53:LEU:HD21	2:E:134:ALA:HA	1.90	0.53
1:5:140:ILE:HD11	1:5:216:PHE:CD1	2.42	0.53
2:A:556:ARG:HE	2:A:571:ARG:HH22	1.56	0.53
2:C:624:PRO:HA	2:C:627:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:682:HIS:CE1	2:B:712:HIS:CE1	2.96	0.53
2:D:26:HIS:CG	2:D:33:HIS:CE1	2.97	0.53
2:D:374:ALA:HA	2:D:394:LEU:HD12	1.90	0.53
2:D:106:GLU:HG2	2:D:107:HIS:CD2	2.43	0.53
2:F:199:ARG:HH21	2:F:310:GLN:HE22	1.55	0.53
2:B:9:ARG:HB3	2:B:105:THR:H	1.72	0.53
2:E:26:HIS:HB2	2:E:33:HIS:CE1	2.43	0.53
2:D:45:ILE:HG23	2:D:141:LEU:HB2	1.91	0.53
2:E:351:LEU:HD13	2:E:391:ALA:HB1	1.91	0.53
2:B:630:LEU:O	2:B:634:LEU:HD13	2.08	0.53
2:C:361:HIS:O	2:C:361:HIS:CG	2.61	0.53
2:E:371:ILE:HD12	2:E:395:ILE:HD13	1.91	0.53
2:E:667:ARG:HH11	2:E:667:ARG:H	1.57	0.53
2:D:355:ARG:HE	2:D:364:VAL:HG12	1.73	0.53
2:A:619:ILE:HG22	2:A:627:PHE:CE1	2.44	0.53
2:E:195:VAL:HG13	2:E:198:ARG:HH11	1.73	0.53
1:6:142:LEU:HD21	1:6:182:LEU:HD22	1.90	0.53
2:C:100:HIS:CG	2:C:102:TYR:O	2.61	0.53
2:F:619:ILE:O	2:F:619:ILE:CG2	2.55	0.53
2:D:542:ILE:HG13	2:D:705:ILE:HD13	1.91	0.53
2:D:476:ILE:O	2:D:480:VAL:HG23	2.09	0.53
2:C:542:ILE:HG13	2:C:705:ILE:HD13	1.91	0.53
2:C:545:GLY:H	2:C:661:GLY:HA3	1.73	0.53
2:F:571:ARG:NH2	2:F:617:ASP:OD2	2.41	0.53
1:3:216:PHE:HA	2:C:440:ALA:HB2	1.91	0.53
2:C:95:ALA:HA	2:C:107:HIS:CD2	2.44	0.53
2:B:361:HIS:CG	2:C:233:ILE:HG12	2.44	0.53
2:F:387:LEU:H	2:F:387:LEU:HD22	1.73	0.53
1:5:133:PHE:CZ	1:5:142:LEU:HD12	2.45	0.52
2:E:46:ALA:HB1	2:E:109:LEU:HB2	1.91	0.52
2:B:53:LEU:HD21	2:B:134:ALA:HA	1.90	0.52
2:E:747:ALA:HB1	2:E:801:PHE:CZ	2.45	0.52
1:1:216:PHE:CE1	2:A:440:ALA:HA	2.44	0.52
2:C:506:LEU:HD21	2:C:558:LEU:HD23	1.91	0.52
2:D:26:HIS:HB2	2:D:33:HIS:CE1	2.44	0.52
2:B:619:ILE:HG22	2:B:697:PHE:HE1	1.74	0.52
2:F:362:HIS:HB2	2:F:403:ARG:HH21	1.74	0.52
2:A:374:ALA:HA	2:A:476:ILE:HG21	1.90	0.52
2:D:26:HIS:CD2	2:D:33:HIS:NE2	2.77	0.52
2:E:361:HIS:HA	2:F:233:ILE:HA	1.90	0.52
2:B:394:LEU:HD13	2:B:480:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:630:LEU:O	2:F:634:LEU:HD13	2.09	0.52
2:C:21:ALA:HA	2:C:33:HIS:CE1	2.45	0.52
2:F:423:VAL:HG11	2:F:445:THR:HB	1.92	0.52
2:F:639:LEU:HD13	2:F:640:THR:H	1.74	0.52
2:E:342:PRO:HG2	2:E:350:ILE:HD11	1.92	0.52
1:6:203:ILE:HA	2:F:434:GLN:HE22	1.74	0.52
2:D:702:ILE:HA	2:D:705:ILE:HD12	1.91	0.51
2:F:786:ILE:HD12	2:F:792:ILE:HD13	1.91	0.51
2:B:669:LYS:HD3	2:B:712:HIS:CD2	2.44	0.51
2:D:394:LEU:HD23	2:D:479:VAL:HG22	1.92	0.51
2:B:355:ARG:HD3	2:B:366:ILE:H	1.75	0.51
2:A:619:ILE:O	2:A:619:ILE:HG22	2.09	0.51
2:B:26:HIS:CG	2:B:33:HIS:CE1	2.98	0.51
2:D:21:ALA:HA	2:D:33:HIS:CE1	2.45	0.51
1:2:216:PHE:HA	2:B:440:ALA:HB2	1.92	0.51
2:F:111:GLY:HA2	2:F:114:ARG:HH11	1.75	0.51
2:D:540:SER:HB2	2:D:706:ASP:H	1.74	0.51
2:A:26:HIS:CG	2:A:33:HIS:CE1	2.98	0.51
2:B:741:ILE:HG22	2:B:792:ILE:HB	1.92	0.51
2:B:427:LYS:O	2:B:431:VAL:HG23	2.09	0.51
2:D:701:PHE:CE2	2:D:705:ILE:HD11	2.46	0.51
2:F:26:HIS:CD2	2:F:33:HIS:HE1	2.26	0.51
2:D:46:ALA:HB2	2:D:105:THR:O	2.09	0.51
2:A:423:VAL:HG11	2:A:445:THR:HB	1.92	0.51
2:D:235:ARG:HH22	2:D:238:ARG:HH22	1.58	0.51
1:1:154:LEU:HD11	1:1:161:TYR:HB3	1.92	0.51
2:C:403:ARG:HE	2:D:231:PRO:HB2	1.76	0.51
2:C:46:ALA:H	2:C:105:THR:HB	1.75	0.51
2:D:619:ILE:HG23	2:D:627:PHE:CE1	2.26	0.51
2:A:26:HIS:CE1	2:A:68:ILE:HB	2.46	0.51
2:A:363:ARG:HD2	2:A:403:ARG:HB2	1.93	0.51
2:A:777:LEU:HD22	2:A:792:ILE:HG21	1.93	0.51
2:C:303:SER:HB3	2:C:309:LEU:HB2	1.92	0.51
2:D:109:LEU:HD23	2:D:138:VAL:HG22	1.92	0.51
2:C:254:ARG:HD3	2:C:254:ARG:H	1.76	0.51
2:E:363:ARG:CZ	2:E:471:VAL:HA	2.41	0.51
2:A:731:THR:HG22	2:A:741:ILE:O	2.10	0.51
2:F:507:HIS:CD2	2:F:517:VAL:HG11	2.46	0.51
2:F:355:ARG:HB3	2:F:365:SER:HA	1.92	0.50
1:3:142:LEU:HD22	1:3:209:LEU:HD13	1.93	0.50
2:F:398:ALA:HB1	2:F:475:ASP:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:742:GLU:HB3	2:C:791:HIS:CE1	2.46	0.50
1:4:140:ILE:HG21	2:D:443:ARG:HE	1.76	0.50
2:B:743:LEU:HD21	2:B:773:VAL:HG22	1.93	0.50
2:B:423:VAL:HG11	2:B:445:THR:HB	1.94	0.50
2:E:394:LEU:HD13	2:E:480:VAL:HG22	1.92	0.50
2:A:192:VAL:HG13	2:A:204:PRO:HG2	1.93	0.50
2:C:743:LEU:HG	2:C:794:LEU:HD23	1.93	0.50
2:C:619:ILE:HG23	2:C:622:ALA:CB	2.41	0.50
2:C:26:HIS:CE1	2:C:68:ILE:HB	2.46	0.50
1:4:164:TYR:CG	1:4:193:ILE:HD13	2.46	0.50
2:B:93:ASP:HB3	2:C:158:ALA:H	1.77	0.50
2:E:543:PHE:HB2	2:E:657:THR:HA	1.92	0.50
2:E:685:MET:O	2:E:689:VAL:HG23	2.11	0.50
2:F:195:VAL:HA	2:F:198:ARG:HE	1.76	0.50
2:B:38:LEU:O	2:B:47:ALA:HB2	2.12	0.50
2:F:498:LYS:HB2	2:F:528:ARG:HH12	1.76	0.50
2:A:544:LEU:HD22	2:A:660:VAL:HG12	1.93	0.50
2:E:29:ILE:HA	2:E:33:HIS:HD1	1.77	0.50
1:3:136:PHE:CG	2:C:431:VAL:HG11	2.47	0.50
2:D:45:ILE:HG22	2:D:138:VAL:HG12	1.94	0.50
2:B:727:SER:HB3	2:B:743:LEU:HD13	1.94	0.50
2:B:424:ARG:HE	2:B:427:LYS:HD3	1.77	0.50
2:A:348:ILE:HG22	2:A:352:GLN:HE21	1.77	0.50
2:F:18:GLN:O	2:F:21:ALA:HB3	2.12	0.50
2:E:371:ILE:O	2:E:374:ALA:HB3	2.12	0.50
2:F:36:LEU:HB3	2:F:40:ARG:HE	1.77	0.50
2:D:627:PHE:HB2	2:D:698:ARG:HE	1.77	0.49
2:E:98:LEU:CD1	2:E:110:LEU:HD13	2.42	0.49
2:C:370:ALA:HB1	2:C:471:VAL:HG13	1.94	0.49
2:F:394:LEU:HD23	2:F:479:VAL:HG22	1.94	0.49
2:A:46:ALA:HB2	2:A:105:THR:O	2.12	0.49
1:5:142:LEU:HD11	1:5:182:LEU:HD22	1.94	0.49
2:F:184:GLY:HA2	2:F:185:ARG:HB2	1.94	0.49
2:A:20:GLU:HB3	2:A:33:HIS:CD2	2.47	0.49
2:E:18:GLN:O	2:E:21:ALA:HB3	2.12	0.49
2:D:371:ILE:O	2:D:374:ALA:HB3	2.13	0.49
2:B:571:ARG:NE	2:B:617:ASP:OD2	2.46	0.49
1:2:203:ILE:HG23	2:B:434:GLN:HE21	1.78	0.49
2:B:39:VAL:HG11	2:B:60:ILE:HD12	1.93	0.49
2:C:36:LEU:HB3	2:C:40:ARG:HE	1.78	0.49
2:B:506:LEU:HB2	2:B:517:VAL:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:777:LEU:CD2	2:A:792:ILE:HG21	2.43	0.49
2:E:49:ALA:O	2:E:53:LEU:HD22	2.13	0.49
1:2:136:PHE:CE2	1:2:216:PHE:CD2	3.00	0.49
2:B:303:SER:HB3	2:B:309:LEU:HB2	1.95	0.49
2:C:355:ARG:HB2	2:C:364:VAL:HG12	1.94	0.49
1:5:216:PHE:CE1	2:E:440:ALA:HA	2.48	0.49
2:B:355:ARG:CD	2:B:366:ILE:H	2.25	0.49
2:B:355:ARG:CG	2:B:366:ILE:H	2.26	0.49
1:4:195:ARG:HH21	1:4:195:ARG:HA	1.78	0.49
2:D:398:ALA:HB1	2:D:475:ASP:CB	2.42	0.49
2:A:631:LEU:HD13	2:A:698:ARG:HH12	1.78	0.49
2:B:36:LEU:HD11	2:B:64:VAL:HG11	1.95	0.49
2:F:26:HIS:CG	2:F:33:HIS:HE1	2.30	0.48
2:E:98:LEU:HD12	2:E:110:LEU:HD13	1.94	0.48
2:E:544:LEU:HD23	2:E:689:VAL:HG11	1.95	0.48
2:C:285:ILE:HD11	2:C:323:TYR:CE1	2.47	0.48
1:3:152:THR:OG1	1:3:163:LEU:HD21	2.13	0.48
2:D:741:ILE:HD13	2:D:777:LEU:CD1	2.43	0.48
2:B:46:ALA:HB2	2:B:105:THR:O	2.13	0.48
2:B:198:ARG:HB2	2:B:202:ASN:HA	1.95	0.48
2:D:522:LYS:HA	2:D:525:ARG:HE	1.78	0.48
2:A:743:LEU:HD11	2:A:773:VAL:CG2	2.43	0.48
1:1:142:LEU:HD23	1:1:185:TYR:CE2	2.48	0.48
2:C:364:VAL:HG22	2:C:471:VAL:CG2	2.43	0.48
1:4:136:PHE:CE2	1:4:216:PHE:CE2	3.02	0.48
2:C:387:LEU:H	2:C:387:LEU:HD12	1.78	0.48
2:A:619:ILE:HG22	2:A:697:PHE:CE1	2.47	0.48
1:6:139:VAL:HG11	1:6:154:LEU:HD13	1.96	0.48
2:A:77:THR:HG21	2:A:450:ARG:HH22	1.79	0.48
2:D:639:LEU:HD13	2:D:640:THR:H	1.79	0.48
2:B:619:ILE:CD1	2:B:656:MET:CB	2.75	0.48
2:E:21:ALA:HB2	2:E:29:ILE:HG12	1.94	0.48
2:E:46:ALA:HB2	2:E:105:THR:O	2.13	0.48
2:F:667:ARG:HH22	2:F:684:ASP:HB2	1.78	0.48
2:D:715:GLU:HB3	2:D:717:LYS:HZ3	1.79	0.48
2:D:627:PHE:HB3	2:D:701:PHE:CG	2.48	0.48
1:3:164:TYR:CD1	1:3:193:ILE:HD13	2.48	0.48
2:B:361:HIS:HA	2:C:233:ILE:HA	1.96	0.48
2:D:762:ALA:HB1	2:D:765:LEU:CD1	2.43	0.48
2:D:751:VAL:HG22	2:D:772:HIS:CD2	2.49	0.48
1:5:203:ILE:HG23	2:E:434:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:53:LEU:HD21	2:A:134:ALA:HA	1.95	0.48
2:D:377:LEU:HD21	2:D:492:ALA:HA	1.95	0.48
2:D:483:TRP:HE1	2:E:198:ARG:HH22	1.62	0.48
2:E:188:GLU:HG3	2:E:339:VAL:HA	1.95	0.48
1:3:136:PHE:CE2	1:3:216:PHE:CD2	3.02	0.47
1:3:153:THR:O	1:3:163:LEU:HD22	2.14	0.47
2:A:49:ALA:O	2:A:53:LEU:HD22	2.14	0.47
2:F:38:LEU:O	2:F:47:ALA:HB2	2.14	0.47
2:F:705:ILE:HG21	2:F:708:ILE:HD13	1.95	0.47
2:C:619:ILE:HD12	2:C:656:MET:HB3	1.95	0.47
2:E:100:HIS:HB2	2:E:107:HIS:CE1	2.48	0.47
2:E:506:LEU:HB2	2:E:517:VAL:HG13	1.96	0.47
2:F:751:VAL:HG22	2:F:772:HIS:HB3	1.95	0.47
1:1:142:LEU:HD23	1:1:185:TYR:CD2	2.49	0.47
2:C:38:LEU:O	2:C:47:ALA:HB2	2.13	0.47
2:F:563:PHE:CE1	2:F:611:TYR:CD1	3.02	0.47
2:F:27:ASN:HA	2:F:75:SER:HA	1.97	0.47
2:C:98:LEU:HD11	2:C:139:LEU:HD22	1.96	0.47
2:A:507:HIS:CD2	2:A:517:VAL:HG11	2.50	0.47
2:A:394:LEU:HD11	2:A:483:TRP:CZ3	2.49	0.47
2:B:370:ALA:HB1	2:B:476:ILE:HD12	1.96	0.47
2:F:543:PHE:HB2	2:F:657:THR:HG22	1.95	0.47
2:C:484:THR:HG23	2:C:611:TYR:CE2	2.48	0.47
1:1:180:SER:HB3	2:A:68:ILE:HD11	1.96	0.47
1:1:140:ILE:HG21	2:A:443:ARG:HD2	1.97	0.47
2:B:27:ASN:HA	2:B:75:SER:HA	1.97	0.47
2:F:431:VAL:HG22	2:F:439:ALA:HB1	1.97	0.47
2:D:623:HIS:CD2	2:D:624:PRO:HD2	2.49	0.47
2:A:363:ARG:HE	2:A:467:GLU:HB3	1.79	0.47
2:A:364:VAL:HG11	2:A:471:VAL:HG21	1.96	0.47
2:A:743:LEU:HD12	2:A:794:LEU:HD13	1.96	0.47
1:3:204:ILE:HD11	1:3:212:ILE:HD11	1.96	0.47
1:3:154:LEU:HD22	1:3:212:ILE:HD11	1.96	0.47
1:3:195:ARG:HH21	2:D:144:SER:H	1.62	0.47
2:E:271:ALA:HB2	2:E:308:GLU:HA	1.96	0.47
2:A:747:ALA:HB1	2:A:801:PHE:CZ	2.50	0.47
2:E:670:TYR:CE1	2:E:756:VAL:HG13	2.50	0.47
2:B:403:ARG:HG2	2:B:403:ARG:HH11	1.80	0.47
2:C:18:GLN:O	2:C:21:ALA:HB3	2.14	0.47
2:C:403:ARG:HE	2:D:231:PRO:CB	2.27	0.47
2:F:786:ILE:HG21	2:F:792:ILE:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:743:LEU:HD11	2:E:773:VAL:HG22	1.97	0.47
2:E:623:HIS:CD2	2:E:624:PRO:HD2	2.50	0.47
2:D:362:HIS:O	2:E:233:ILE:HD11	2.15	0.46
2:C:363:ARG:HH21	2:C:470:GLU:CD	2.18	0.46
2:A:381:TYR:HB2	2:A:484:THR:HG21	1.97	0.46
2:B:100:HIS:HB2	2:B:107:HIS:CE1	2.50	0.46
2:B:95:ALA:HB2	2:B:107:HIS:CG	2.50	0.46
2:E:109:LEU:HD23	2:E:138:VAL:CG2	2.45	0.46
2:B:60:ILE:HG23	2:B:123:VAL:HG11	1.97	0.46
2:B:751:VAL:HG22	2:B:772:HIS:HB2	1.97	0.46
2:A:563:PHE:CD2	2:A:611:TYR:CD1	3.04	0.46
2:A:413:LEU:HB2	2:A:460:TRP:HE1	1.81	0.46
2:D:427:LYS:HA	2:D:442:LEU:HB2	1.98	0.46
2:A:276:LEU:HD23	2:A:309:LEU:HA	1.97	0.46
2:B:402:VAL:HG23	2:B:475:ASP:OD1	2.16	0.46
2:F:31:THR:HB	2:F:120:ALA:HB2	1.96	0.46
2:C:423:VAL:HG11	2:C:445:THR:HB	1.97	0.46
2:A:420:LEU:O	2:A:420:LEU:HD23	2.16	0.46
1:2:142:LEU:HD21	1:2:182:LEU:HG	1.98	0.46
2:B:139:LEU:O	2:B:142:LEU:HD13	2.16	0.46
2:C:660:VAL:HG21	2:C:697:PHE:CE2	2.51	0.46
2:E:787:HIS:H	2:E:790:GLN:HG2	1.80	0.46
2:C:619:ILE:HG21	2:C:627:PHE:HE1	1.78	0.46
2:D:17:ALA:HB1	2:D:29:ILE:CG2	2.46	0.46
2:A:559:ALA:HA	2:A:563:PHE:CD1	2.51	0.46
2:E:727:SER:O	2:E:731:THR:HG23	2.16	0.46
2:B:623:HIS:CD2	2:B:624:PRO:HD2	2.51	0.46
2:D:363:ARG:NH1	2:D:399:GLY:HA2	2.30	0.46
1:2:142:LEU:HD22	1:2:146:ASN:HB2	1.98	0.46
2:F:665:LEU:HG	2:F:689:VAL:HG21	1.98	0.46
2:B:747:ALA:HB1	2:B:801:PHE:CE1	2.51	0.46
2:A:109:LEU:HD23	2:A:138:VAL:HG22	1.97	0.46
1:4:154:LEU:HD22	1:4:212:ILE:HD11	1.98	0.46
2:A:619:ILE:O	2:A:619:ILE:CG2	2.63	0.46
2:A:374:ALA:CA	2:A:476:ILE:HG21	2.45	0.46
1:2:136:PHE:CD1	2:B:431:VAL:HG11	2.51	0.46
2:A:396:ASP:HB3	2:B:198:ARG:HB3	1.96	0.46
2:B:87:VAL:HG13	2:B:112:LEU:HA	1.97	0.46
2:E:574:MET:SD	2:E:626:VAL:HG11	2.56	0.45
2:B:20:GLU:HB3	2:B:23:ARG:HH21	1.80	0.45
2:B:26:HIS:CE1	2:B:68:ILE:HB	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:777:LEU:HD21	2:D:794:LEU:HD11	1.97	0.45
2:D:34:ILE:HD11	2:D:84:ALA:HB1	1.98	0.45
2:D:571:ARG:NE	2:D:617:ASP:OD2	2.49	0.45
2:E:739:LEU:HD11	2:E:792:ILE:HD11	1.98	0.45
2:D:370:ALA:HB1	2:D:471:VAL:HG13	1.99	0.45
2:F:751:VAL:HA	2:F:772:HIS:CD2	2.52	0.45
2:D:21:ALA:HB2	2:D:29:ILE:HD11	1.98	0.45
2:B:727:SER:O	2:B:731:THR:HG23	2.16	0.45
2:E:352:GLN:HG3	2:E:371:ILE:HG21	1.98	0.45
2:C:542:ILE:CG1	2:C:705:ILE:HD13	2.46	0.45
2:B:406:SER:HB3	2:B:407:PHE:CD1	2.51	0.45
2:D:723:VAL:HG21	2:D:752:ALA:HA	1.97	0.45
2:B:26:HIS:HE1	2:B:68:ILE:HB	1.81	0.45
1:2:164:TYR:CD1	1:2:193:ILE:HD13	2.50	0.45
2:E:32:GLU:HB2	2:E:64:VAL:HG13	1.97	0.45
2:A:199:ARG:H	2:F:396:ASP:HB3	1.80	0.45
2:E:106:GLU:HG3	2:E:107:HIS:CD2	2.52	0.45
2:F:751:VAL:HG22	2:F:772:HIS:HB2	1.99	0.45
1:4:137:GLU:HA	1:4:140:ILE:HD12	1.99	0.45
1:5:136:PHE:CE2	1:5:203:ILE:HG21	2.51	0.45
2:C:410:PRO:HG2	2:C:412:ASN:H	1.82	0.45
2:A:355:ARG:HD3	2:A:366:ILE:H	1.82	0.45
2:F:100:HIS:CD2	2:F:107:HIS:CE1	3.04	0.45
1:4:203:ILE:CG2	2:D:434:GLN:HE21	2.29	0.45
2:B:394:LEU:HD23	2:B:479:VAL:HG22	1.97	0.45
2:B:348:ILE:HG22	2:B:352:GLN:HE21	1.82	0.45
2:A:38:LEU:O	2:A:47:ALA:HB2	2.17	0.45
2:C:661:GLY:HA2	2:C:689:VAL:HG22	1.99	0.45
2:A:685:MET:HA	2:A:689:VAL:HG23	1.99	0.45
2:F:616:LEU:CB	2:F:619:ILE:HD11	2.46	0.45
2:A:363:ARG:HA	2:A:468:ASN:HA	1.99	0.45
2:B:743:LEU:HB3	2:B:747:ALA:HB3	1.98	0.45
2:E:483:TRP:HE1	2:F:198:ARG:HH12	1.63	0.45
2:F:100:HIS:HB3	2:F:107:HIS:CE1	2.51	0.45
2:E:674:ASN:HB3	2:E:676:GLN:H	1.82	0.45
2:F:587:VAL:HG22	2:F:589:SER:H	1.82	0.45
2:C:363:ARG:HG3	2:C:403:ARG:HB2	1.98	0.45
2:E:476:ILE:O	2:E:480:VAL:HG23	2.17	0.45
2:C:574:MET:CG	2:C:619:ILE:HG12	2.46	0.45
2:C:403:ARG:HG3	2:D:231:PRO:HB3	1.99	0.45
1:6:142:LEU:HD23	1:6:182:LEU:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:394:LEU:HD23	2:E:479:VAL:HG22	1.99	0.45
2:D:53:LEU:HB3	2:D:129:VAL:HG21	1.99	0.45
2:D:278:ILE:HD11	2:D:309:LEU:HD23	1.99	0.45
2:A:619:ILE:HG23	2:A:627:PHE:HE1	1.81	0.44
2:A:371:ILE:O	2:A:374:ALA:HB3	2.17	0.44
2:B:363:ARG:HH12	2:B:471:VAL:HA	1.82	0.44
2:A:32:GLU:HG2	2:A:33:HIS:CD2	2.52	0.44
1:1:133:PHE:CE2	1:1:163:LEU:HD12	2.52	0.44
2:D:731:THR:HG22	2:D:741:ILE:HD12	1.99	0.44
2:D:777:LEU:CD2	2:D:792:ILE:HG21	2.47	0.44
2:E:26:HIS:CE1	2:E:68:ILE:HB	2.52	0.44
2:F:623:HIS:CD2	2:F:624:PRO:HD2	2.52	0.44
2:E:355:ARG:HG3	2:E:371:ILE:HD11	1.99	0.44
2:A:510:VAL:HG21	2:A:554:LEU:HA	1.99	0.44
2:A:113:ILE:HG21	2:A:135:ARG:HB2	2.00	0.44
1:6:204:ILE:HG21	1:6:211:THR:HB	2.00	0.44
2:D:624:PRO:HA	2:D:627:PHE:CD2	2.52	0.44
2:E:394:LEU:HD21	2:E:483:TRP:CZ2	2.53	0.44
2:F:100:HIS:CD2	2:F:107:HIS:HE1	2.35	0.44
2:A:665:LEU:HD21	2:A:689:VAL:HG21	1.99	0.44
2:F:669:LYS:HG2	2:F:712:HIS:CE1	2.52	0.44
2:D:77:THR:HB	2:D:79:HIS:CD2	2.53	0.44
2:C:714:LEU:HD22	2:C:718:HIS:CD2	2.51	0.44
1:4:181:ILE:HD12	1:4:181:ILE:H	1.81	0.44
2:B:693:LEU:O	2:B:697:PHE:CD2	2.70	0.44
2:D:394:LEU:CD1	2:D:480:VAL:HG22	2.47	0.44
2:A:665:LEU:CD2	2:A:689:VAL:HG21	2.48	0.44
2:B:420:LEU:HD13	2:B:453:VAL:HG21	1.99	0.44
2:F:417:GLU:CD	2:F:417:GLU:H	2.21	0.44
2:F:420:LEU:HD23	2:F:420:LEU:O	2.18	0.44
2:D:26:HIS:HB2	2:D:33:HIS:HE1	1.83	0.44
2:E:55:LEU:HD11	2:E:129:VAL:HG11	2.00	0.44
1:3:139:VAL:CG1	1:3:212:ILE:HD13	2.47	0.44
1:5:204:ILE:HD11	1:5:212:ILE:HD11	1.99	0.44
2:C:6:PHE:HA	2:C:102:TYR:HA	2.00	0.44
1:1:203:ILE:HG22	1:1:204:ILE:HD13	1.99	0.44
2:A:431:VAL:HG13	2:A:439:ALA:HB1	1.99	0.44
2:E:10:ALA:HB1	2:E:108:ILE:HD11	1.99	0.44
2:E:579:GLU:HA	2:E:593:TYR:CD2	2.53	0.44
2:B:282:HIS:CE1	2:B:283:THR:HG23	2.52	0.44
2:B:45:ILE:HG22	2:B:138:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:371:ILE:O	2:C:374:ALA:HB3	2.17	0.44
2:F:739:LEU:HD11	2:F:792:ILE:HD11	1.98	0.44
2:A:363:ARG:HH11	2:A:399:GLY:HA2	1.82	0.44
2:A:631:LEU:HA	2:A:634:LEU:HD22	2.00	0.44
2:D:660:VAL:HG21	2:D:696:ALA:HB2	1.99	0.44
2:E:382:ILE:HG12	2:E:651:ASN:HD21	1.82	0.44
2:F:468:ASN:HD22	2:F:468:ASN:H	1.65	0.44
2:C:476:ILE:O	2:C:480:VAL:HG23	2.18	0.44
2:A:20:GLU:HB2	2:A:33:HIS:CG	2.52	0.44
2:E:20:GLU:HB3	2:E:33:HIS:CD2	2.52	0.44
2:A:53:LEU:HD11	2:A:137:GLN:HB2	2.00	0.44
2:C:32:GLU:HB2	2:C:64:VAL:HG13	1.99	0.44
2:B:59:LYS:HG2	2:B:127:LEU:HD22	1.99	0.44
2:B:619:ILE:O	2:B:619:ILE:HG22	2.18	0.44
2:C:55:LEU:HD11	2:C:129:VAL:HG11	1.99	0.44
2:E:398:ALA:HB1	2:E:475:ASP:HB3	2.00	0.44
2:C:24:LEU:HD13	2:C:69:GLY:HA2	2.00	0.43
2:B:32:GLU:HB2	2:B:64:VAL:HG13	2.00	0.43
2:B:402:VAL:HG22	2:B:405:ARG:CZ	2.48	0.43
2:A:351:LEU:HD22	2:A:392:ILE:HG12	1.99	0.43
2:C:384:ASP:HB3	2:C:385:ARG:HE	1.82	0.43
2:D:619:ILE:HG22	2:D:619:ILE:O	2.17	0.43
2:A:702:ILE:HA	2:A:705:ILE:HD12	2.01	0.43
2:D:394:LEU:HD21	2:D:483:TRP:CH2	2.53	0.43
2:A:510:VAL:HG12	2:A:512:GLY:H	1.84	0.43
2:C:398:ALA:C	2:C:400:SER:H	2.21	0.43
2:A:639:LEU:HD23	2:A:640:THR:H	1.83	0.43
2:F:21:ALA:HA	2:F:33:HIS:ND1	2.33	0.43
2:B:399:GLY:O	2:C:233:ILE:HD11	2.17	0.43
2:C:198:ARG:HD2	2:C:202:ASN:HA	1.99	0.43
2:A:231:PRO:HB2	2:F:403:ARG:HD3	2.00	0.43
2:B:371:ILE:O	2:B:374:ALA:HB3	2.18	0.43
2:E:59:LYS:HG2	2:E:127:LEU:HD22	1.99	0.43
2:D:701:PHE:CZ	2:D:705:ILE:HD11	2.54	0.43
2:A:402:VAL:HG21	2:A:475:ASP:CG	2.38	0.43
2:E:623:HIS:CG	2:E:624:PRO:HD2	2.53	0.43
1:6:133:PHE:CZ	1:6:186:ALA:HB2	2.52	0.43
2:D:193:ILE:HD13	2:D:225:ILE:HG12	2.00	0.43
2:F:59:LYS:HG2	2:F:127:LEU:HD22	1.99	0.43
1:6:153:THR:O	1:6:163:LEU:HD22	2.18	0.43
2:E:627:PHE:HB3	2:E:701:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:627:PHE:HB2	2:C:698:ARG:HE	1.83	0.43
2:D:712:HIS:H	2:D:712:HIS:CD2	2.35	0.43
1:3:133:PHE:CD2	1:3:139:VAL:HG22	2.53	0.43
2:C:348:ILE:HG21	2:C:372:GLU:HG2	2.01	0.43
2:E:520:VAL:HG11	2:E:558:LEU:HD11	2.01	0.43
2:E:6:PHE:HA	2:E:102:TYR:HA	2.00	0.43
2:B:301:LYS:HB2	2:B:302:PRO:HD3	2.00	0.43
2:E:110:LEU:HD23	2:E:135:ARG:HG2	2.00	0.43
2:E:21:ALA:CB	2:E:29:ILE:HG12	2.49	0.43
2:B:374:ALA:HA	2:B:394:LEU:HD12	2.01	0.43
2:C:381:TYR:HB2	2:C:611:TYR:CE2	2.54	0.43
2:A:588:GLY:HA3	2:B:594:VAL:H	1.84	0.43
2:D:665:LEU:HD22	2:D:712:HIS:HA	2.00	0.43
1:3:140:ILE:HD11	1:3:216:PHE:CD1	2.54	0.43
1:6:137:GLU:HA	1:6:140:ILE:HD12	2.00	0.43
2:C:730:LEU:HD11	2:C:774:GLU:HG2	2.00	0.43
2:D:580:LYS:HD3	2:D:581:HIS:CE1	2.54	0.43
2:B:394:LEU:HD21	2:B:483:TRP:CH2	2.54	0.43
2:F:664:GLU:HA	2:F:667:ARG:HE	1.84	0.43
2:F:31:THR:HG23	2:F:83:ARG:HG3	2.01	0.43
2:B:406:SER:HB2	2:B:463:LYS:HE2	2.01	0.43
2:F:402:VAL:HG12	2:F:467:GLU:HB3	2.00	0.43
2:C:363:ARG:HH12	2:C:475:ASP:HB3	1.84	0.43
2:B:742:GLU:OE1	2:B:793:VAL:HG13	2.19	0.43
2:D:510:VAL:HG12	2:D:512:GLY:H	1.84	0.43
2:D:22:LEU:H	2:D:22:LEU:HD12	1.82	0.43
2:E:394:LEU:HD21	2:E:483:TRP:CE2	2.54	0.43
2:C:410:PRO:HB2	2:C:411:PRO:HD2	2.00	0.43
2:F:53:LEU:HD21	2:F:134:ALA:HA	2.00	0.43
2:E:367:THR:O	2:E:370:ALA:HB3	2.19	0.43
2:A:619:ILE:HD11	2:A:656:MET:CG	2.44	0.42
2:A:363:ARG:HD2	2:A:403:ARG:H	1.83	0.42
2:D:747:ALA:O	2:D:751:VAL:HG23	2.19	0.42
2:B:407:PHE:CD1	2:C:229:GLU:HB3	2.53	0.42
2:A:398:ALA:C	2:A:400:SER:H	2.22	0.42
2:D:370:ALA:HB2	2:D:472:THR:HA	2.01	0.42
2:A:20:GLU:CB	2:A:33:HIS:CD2	3.02	0.42
2:E:397:GLU:CB	2:E:479:VAL:HG21	2.50	0.42
2:D:6:PHE:CD2	2:D:103:VAL:HG23	2.54	0.42
2:F:192:VAL:HG13	2:F:204:PRO:HG2	2.01	0.42
2:E:359:GLU:HA	2:E:362:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:HIS:CD2	2:D:33:HIS:CE1	3.07	0.42
2:B:53:LEU:HD12	2:B:129:VAL:HG13	2.01	0.42
2:C:46:ALA:HB2	2:C:105:THR:O	2.19	0.42
2:B:546:PRO:HD2	2:B:549:VAL:HG21	1.99	0.42
2:E:410:PRO:HG2	2:E:413:LEU:H	1.85	0.42
2:E:513:GLN:HA	2:E:718:HIS:CE1	2.54	0.42
1:5:144:LYS:HZ1	1:5:213:LYS:HA	1.85	0.42
2:F:98:LEU:HD12	2:F:110:LEU:HD13	2.00	0.42
2:D:351:LEU:CD1	2:D:391:ALA:HB1	2.49	0.42
2:A:46:ALA:HB1	2:A:109:LEU:HB2	2.00	0.42
1:5:175:VAL:HA	1:5:178:GLN:HE21	1.84	0.42
2:D:742:GLU:HB3	2:D:791:HIS:CE1	2.54	0.42
2:E:166:LEU:HA	2:E:167:ALA:CB	2.49	0.42
2:F:371:ILE:O	2:F:374:ALA:HB3	2.20	0.42
1:1:216:PHE:HA	2:A:440:ALA:HB2	2.00	0.42
2:A:743:LEU:HB3	2:A:747:ALA:HB3	2.02	0.42
2:A:22:LEU:H	2:A:22:LEU:HD22	1.85	0.42
2:F:374:ALA:HB1	2:F:391:ALA:HA	2.01	0.42
2:D:549:VAL:HG13	2:D:714:LEU:CD2	2.49	0.42
1:6:142:LEU:HB2	1:6:185:TYR:CD2	2.55	0.42
2:B:571:ARG:NH2	2:B:617:ASP:OD2	2.52	0.42
2:F:100:HIS:CE1	2:F:102:TYR:HB2	2.55	0.42
2:D:6:PHE:HA	2:D:102:TYR:HA	2.01	0.42
2:D:392:ILE:HA	2:D:395:ILE:HD12	2.01	0.42
2:E:581:HIS:CE1	2:E:585:ARG:CZ	3.02	0.42
2:D:271:ALA:HA	2:D:274:ILE:HG22	2.02	0.42
1:2:154:LEU:HB2	1:2:208:ALA:HB1	2.01	0.42
1:5:216:PHE:CE2	2:E:439:ALA:HB3	2.55	0.42
2:E:483:TRP:CD1	2:F:335:GLN:HG3	2.55	0.42
2:C:281:LEU:HG	2:C:285:ILE:HD13	2.01	0.42
2:B:113:ILE:HG21	2:B:135:ARG:HB2	2.01	0.42
2:F:46:ALA:H	2:F:105:THR:HB	1.84	0.42
1:2:215:HIS:HB2	2:B:436:PHE:HB3	2.00	0.42
2:B:26:HIS:CD2	2:B:33:HIS:NE2	2.86	0.42
2:D:361:HIS:CG	2:E:233:ILE:HG23	2.55	0.42
2:F:374:ALA:HB2	2:F:476:ILE:HG12	2.02	0.42
2:D:682:HIS:CD2	2:D:712:HIS:CE1	3.07	0.42
2:A:403:ARG:HA	2:A:467:GLU:HG3	2.01	0.42
2:B:777:LEU:HD11	2:B:794:LEU:HD11	2.02	0.42
2:B:743:LEU:HA	2:B:794:LEU:HB2	2.02	0.42
2:E:370:ALA:HB2	2:E:472:THR:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:627:PHE:HB3	2:D:701:PHE:CD2	2.55	0.42
2:A:786:ILE:HD12	2:A:792:ILE:HD13	2.00	0.42
2:B:427:LYS:HD2	2:B:443:ARG:HA	2.02	0.42
2:B:398:ALA:HB1	2:B:475:ASP:HB3	2.01	0.42
2:E:634:LEU:HD22	2:E:701:PHE:CE1	2.54	0.42
1:1:133:PHE:CZ	1:1:163:LEU:HD12	2.55	0.42
2:A:739:LEU:HD21	2:A:792:ILE:HD11	2.02	0.42
2:B:355:ARG:HA	2:B:358:TYR:CZ	2.55	0.42
1:1:128:GLN:HG3	1:1:166:ASP:HA	2.02	0.42
2:C:373:ALA:HB2	2:C:473:VAL:HG13	2.02	0.42
2:F:502:MET:HA	2:F:505:ILE:HG12	2.02	0.42
2:F:392:ILE:HA	2:F:395:ILE:HD12	2.02	0.41
2:B:507:HIS:CD2	2:B:517:VAL:CG1	3.02	0.41
2:A:383:SER:H	2:A:390:LYS:CD	2.31	0.41
2:E:743:LEU:HD21	2:E:773:VAL:HG22	2.02	0.41
2:F:382:ILE:H	2:F:383:SER:HB2	1.84	0.41
2:D:631:LEU:HA	2:D:634:LEU:HD22	2.02	0.41
2:C:413:LEU:HB2	2:C:460:TRP:CZ2	2.55	0.41
2:A:142:LEU:HG	2:A:144:SER:H	1.85	0.41
2:F:395:ILE:HA	2:F:476:ILE:HD11	2.02	0.41
2:D:20:GLU:HB2	2:D:33:HIS:CG	2.55	0.41
2:C:361:HIS:CE1	2:C:396:ASP:HA	2.55	0.41
2:E:366:ILE:HB	2:E:367:THR:HA	2.02	0.41
2:B:183:ILE:HD12	2:B:350:ILE:HA	2.01	0.41
2:F:427:LYS:HG3	2:F:443:ARG:CA	2.48	0.41
2:D:714:LEU:HD12	2:D:762:ALA:HB2	2.02	0.41
2:F:507:HIS:CE1	2:F:518:VAL:HG22	2.56	0.41
2:A:165:SER:HB2	2:A:166:LEU:HB2	2.02	0.41
2:D:507:HIS:CE1	2:D:518:VAL:HG22	2.56	0.41
2:B:106:GLU:CG	2:B:142:LEU:HD11	2.50	0.41
2:E:9:ARG:HB2	2:E:105:THR:HB	2.03	0.41
2:B:476:ILE:O	2:B:479:VAL:HG13	2.21	0.41
2:D:747:ALA:HB1	2:D:801:PHE:CZ	2.56	0.41
2:F:484:THR:HG22	2:F:563:PHE:HA	2.02	0.41
2:D:427:LYS:C	2:D:427:LYS:HD3	2.41	0.41
2:F:53:LEU:HD12	2:F:129:VAL:HG13	2.02	0.41
2:E:303:SER:HB3	2:E:309:LEU:HB2	2.02	0.41
2:C:357:ARG:C	2:C:359:GLU:H	2.24	0.41
2:B:364:VAL:HG11	2:B:471:VAL:HG13	2.03	0.41
1:1:140:ILE:HG23	1:1:216:PHE:HB3	2.03	0.41
2:F:474:ASP:HA	2:F:493:GLN:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:445:THR:O	2:E:449:LEU:HD23	2.20	0.41
2:D:400:SER:HA	2:E:233:ILE:HD12	2.02	0.41
2:D:21:ALA:HB2	2:D:29:ILE:CD1	2.51	0.41
2:C:304:LEU:HD22	2:C:311:CYS:SG	2.60	0.41
2:F:579:GLU:HA	2:F:593:TYR:CD1	2.55	0.41
1:6:210:GLU:CD	1:6:210:GLU:H	2.23	0.41
2:D:70:ARG:HD2	2:D:70:ARG:H	1.85	0.41
2:C:417:GLU:H	2:C:417:GLU:CD	2.24	0.41
2:B:627:PHE:CE2	2:B:697:PHE:HA	2.55	0.41
2:B:26:HIS:CB	2:B:33:HIS:HE1	2.33	0.41
2:B:632:GLN:HB2	2:B:639:LEU:HD22	2.03	0.41
2:C:437:GLU:HA	2:C:440:ALA:HB3	2.01	0.41
1:4:203:ILE:HG21	2:D:434:GLN:HE21	1.85	0.41
1:6:127:LEU:CB	1:6:175:VAL:HG21	2.50	0.41
2:C:615:LEU:HD21	2:C:657:THR:HG23	2.03	0.41
1:2:216:PHE:CZ	2:B:439:ALA:HB3	2.55	0.41
2:C:5:ARG:HH22	2:C:357:ARG:HH21	1.69	0.41
2:A:362:HIS:CE1	2:B:232:GLU:OE2	2.74	0.41
1:1:194:HIS:CD2	2:B:141:LEU:HD22	2.55	0.41
2:A:324:ILE:HD13	2:F:385:ARG:HH12	1.86	0.41
1:4:128:GLN:HG3	1:4:166:ASP:HA	2.02	0.41
1:3:171:THR:O	1:3:175:VAL:HG23	2.21	0.41
2:D:110:LEU:HD21	2:D:138:VAL:HB	2.03	0.41
2:B:739:LEU:HD13	2:B:741:ILE:HG23	2.03	0.41
2:C:545:GLY:N	2:C:661:GLY:HA3	2.36	0.41
2:F:100:HIS:HD2	2:F:107:HIS:CE1	2.39	0.41
2:B:109:LEU:HD23	2:B:138:VAL:HG22	2.02	0.41
2:F:746:ALA:HB1	2:F:796:VAL:HB	2.03	0.41
2:F:201:LYS:C	2:F:203:ASN:H	2.24	0.41
2:B:589:SER:H	2:C:584:SER:HA	1.86	0.41
2:D:59:LYS:HG2	2:D:127:LEU:HD22	2.02	0.41
2:C:741:ILE:HA	2:C:792:ILE:HB	2.01	0.41
1:4:147:VAL:HG13	1:4:148:ASN:H	1.85	0.41
2:C:480:VAL:HG13	2:C:483:TRP:CZ3	2.56	0.41
2:B:395:ILE:HA	2:B:471:VAL:HG11	2.03	0.41
2:B:361:HIS:HB2	2:C:233:ILE:HG23	2.03	0.41
2:D:665:LEU:HD11	2:D:710:VAL:HG13	2.02	0.41
2:B:719:LEU:HD12	2:B:752:ALA:HB1	2.02	0.41
2:D:394:LEU:CD2	2:D:479:VAL:HG22	2.51	0.41
2:B:188:GLU:HG3	2:B:339:VAL:HA	2.02	0.41
2:B:624:PRO:HA	2:B:627:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:GLU:HB3	2:D:33:HIS:CD2	2.56	0.40
2:D:98:LEU:HD12	2:D:110:LEU:HD13	2.02	0.40
2:E:741:ILE:HG22	2:E:792:ILE:HD12	2.04	0.40
2:F:544:LEU:HD13	2:F:690:MET:CE	2.51	0.40
2:E:29:ILE:HG23	2:E:33:HIS:HD1	1.86	0.40
2:E:686:LYS:HB2	2:E:712:HIS:HE1	1.86	0.40
2:F:94:GLU:O	2:F:107:HIS:CD2	2.74	0.40
2:D:620:GLU:O	2:D:696:ALA:HB1	2.21	0.40
1:6:127:LEU:HA	1:6:175:VAL:HG21	2.03	0.40
2:F:271:ALA:HB2	2:F:308:GLU:HA	2.03	0.40
2:C:427:LYS:HG3	2:C:443:ARG:HA	2.03	0.40
2:C:685:MET:HB2	2:C:712:HIS:CE1	2.56	0.40
2:B:387:LEU:HD22	2:B:387:LEU:H	1.86	0.40
2:D:55:LEU:HD11	2:D:129:VAL:HG11	2.04	0.40
1:2:133:PHE:CD1	1:2:186:ALA:HB2	2.57	0.40
2:E:710:VAL:CG1	2:E:712:HIS:CE1	3.04	0.40
2:B:742:GLU:O	2:B:794:LEU:HD12	2.22	0.40
1:3:139:VAL:HG11	1:3:212:ILE:HD13	2.03	0.40
2:B:235:ARG:NE	2:B:236:ASP:H	2.19	0.40
2:B:570:ILE:HG13	2:B:606:VAL:HG22	2.03	0.40
2:D:14:LEU:O	2:D:17:ALA:HB3	2.22	0.40
2:D:727:SER:O	2:D:731:THR:HG23	2.22	0.40
2:A:370:ALA:CB	2:A:471:VAL:HG13	2.51	0.40
2:C:363:ARG:HD3	2:C:399:GLY:HA2	2.02	0.40
2:D:714:LEU:HD22	2:D:718:HIS:CD2	2.56	0.40
2:A:110:LEU:HD11	2:A:142:LEU:HD13	2.04	0.40
2:E:484:THR:HG23	2:E:611:TYR:CD2	2.57	0.40
2:A:87:VAL:HG13	2:A:112:LEU:HA	2.02	0.40
2:D:506:LEU:HD21	2:D:558:LEU:HD23	2.04	0.40
2:C:627:PHE:CD2	2:C:697:PHE:HA	2.57	0.40
2:E:484:THR:HG23	2:E:611:TYR:CE2	2.57	0.40
2:D:91:SER:HB2	2:D:108:ILE:HD13	2.03	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%)	78 (85%)	8 (9%)	6 (6%)	1	25
1	2	92/218 (42%)	78 (85%)	9 (10%)	5 (5%)	2	29
1	3	92/218 (42%)	74 (80%)	12 (13%)	6 (6%)	1	25
1	4	92/218 (42%)	79 (86%)	8 (9%)	5 (5%)	2	29
1	5	92/218 (42%)	76 (83%)	12 (13%)	4 (4%)	3	34
1	6	92/218 (42%)	76 (83%)	13 (14%)	3 (3%)	5	40
2	A	794/810 (98%)	627 (79%)	109 (14%)	58 (7%)	1	21
2	B	794/810 (98%)	625 (79%)	117 (15%)	52 (6%)	1	25
2	C	794/810 (98%)	623 (78%)	118 (15%)	53 (7%)	1	24
2	D	794/810 (98%)	614 (77%)	125 (16%)	55 (7%)	1	23
2	E	794/810 (98%)	629 (79%)	107 (14%)	58 (7%)	1	21
2	F	794/810 (98%)	628 (79%)	112 (14%)	54 (7%)	1	23
All	All	5316/6168 (86%)	4207 (79%)	750 (14%)	359 (7%)	3	23

All (359) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	207	HIS
1	2	145	LEU
1	2	147	VAL
1	3	145	LEU
1	3	146	ASN
1	5	148	ASN
2	A	100	HIS
2	A	271	ALA
2	A	294	ILE
2	A	366	ILE
2	A	412	ASN
2	A	468	ASN
2	A	472	THR
2	A	493	GLN
2	A	579	GLU
2	A	650	ARG
2	A	669	LYS
2	B	100	HIS

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Mol	Chain	Res	Type
2	B	150	SER
2	B	151	ALA
2	B	343	SER
2	B	365	SER
2	B	366	ILE
2	B	410	PRO
2	B	468	ASN
2	B	470	GLU
2	B	493	GLN
2	B	531	LEU
2	B	652	THR
2	B	667	ARG
2	C	78	ILE
2	C	271	ALA
2	C	294	ILE
2	C	363	ARG
2	C	365	SER
2	C	366	ILE
2	C	434	GLN
2	C	468	ASN
2	C	472	THR
2	C	493	GLN
2	C	547	THR
2	C	589	SER
2	C	590	PRO
2	C	642	SER
2	C	713	SER
2	D	293	ALA
2	D	333	ARG
2	D	339	VAL
2	D	365	SER
2	D	410	PRO
2	D	412	ASN
2	D	468	ASN
2	D	471	VAL
2	D	473	VAL
2	D	535	LYS
2	D	591	PRO
2	D	669	LYS
2	D	762	ALA
2	E	150	SER
2	E	167	ALA

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Mol	Chain	Res	Type
2	E	183	ILE
2	E	293	ALA
2	E	363	ARG
2	E	366	ILE
2	E	412	ASN
2	E	468	ASN
2	E	473	VAL
2	E	493	GLN
2	E	585	ARG
2	E	674	ASN
2	F	7	THR
2	F	78	ILE
2	F	117	GLU
2	F	183	ILE
2	F	294	ILE
2	F	410	PRO
2	F	412	ASN
2	F	434	GLN
2	F	468	ASN
2	F	472	THR
2	F	493	GLN
2	F	547	THR
2	F	668	ASN
2	F	670	TYR
1	1	147	VAL
1	4	145	LEU
1	4	147	VAL
1	5	147	VAL
1	6	145	LEU
2	A	68	ILE
2	A	144	SER
2	A	157	ASN
2	A	165	SER
2	A	183	ILE
2	A	391	ALA
2	A	471	VAL
2	A	473	VAL
2	A	652	THR
2	A	662	ALA
2	A	675	VAL
2	B	99	GLY
2	B	163	LEU

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Mol	Chain	Res	Type
2	B	165	SER
2	B	177	ASP
2	B	212	VAL
2	B	271	ALA
2	B	291	GLU
2	B	294	ILE
2	B	383	SER
2	B	547	THR
2	B	579	GLU
2	B	642	SER
2	B	659	ASN
2	B	662	ALA
2	B	674	ASN
2	B	716	LYS
2	B	757	ASP
2	C	99	GLY
2	C	150	SER
2	C	165	SER
2	C	212	VAL
2	C	293	ALA
2	C	362	HIS
2	C	412	ASN
2	C	568	SER
2	C	662	ALA
2	D	72	GLN
2	D	99	GLY
2	D	100	HIS
2	D	165	SER
2	D	166	LEU
2	D	178	SER
2	D	183	ILE
2	D	362	HIS
2	D	363	ARG
2	D	366	ILE
2	D	413	LEU
2	D	493	GLN
2	D	578	MET
2	D	662	ALA
2	D	738	ASP
2	E	100	HIS
2	E	152	ALA
2	E	165	SER

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Mol	Chain	Res	Type
2	E	177	ASP
2	E	271	ALA
2	E	365	SER
2	E	383	SER
2	E	384	ASP
2	E	410	PRO
2	E	434	GLN
2	E	618	ALA
2	E	642	SER
2	E	662	ALA
2	E	738	ASP
2	E	759	GLU
2	F	100	HIS
2	F	118	GLY
2	F	150	SER
2	F	165	SER
2	F	168	ARG
2	F	271	ALA
2	F	343	SER
2	F	366	ILE
2	F	662	ALA
2	F	673	PHE
2	F	717	LYS
2	F	757	ASP
1	1	144	LYS
1	1	177	ASN
1	2	144	LYS
1	2	177	ASN
1	3	144	LYS
1	3	177	ASN
1	4	144	LYS
1	4	177	ASN
1	5	177	ASN
1	6	177	ASN
2	A	99	GLY
2	A	151	ALA
2	A	162	THR
2	A	163	LEU
2	A	167	ALA
2	A	330	LEU
2	A	375	VAL
2	A	388	PRO

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Mol	Chain	Res	Type
2	A	410	PRO
2	A	413	LEU
2	A	585	ARG
2	A	707	GLU
2	A	738	ASP
2	A	760	TYR
2	B	364	VAL
2	B	384	ASP
2	B	391	ALA
2	B	591	PRO
2	B	738	ASP
2	C	148	GLY
2	C	162	THR
2	C	163	LEU
2	C	364	VAL
2	C	375	VAL
2	C	391	ALA
2	C	410	PRO
2	C	413	LEU
2	C	550	GLY
2	C	580	LYS
2	C	757	ASP
2	C	761	GLY
2	C	788	LYS
2	D	143	GLY
2	D	150	SER
2	D	163	LEU
2	D	291	GLU
2	D	326	LYS
2	D	375	VAL
2	D	388	PRO
2	D	391	ALA
2	D	400	SER
2	D	472	THR
2	D	592	GLY
2	E	72	GLN
2	E	73	GLU
2	E	162	THR
2	E	163	LEU
2	E	210	PRO
2	E	391	ALA
2	E	413	LEU

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Mol	Chain	Res	Type
2	E	472	THR
2	E	580	LYS
2	F	152	ALA
2	F	162	THR
2	F	163	LEU
2	F	177	ASP
2	F	185	ARG
2	F	384	ASP
2	F	388	PRO
2	F	391	ALA
2	F	413	LEU
2	F	568	SER
2	F	738	ASP
1	1	145	LEU
1	4	217	ALA
1	6	144	LYS
2	A	150	SER
2	A	152	ALA
2	A	210	PRO
2	A	293	ALA
2	A	343	SER
2	A	550	GLY
2	A	690	MET
2	B	152	ALA
2	B	162	THR
2	B	226	ILE
2	B	388	PRO
2	B	400	SER
2	B	413	LEU
2	B	550	GLY
2	C	226	ILE
2	C	384	ASP
2	C	388	PRO
2	C	471	VAL
2	C	661	GLY
2	C	686	LYS
2	D	145	ASN
2	D	162	THR
2	D	197	SER
2	D	364	VAL
2	D	550	GLY
2	D	686	LYS

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Mol	Chain	Res	Type
2	E	143	GLY
2	E	231	PRO
2	E	375	VAL
2	E	388	PRO
2	E	400	SER
2	E	550	GLY
2	E	586	LEU
2	E	686	LYS
2	F	166	LEU
2	F	293	ALA
2	F	375	VAL
2	F	531	LEU
2	F	550	GLY
2	F	642	SER
2	F	671	VAL
1	1	191	ILE
1	5	144	LYS
2	A	70	ARG
2	A	198	ARG
2	A	202	ASN
2	A	226	ILE
2	A	228	ASN
2	A	400	SER
2	A	469	SER
2	A	642	SER
2	B	375	VAL
2	B	434	GLN
2	B	472	THR
2	B	717	LYS
2	C	147	THR
2	C	400	SER
2	C	579	GLU
2	D	167	ALA
2	D	226	ILE
2	D	674	ASN
2	E	209	GLU
2	E	226	ILE
2	E	469	SER
2	E	534	PRO
2	E	690	MET
2	E	698	ARG
2	E	713	SER

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Mol	Chain	Res	Type
2	F	226	ILE
2	F	400	SER
1	3	216	PHE
2	A	434	GLN
2	A	600	GLY
2	B	166	LEU
2	C	118	GLY
2	C	152	ALA
2	C	323	TYR
2	D	228	ASN
2	D	251	THR
2	D	343	SER
2	D	531	LEU
2	D	760	TYR
2	E	5	ARG
2	E	103	VAL
2	E	323	TYR
2	E	600	GLY
2	E	757	ASP
2	F	99	GLY
2	F	686	LYS
2	F	758	LEU
1	3	191	ILE
2	C	210	PRO
2	C	512	GLY
2	E	661	GLY
2	F	212	VAL
2	F	382	ILE
2	F	610	PRO
2	A	212	VAL
2	A	382	ILE
2	B	600	GLY
2	C	588	GLY
2	D	68	ILE
2	E	212	VAL
2	F	471	VAL
1	2	191	ILE
2	A	761	GLY
2	B	182	VAL
2	B	660	VAL
2	D	382	ILE
2	F	210	PRO

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Mol	Chain	Res	Type
2	A	364	VAL
2	B	382	ILE
2	B	534	PRO
2	C	392	ILE
2	A	160	THR

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%)	80 (91%)	8 (9%)	12 43
1	2	88/201 (44%)	79 (90%)	9 (10%)	9 37
1	3	88/201 (44%)	79 (90%)	9 (10%)	9 37
1	4	88/201 (44%)	81 (92%)	7 (8%)	15 50
1	5	88/201 (44%)	80 (91%)	8 (9%)	12 43
1	6	88/201 (44%)	81 (92%)	7 (8%)	15 50
2	A	667/686 (97%)	584 (88%)	83 (12%)	6 30
2	B	667/686 (97%)	585 (88%)	82 (12%)	6 30
2	C	667/686 (97%)	591 (89%)	76 (11%)	7 33
2	D	667/686 (97%)	589 (88%)	78 (12%)	7 32
2	E	667/686 (97%)	597 (90%)	70 (10%)	8 36
2	F	667/686 (97%)	597 (90%)	70 (10%)	8 36
All	All	4530/5322 (85%)	4023 (89%)	507 (11%)	12 33

All (507) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	136	PHE
1	1	137	GLU
1	1	145	LEU
1	1	147	VAL
1	1	151	LYS

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Mol	Chain	Res	Type
1	1	175	VAL
1	1	204	ILE
1	1	216	PHE
1	2	140	ILE
1	2	142	LEU
1	2	145	LEU
1	2	147	VAL
1	2	151	LYS
1	2	170	MET
1	2	214	LYS
1	2	215	HIS
1	2	216	PHE
1	3	145	LEU
1	3	151	LYS
1	3	152	THR
1	3	165	VAL
1	3	195	ARG
1	3	204	ILE
1	3	210	GLU
1	3	214	LYS
1	3	216	PHE
1	4	136	PHE
1	4	145	LEU
1	4	147	VAL
1	4	151	LYS
1	4	170	MET
1	4	195	ARG
1	4	204	ILE
1	5	137	GLU
1	5	142	LEU
1	5	144	LYS
1	5	151	LYS
1	5	170	MET
1	5	176	GLU
1	5	204	ILE
1	5	216	PHE
1	6	130	VAL
1	6	136	PHE
1	6	142	LEU
1	6	145	LEU
1	6	151	LYS
1	6	170	MET

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Mol	Chain	Res	Type
1	6	215	HIS
2	A	3	PHE
2	A	5	ARG
2	A	8	GLU
2	A	9	ARG
2	A	19	GLU
2	A	22	LEU
2	A	41	GLU
2	A	43	GLU
2	A	53	LEU
2	A	62	LYS
2	A	74	MET
2	A	76	GLN
2	A	78	ILE
2	A	92	MET
2	A	94	GLU
2	A	105	THR
2	A	106	GLU
2	A	117	GLU
2	A	138	VAL
2	A	139	LEU
2	A	142	LEU
2	A	155	ASN
2	A	170	LEU
2	A	185	ARG
2	A	187	LYS
2	A	194	GLU
2	A	209	GLU
2	A	224	GLN
2	A	238	ARG
2	A	262	LYS
2	A	268	ILE
2	A	269	ARG
2	A	294	ILE
2	A	303	SER
2	A	315	THR
2	A	335	GLN
2	A	337	ILE
2	A	341	GLN
2	A	354	LEU
2	A	355	ARG
2	A	364	VAL

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Mol	Chain	Res	Type
2	A	379	ASP
2	A	380	ARG
2	A	392	ILE
2	A	415	GLU
2	A	423	VAL
2	A	424	ARG
2	A	443	ARG
2	A	449	LEU
2	A	452	GLN
2	A	457	LYS
2	A	461	LYS
2	A	463	LYS
2	A	470	GLU
2	A	471	VAL
2	A	475	ASP
2	A	497	ASP
2	A	503	GLU
2	A	509	ARG
2	A	511	ILE
2	A	563	PHE
2	A	578	MET
2	A	597	ASP
2	A	624	PRO
2	A	626	VAL
2	A	632	GLN
2	A	634	LEU
2	A	641	ASP
2	A	647	VAL
2	A	673	PHE
2	A	674	ASN
2	A	675	VAL
2	A	676	GLN
2	A	687	ASP
2	A	690	MET
2	A	694	LYS
2	A	700	GLU
2	A	713	SER
2	A	729	GLN
2	A	730	LEU
2	A	741	ILE
2	A	763	ARG
2	A	795	ASP

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Mol	Chain	Res	Type
2	B	3	PHE
2	B	5	ARG
2	B	11	GLN
2	B	18	GLN
2	B	20	GLU
2	B	27	ASN
2	B	41	GLU
2	B	62	LYS
2	B	72	GLN
2	B	74	MET
2	B	78	ILE
2	B	83	ARG
2	B	96	ARG
2	B	100	HIS
2	B	105	THR
2	B	115	GLU
2	B	117	GLU
2	B	137	GLN
2	B	138	VAL
2	B	139	LEU
2	B	166	LEU
2	B	170	LEU
2	B	185	ARG
2	B	194	GLU
2	B	214	LYS
2	B	230	VAL
2	B	232	GLU
2	B	235	ARG
2	B	265	MET
2	B	268	ILE
2	B	269	ARG
2	B	308	GLU
2	B	309	LEU
2	B	355	ARG
2	B	358	TYR
2	B	359	GLU
2	B	361	HIS
2	B	363	ARG
2	B	364	VAL
2	B	380	ARG
2	B	385	ARG
2	B	387	LEU

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Mol	Chain	Res	Type
2	B	392	ILE
2	B	415	GLU
2	B	423	VAL
2	B	424	ARG
2	B	425	LYS
2	B	443	ARG
2	B	451	GLU
2	B	452	GLN
2	B	457	LYS
2	B	472	THR
2	B	478	MET
2	B	479	VAL
2	B	480	VAL
2	B	481	SER
2	B	483	TRP
2	B	503	GLU
2	B	509	ARG
2	B	511	ILE
2	B	531	LEU
2	B	567	GLU
2	B	578	MET
2	B	586	LEU
2	B	597	ASP
2	B	609	LYS
2	B	620	GLU
2	B	624	PRO
2	B	639	LEU
2	B	641	ASP
2	B	643	LYS
2	B	682	HIS
2	B	693	LEU
2	B	695	ARG
2	B	716	LYS
2	B	719	LEU
2	B	729	GLN
2	B	730	LEU
2	B	739	LEU
2	B	742	GLU
2	B	790	GLN
2	B	795	ASP
2	C	5	ARG
2	C	11	GLN

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Mol	Chain	Res	Type
2	C	18	GLN
2	C	19	GLU
2	C	20	GLU
2	C	27	ASN
2	C	31	THR
2	C	32	GLU
2	C	45	ILE
2	C	53	LEU
2	C	62	LYS
2	C	72	GLN
2	C	74	MET
2	C	83	ARG
2	C	105	THR
2	C	106	GLU
2	C	135	ARG
2	C	138	VAL
2	C	139	LEU
2	C	202	ASN
2	C	254	ARG
2	C	269	ARG
2	C	285	ILE
2	C	308	GLU
2	C	323	TYR
2	C	342	PRO
2	C	346	GLU
2	C	357	ARG
2	C	362	HIS
2	C	363	ARG
2	C	379	ASP
2	C	380	ARG
2	C	385	ARG
2	C	392	ILE
2	C	397	GLU
2	C	410	PRO
2	C	415	GLU
2	C	423	VAL
2	C	424	ARG
2	C	427	LYS
2	C	431	VAL
2	C	434	GLN
2	C	443	ARG
2	C	449	LEU

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Mol	Chain	Res	Type
2	C	452	GLN
2	C	460	TRP
2	C	463	LYS
2	C	478	MET
2	C	495	GLU
2	C	503	GLU
2	C	549	VAL
2	C	565	ASP
2	C	586	LEU
2	C	603	THR
2	C	609	LYS
2	C	611	TYR
2	C	624	PRO
2	C	634	LEU
2	C	639	LEU
2	C	647	VAL
2	C	648	ASP
2	C	665	LEU
2	C	667	ARG
2	C	669	LYS
2	C	679	THR
2	C	680	GLN
2	C	688	LYS
2	C	690	MET
2	C	695	ARG
2	C	713	SER
2	C	729	GLN
2	C	730	LEU
2	C	741	ILE
2	C	742	GLU
2	C	767	ARG
2	C	795	ASP
2	D	11	GLN
2	D	19	GLU
2	D	22	LEU
2	D	31	THR
2	D	32	GLU
2	D	41	GLU
2	D	53	LEU
2	D	62	LYS
2	D	74	MET
2	D	76	GLN

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Mol	Chain	Res	Type
2	D	85	LYS
2	D	90	LEU
2	D	105	THR
2	D	106	GLU
2	D	115	GLU
2	D	117	GLU
2	D	136	GLN
2	D	138	VAL
2	D	139	LEU
2	D	185	ARG
2	D	194	GLU
2	D	224	GLN
2	D	229	GLU
2	D	234	LEU
2	D	235	ARG
2	D	237	LYS
2	D	265	MET
2	D	269	ARG
2	D	308	GLU
2	D	323	TYR
2	D	337	ILE
2	D	342	PRO
2	D	357	ARG
2	D	361	HIS
2	D	364	VAL
2	D	380	ARG
2	D	381	TYR
2	D	387	LEU
2	D	392	ILE
2	D	397	GLU
2	D	403	ARG
2	D	412	ASN
2	D	415	GLU
2	D	423	VAL
2	D	424	ARG
2	D	428	ASP
2	D	431	VAL
2	D	443	ARG
2	D	452	GLN
2	D	457	LYS
2	D	462	GLU
2	D	471	VAL

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Mol	Chain	Res	Type
2	D	479	VAL
2	D	503	GLU
2	D	511	ILE
2	D	546	PRO
2	D	563	PHE
2	D	567	GLU
2	D	570	ILE
2	D	574	MET
2	D	578	MET
2	D	593	TYR
2	D	606	VAL
2	D	609	LYS
2	D	611	TYR
2	D	623	HIS
2	D	634	LEU
2	D	636	ASP
2	D	639	LEU
2	D	648	ASP
2	D	680	GLN
2	D	695	ARG
2	D	729	GLN
2	D	730	LEU
2	D	742	GLU
2	D	758	LEU
2	D	766	ARG
2	D	804	LYS
2	E	11	GLN
2	E	18	GLN
2	E	45	ILE
2	E	53	LEU
2	E	62	LYS
2	E	83	ARG
2	E	100	HIS
2	E	108	ILE
2	E	119	VAL
2	E	139	LEU
2	E	180	ASP
2	E	229	GLU
2	E	262	LYS
2	E	265	MET
2	E	269	ARG
2	E	270	GLN

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Mol	Chain	Res	Type
2	E	299	ILE
2	E	337	ILE
2	E	342	PRO
2	E	355	ARG
2	E	359	GLU
2	E	363	ARG
2	E	378	SER
2	E	380	ARG
2	E	382	ILE
2	E	384	ASP
2	E	393	ASP
2	E	397	GLU
2	E	400	SER
2	E	401	LYS
2	E	410	PRO
2	E	415	GLU
2	E	421	ASP
2	E	423	VAL
2	E	424	ARG
2	E	427	LYS
2	E	428	ASP
2	E	435	GLU
2	E	443	ARG
2	E	452	GLN
2	E	457	LYS
2	E	461	LYS
2	E	462	GLU
2	E	480	VAL
2	E	503	GLU
2	E	509	ARG
2	E	511	ILE
2	E	544	LEU
2	E	593	TYR
2	E	597	ASP
2	E	611	TYR
2	E	624	PRO
2	E	626	VAL
2	E	639	LEU
2	E	641	ASP
2	E	647	VAL
2	E	665	LEU
2	E	667	ARG

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Mol	Chain	Res	Type
2	E	685	MET
2	E	690	MET
2	E	697	PHE
2	E	711	PHE
2	E	719	LEU
2	E	730	LEU
2	E	741	ILE
2	E	759	GLU
2	E	760	TYR
2	E	790	GLN
2	E	791	HIS
2	E	795	ASP
2	F	11	GLN
2	F	19	GLU
2	F	20	GLU
2	F	32	GLU
2	F	62	LYS
2	F	72	GLN
2	F	74	MET
2	F	83	ARG
2	F	96	ARG
2	F	100	HIS
2	F	105	THR
2	F	119	VAL
2	F	137	GLN
2	F	138	VAL
2	F	170	LEU
2	F	185	ARG
2	F	209	GLU
2	F	262	LYS
2	F	269	ARG
2	F	303	SER
2	F	337	ILE
2	F	341	GLN
2	F	351	LEU
2	F	357	ARG
2	F	364	VAL
2	F	379	ASP
2	F	380	ARG
2	F	381	TYR
2	F	387	LEU
2	F	397	GLU

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Mol	Chain	Res	Type
2	F	414	LYS
2	F	415	GLU
2	F	423	VAL
2	F	424	ARG
2	F	431	VAL
2	F	443	ARG
2	F	449	LEU
2	F	452	GLN
2	F	468	ASN
2	F	471	VAL
2	F	473	VAL
2	F	475	ASP
2	F	476	ILE
2	F	478	MET
2	F	479	VAL
2	F	503	GLU
2	F	509	ARG
2	F	579	GLU
2	F	586	LEU
2	F	589	SER
2	F	593	TYR
2	F	611	TYR
2	F	636	ASP
2	F	639	LEU
2	F	641	ASP
2	F	664	GLU
2	F	676	GLN
2	F	690	MET
2	F	692	GLU
2	F	697	PHE
2	F	704	ARG
2	F	710	VAL
2	F	719	LEU
2	F	729	GLN
2	F	730	LEU
2	F	741	ILE
2	F	742	GLU
2	F	760	TYR
2	F	766	ARG
2	F	790	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	194	HIS
1	1	207	HIS
1	3	207	HIS
1	4	207	HIS
1	5	146	ASN
1	5	207	HIS
2	A	26	HIS
2	A	33	HIS
2	A	137	GLN
2	A	155	ASN
2	A	190	GLN
2	A	352	GLN
2	A	507	HIS
2	A	513	GLN
2	A	581	HIS
2	A	682	HIS
2	B	107	HIS
2	B	140	GLN
2	B	224	GLN
2	B	273	ASN
2	B	338	GLN
2	B	352	GLN
2	B	434	GLN
2	B	504	ASN
2	B	507	HIS
2	B	581	HIS
2	B	682	HIS
2	B	718	HIS
2	C	26	HIS
2	C	33	HIS
2	C	224	GLN
2	C	352	GLN
2	C	447	GLN
2	C	504	ASN
2	C	507	HIS
2	C	628	ASN
2	C	703	ASN
2	C	791	HIS
2	D	26	HIS
2	D	72	GLN
2	D	79	HIS
2	D	100	HIS
2	D	137	GLN

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Mol	Chain	Res	Type
2	D	362	HIS
2	D	507	HIS
2	D	703	ASN
2	D	712	HIS
2	D	718	HIS
2	D	772	HIS
2	E	190	GLN
2	E	335	GLN
2	E	507	HIS
2	E	581	HIS
2	E	651	ASN
2	E	772	HIS
2	F	26	HIS
2	F	33	HIS
2	F	100	HIS
2	F	107	HIS
2	F	190	GLN
2	F	203	ASN
2	F	273	ASN
2	F	310	GLN
2	F	361	HIS
2	F	412	ASN
2	F	468	ASN
2	F	507	HIS
2	F	601	GLN
2	F	623	HIS
2	F	681	ASN
2	F	682	HIS
2	F	718	HIS
2	F	737	GLN
2	F	770	GLN
2	F	772	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

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.