wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:03 PM BST

PDB ID	:	4UUK
EMDB ID:	:	EMD-2701
Title	:	Human dynamin 1 K44A superconstricted polymer stabilized with GTP strand 2
Authors	:	Sundborger, A.C.; Fang, S.; Heymann, J.A.; Ray, P.; Chappie, J.S.; Hinshaw, J.E.
Deposited on	:	2014-07-29
Resolution	:	12.50 Å(reported)
Based on PDB ID	:	3ZYC,3SNH,1DYN

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

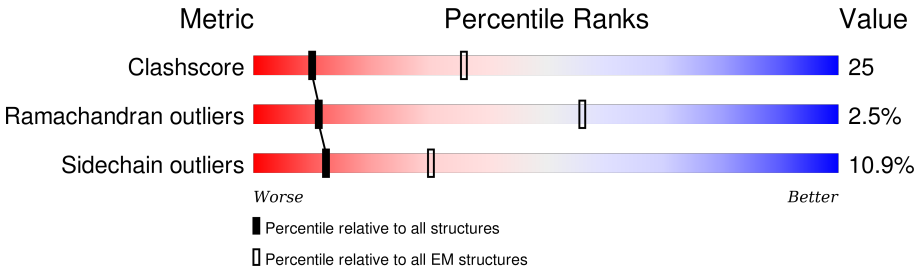
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 12.50 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	A	864	24% 13% • 62%
1	D	864	24% 12% • 61%
1	G	864	24% 12% • 62%
1	K	864	24% 12% • 61%
2	B	864	10% 7% • • 76%
2	C	864	7% 5% •• 87%
2	E	864	8% 11% • • 76%
2	F	864	7% • •• 87%
2	H	864	7% 5% •• 87%

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Mol	Chain	Length	Quality of chain
2	I	864	10% 8% 76%
2	J	864	8% 11% 76%
2	L	864	7% 87%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21116 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 DYNAMIN-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	329	Total 2567	C 1615	N 453	O 489	S 10	0	0
1	D	337	Total 2643	C 1664	N 466	O 503	S 10	0	0
1	G	329	Total 2567	C 1615	N 453	O 489	S 10	0	0
1	K	337	Total 2643	C 1664	N 466	O 503	S 10	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	744	ASN	ASP	VARIANT	UNP Q05193
D	744	ASN	ASP	VARIANT	UNP Q05193
G	744	ASN	ASP	VARIANT	UNP Q05193
K	744	ASN	ASP	VARIANT	UNP Q05193

- Molecule 2 is a protein called DYNAMIN-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	208	Total 1728	C 1097	N 304	O 313	S 14	0	0
2	C	113	Total 946	C 609	N 158	O 175	S 4	0	0
2	E	208	Total 1728	C 1097	N 304	O 313	S 14	0	0
2	F	113	Total 946	C 609	N 158	O 175	S 4	0	0
2	H	113	Total 946	C 609	N 158	O 175	S 4	0	0
2	I	208	Total 1728	C 1097	N 304	O 313	S 14	0	0
2	J	208	Total 1728	C 1097	N 304	O 313	S 14	0	0

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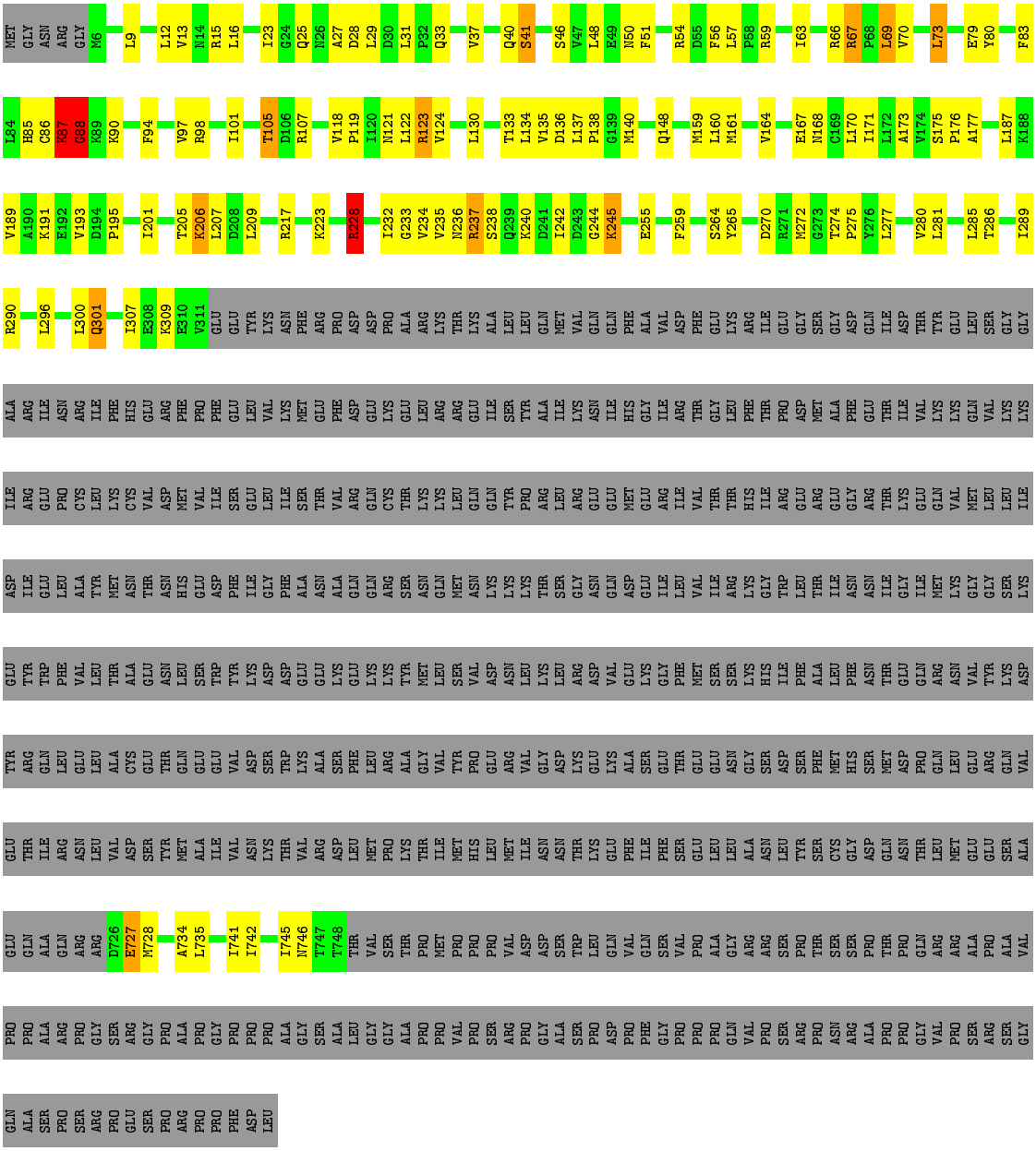
Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	113	Total	C	N	O	S	0	0
			946	609	158	175	4		

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.

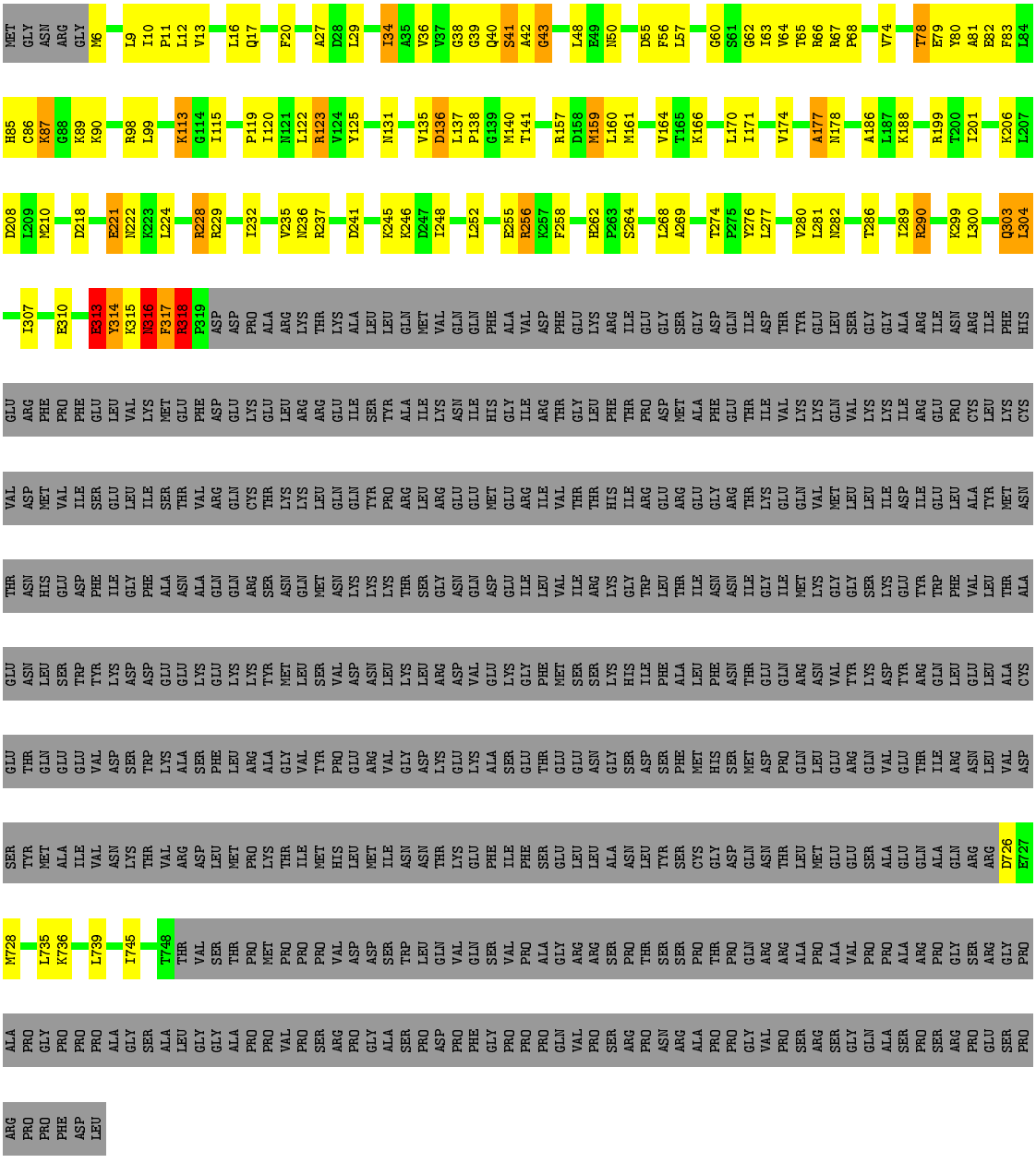
- Molecule 1: DYNAMIN-1

Chain A:



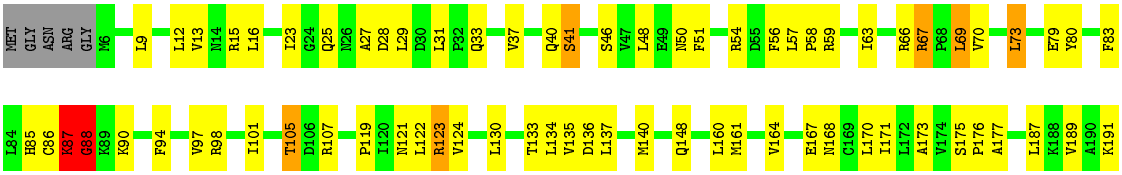
- Molecule 1: DYNAMIN-1

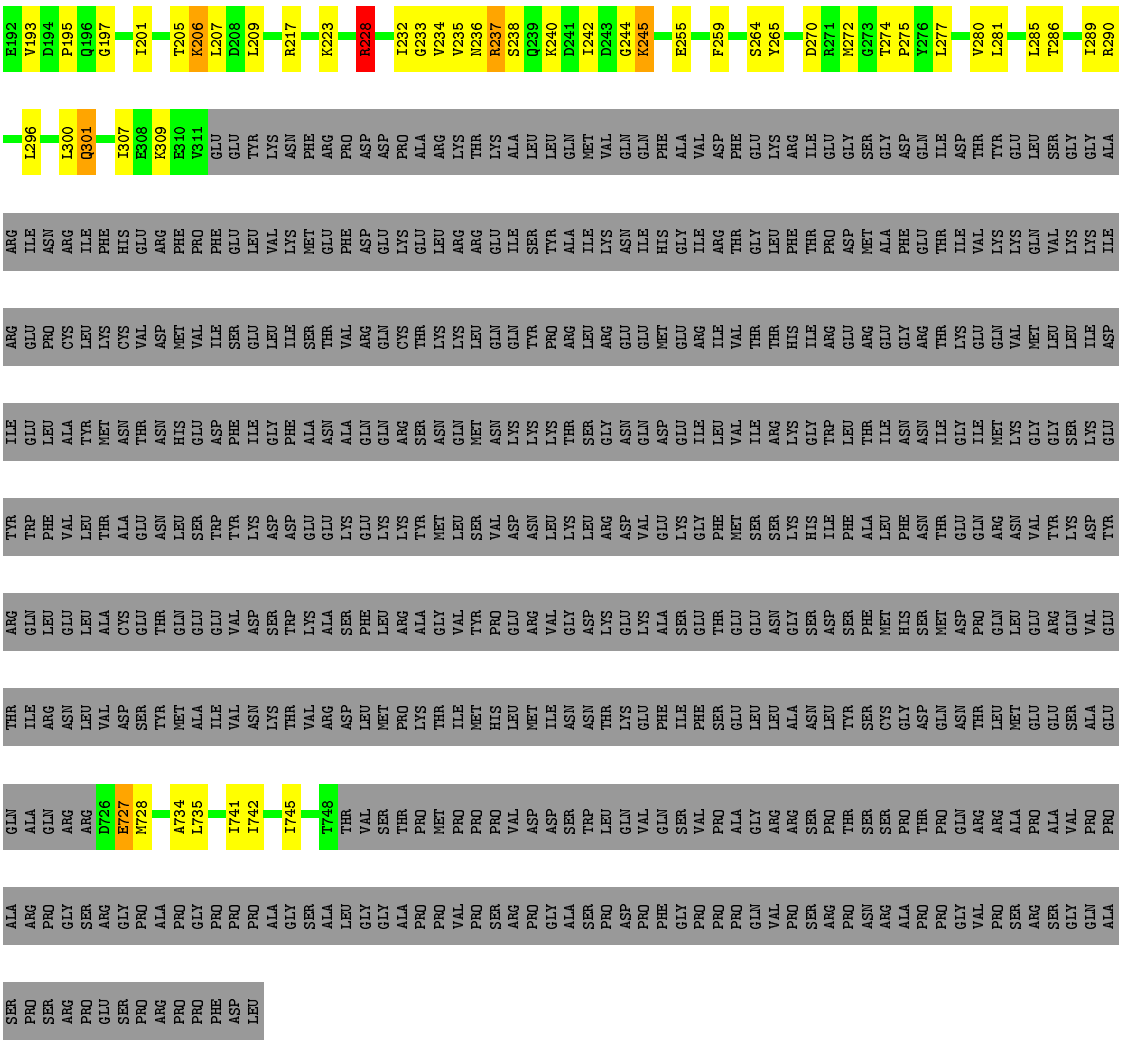
Chain D:



- Molecule 1: DYNAMIN-1

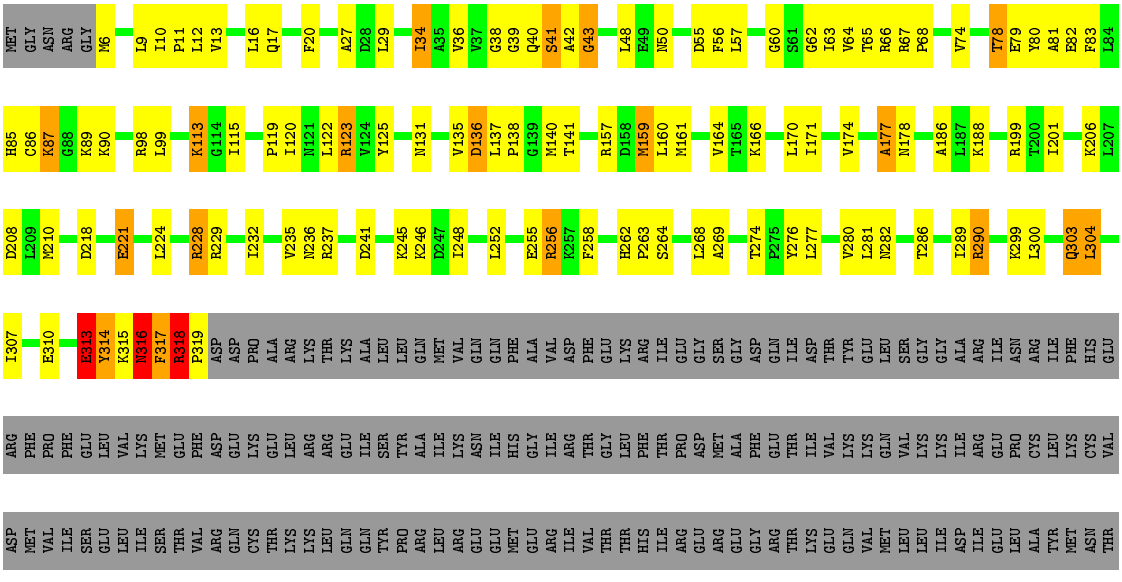
Chain G:

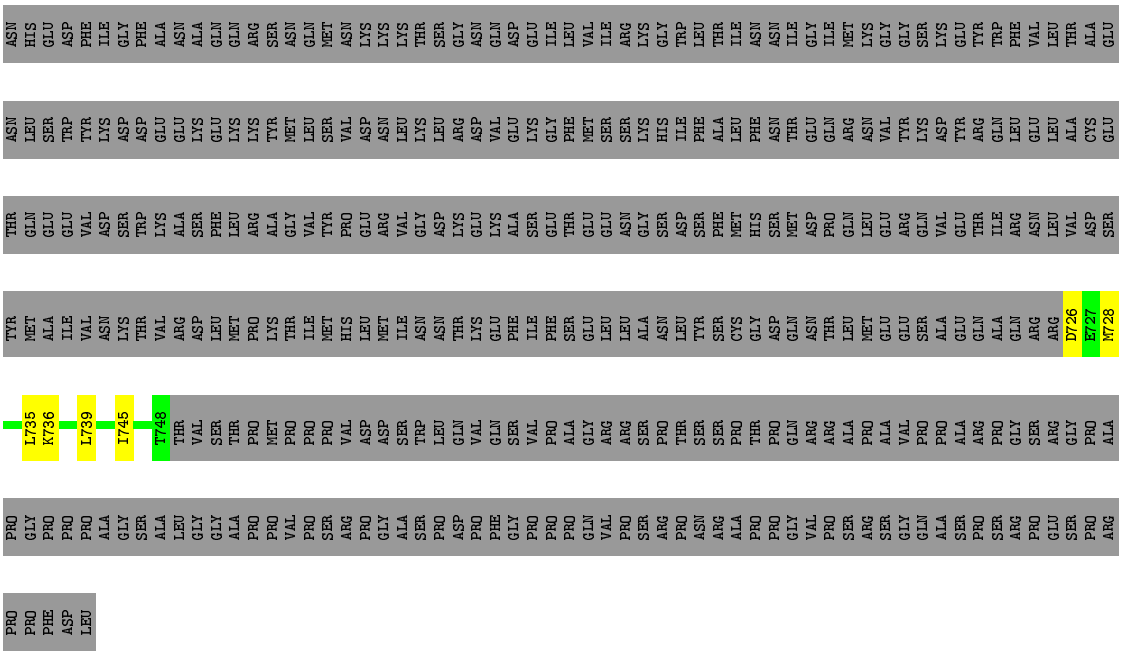




• Molecule 1: DYNAMIN-1

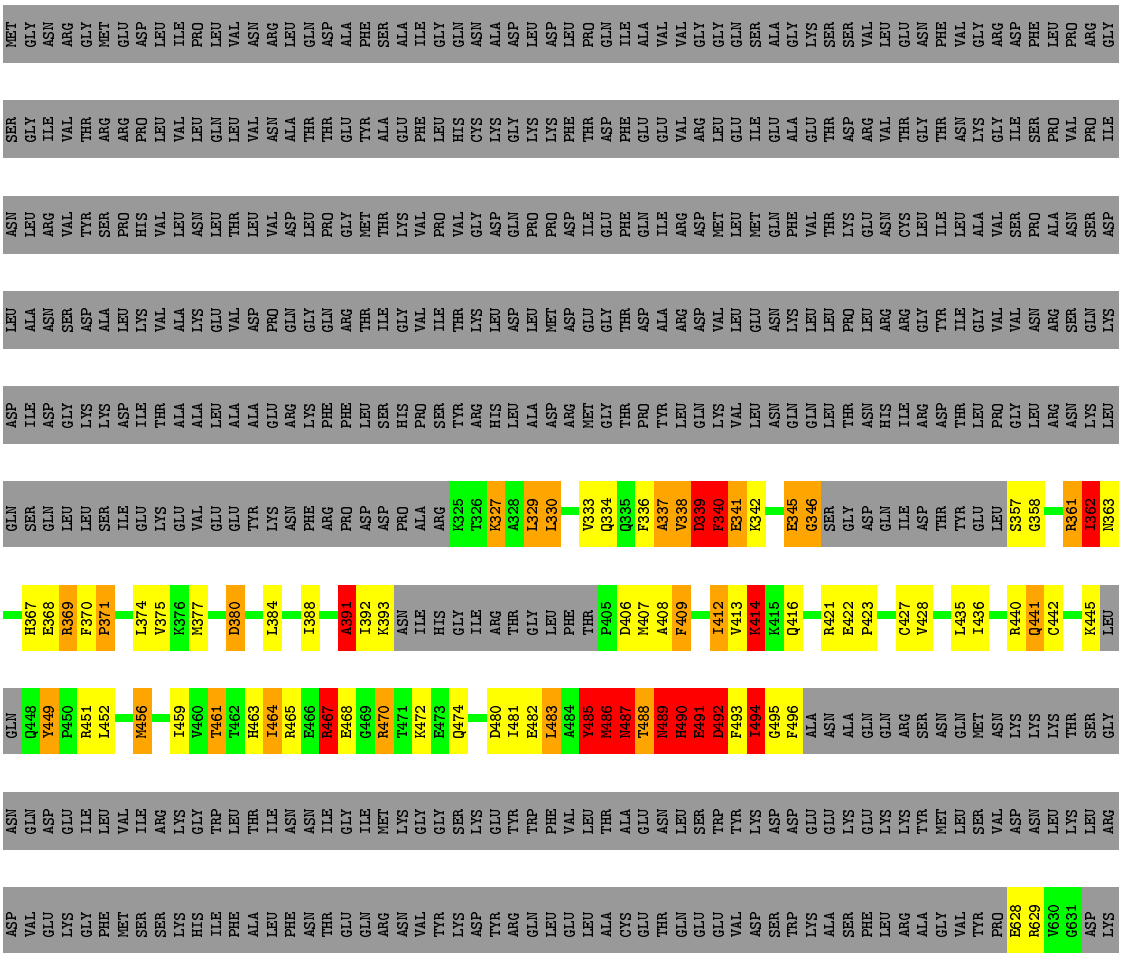
Chain K:

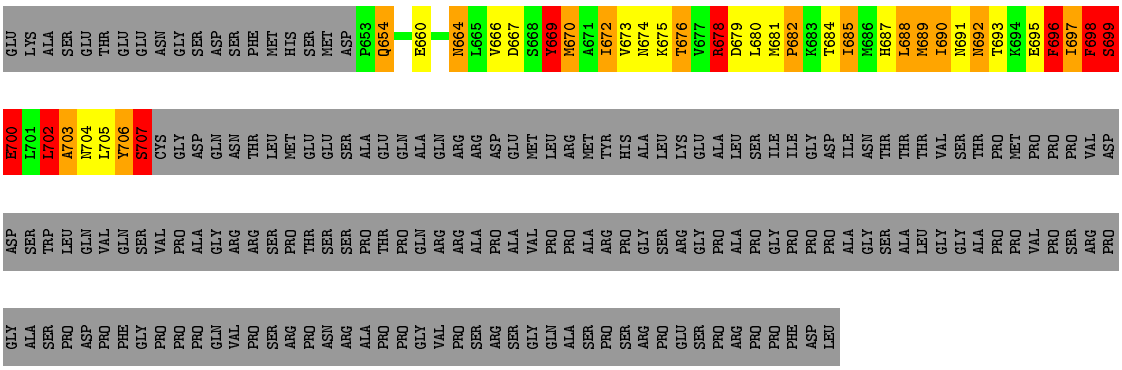




- Molecule 2: DYNAMIN-1

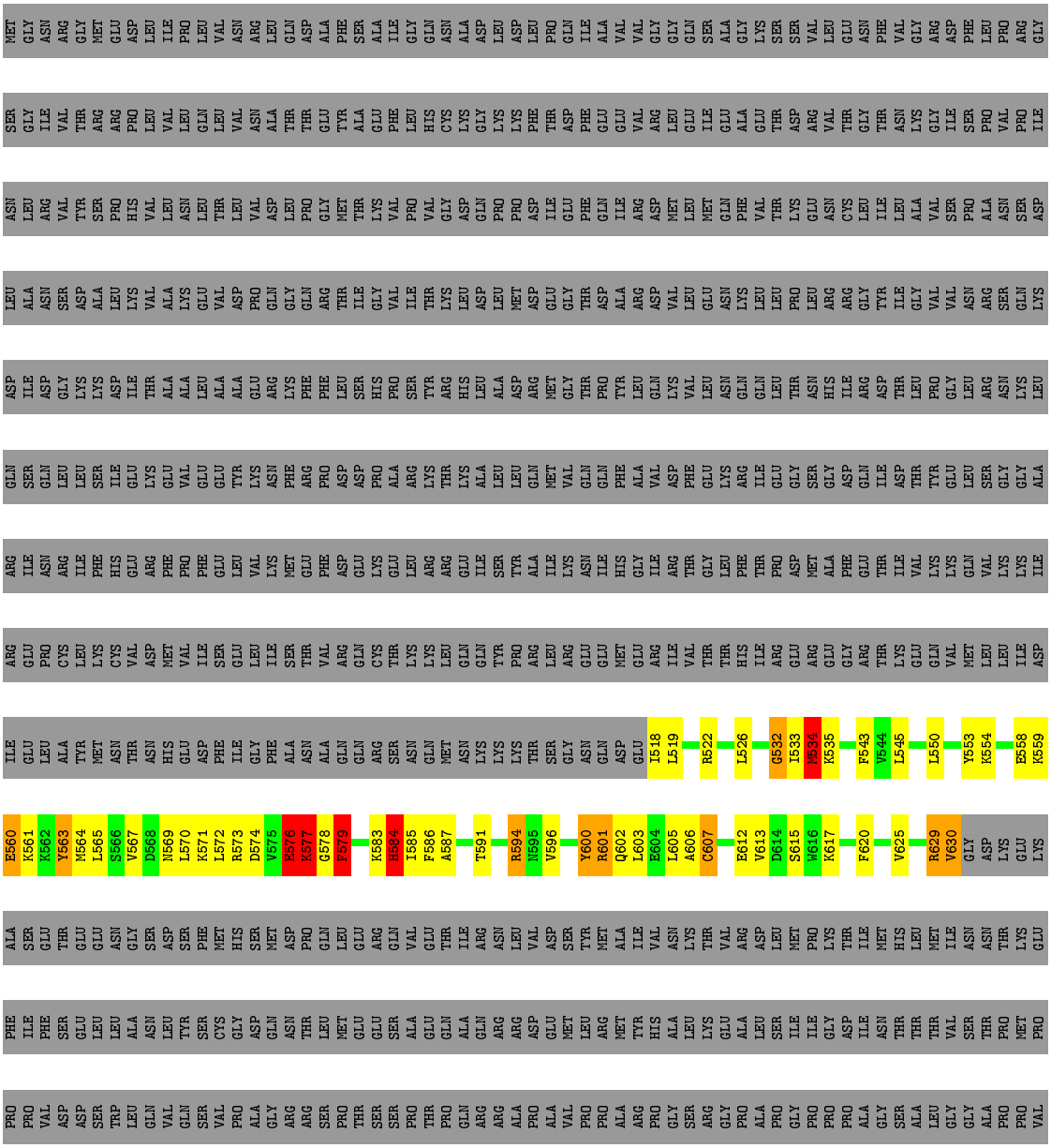
Chain B:





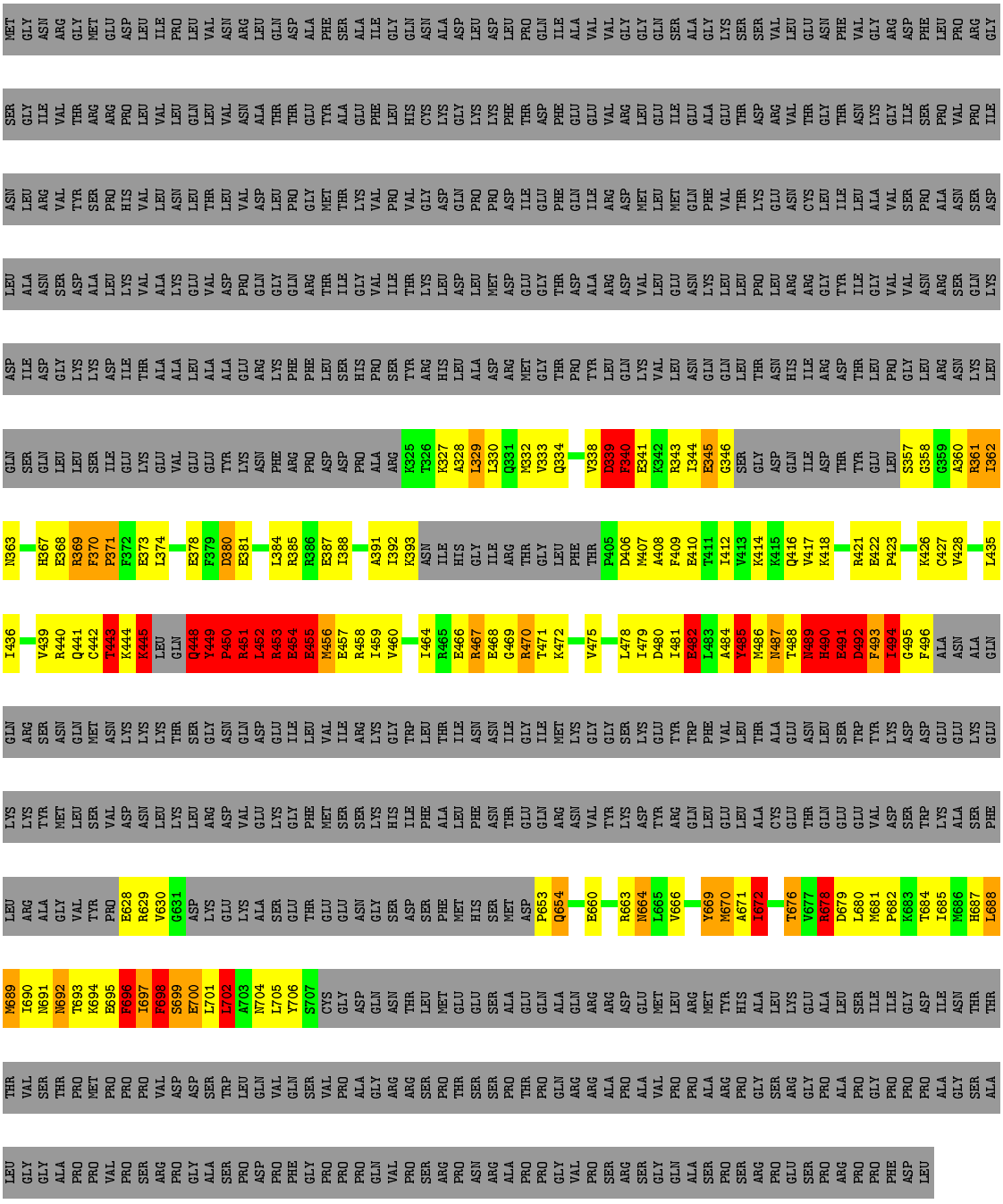
- Molecule 2: DYNAMIN-1

Chain C: 7% 5% •• 87%



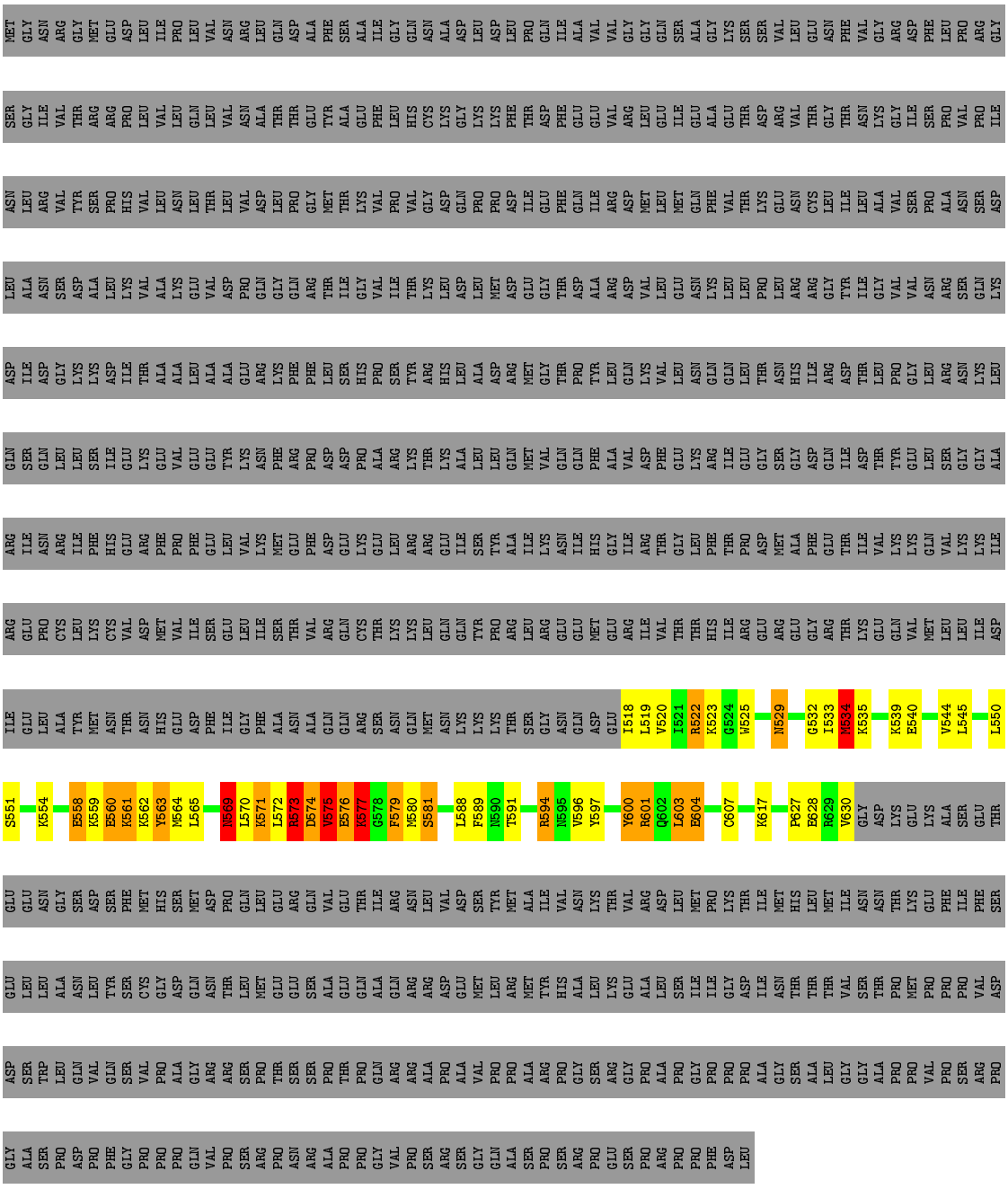
- Molecule 2: DYNAMIN-1

Chain E:



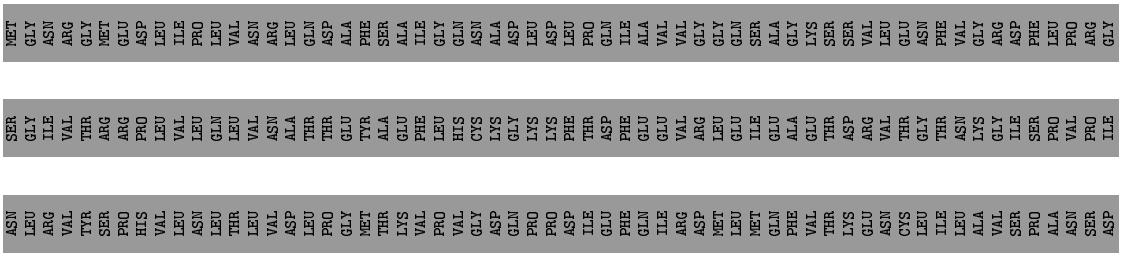
- Molecule 2: DYNAMIN-1

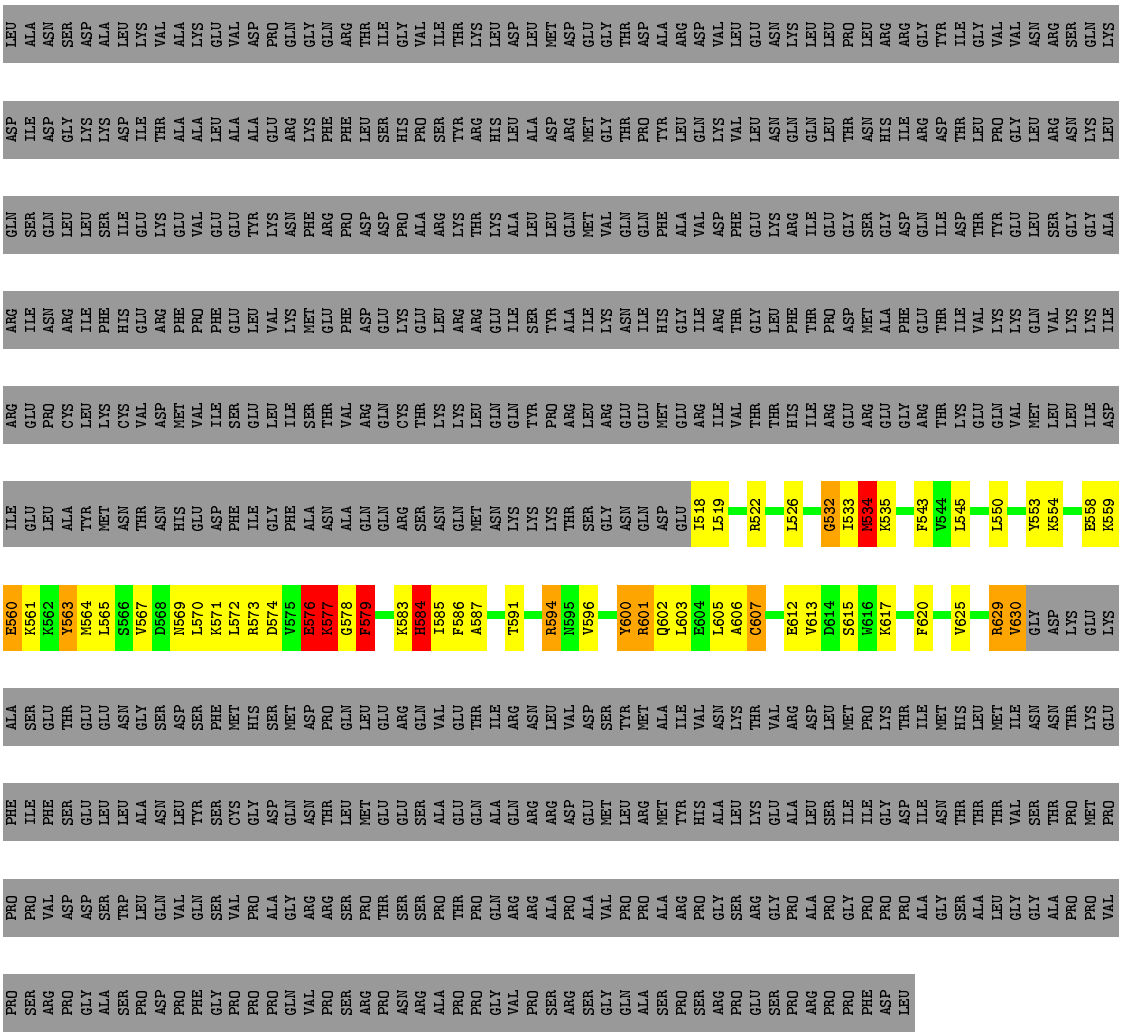
Chain F:



- Molecule 2: DYNAMIN-1

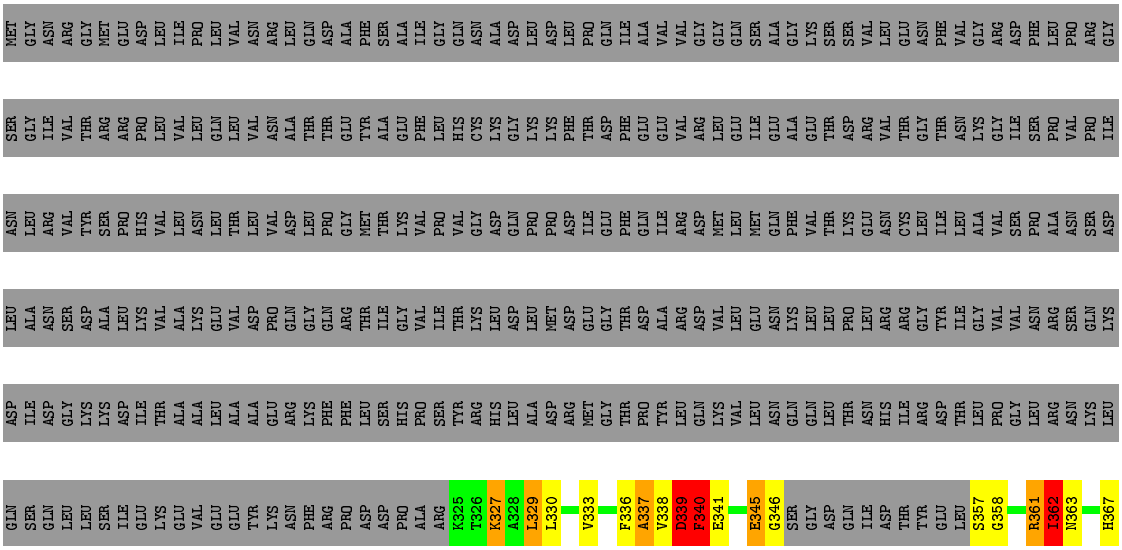
Chain H:

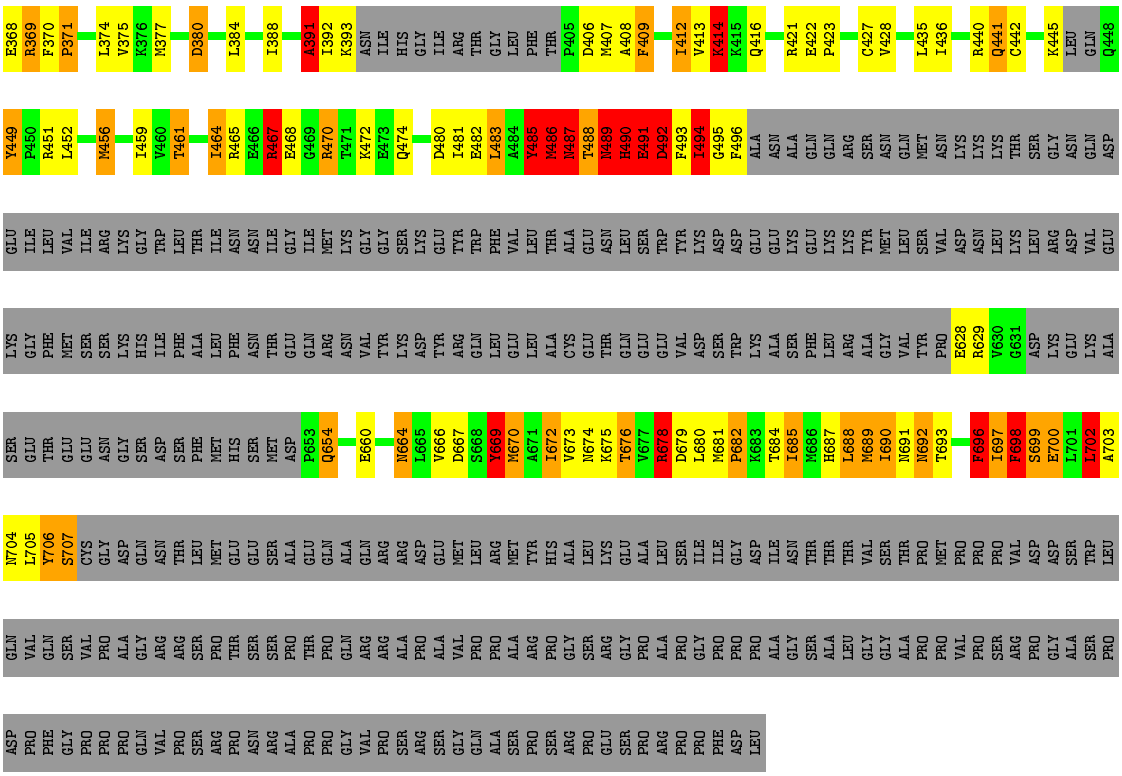




- Molecule 2: DYNAMIN-1

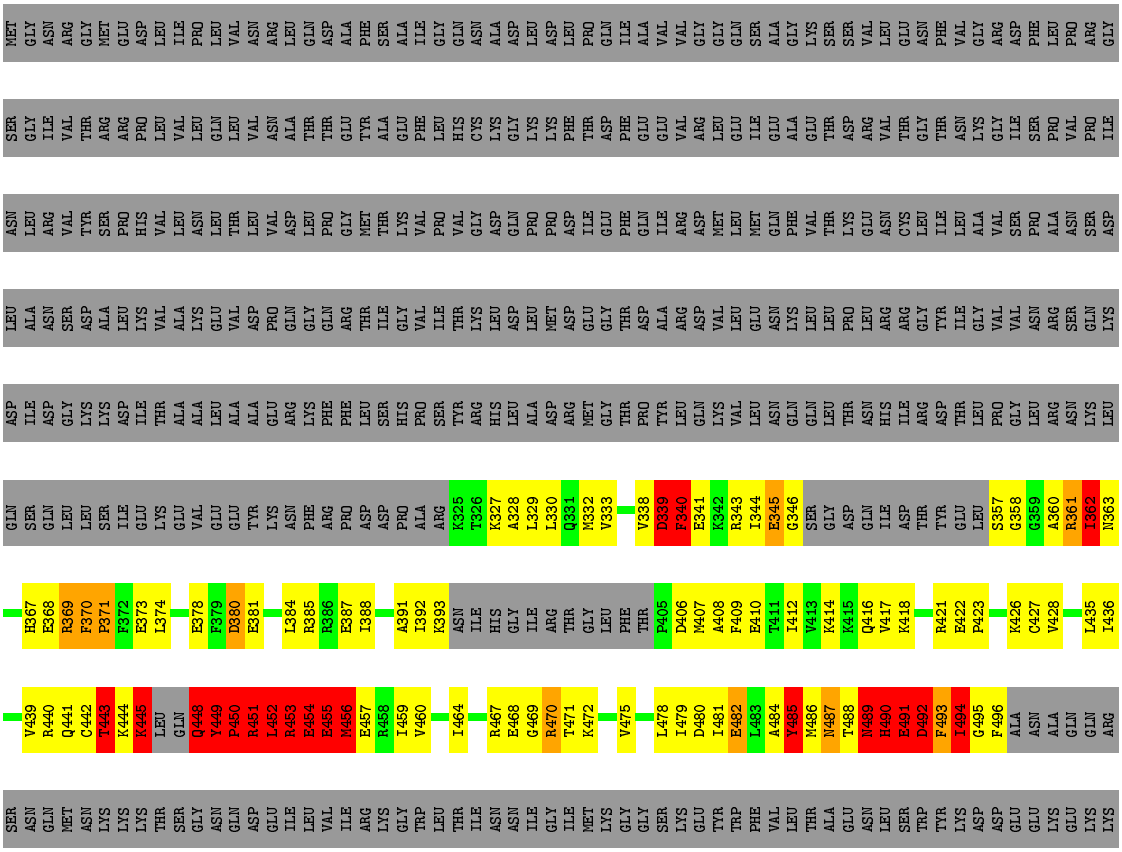
Chain I:

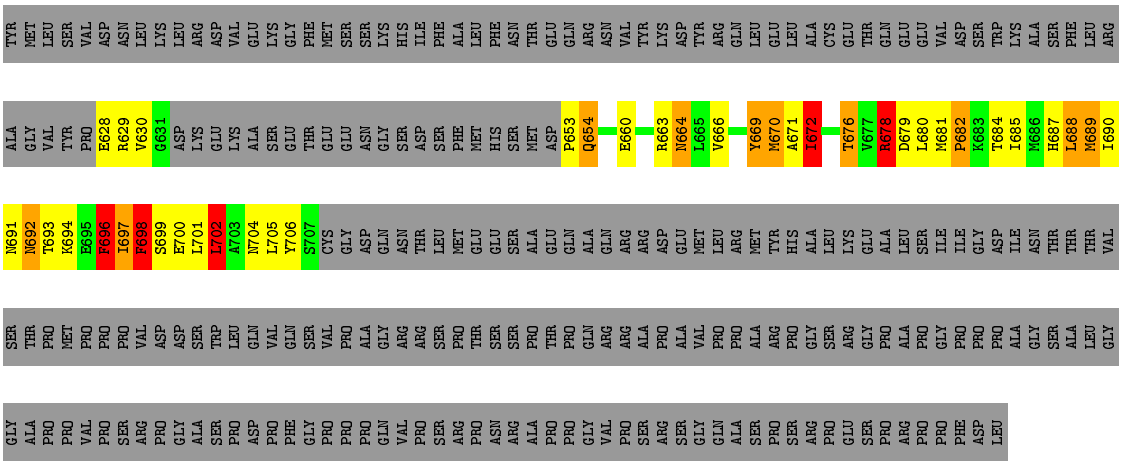




- Molecule 2: DYNAMIN-1

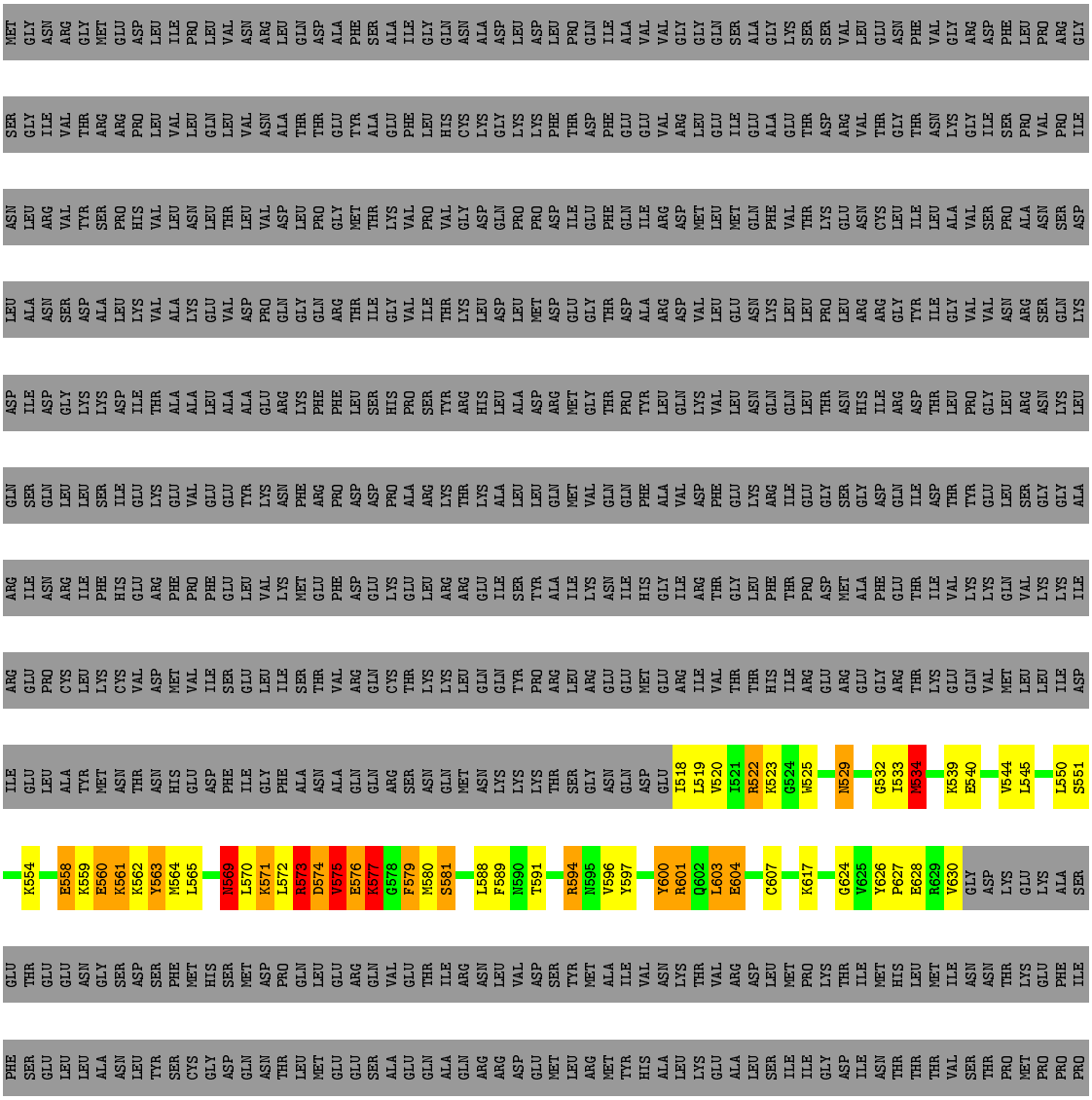
Chain J:





- Molecule 2: DYNAMIN-1

Chain L: 7% 87%



VAL ASP ASP SER TRP LEU GLN VAL GLN SER VAL PRO ALA GLY ARG ARG SER PRO THR SER SER PRO THR PRO GLN ARG ARG ALA PRO ALA VAL PRO PRO ALA ARG PRO GLY SER ARG GLY PRO ALA PRO GLY PRO PRO PRO ALA GLY SER ALA LEU GLY GLY ALA PRO PRO VAL PRO SER

ARG PRO GLY ALA SER PRO ASP PRO PHE GLY PRO PRO PRO GLN VAL PRO SER ARG PRO ASN ARG ALA PRO PRO GLY VAL PRO SER ARG SER GLY GLN ALA SER PRO SER ARG PRO GLU SER PRO ARG PRO PRO PHE ASP LEU

4 Experimental information (i)

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	INDIVIDUAL IMAGES	Depositor
Microscope	FEI/PHILIPS CM300FEG/HE	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK SO-163 FILM	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	A	0.72	2/2604 (0.1%)	1.19	19/3524 (0.5%)
1	D	0.88	6/2683 (0.2%)	1.44	37/3630 (1.0%)
1	G	0.72	2/2604 (0.1%)	1.19	19/3524 (0.5%)
1	K	0.88	6/2683 (0.2%)	1.44	37/3630 (1.0%)
2	B	1.32	14/1748 (0.8%)	2.41	83/2331 (3.6%)
2	C	0.86	2/966 (0.2%)	1.42	20/1298 (1.5%)
2	E	1.39	20/1748 (1.1%)	2.56	104/2331 (4.5%)
2	F	1.15	7/966 (0.7%)	1.82	37/1298 (2.9%)
2	H	0.86	2/966 (0.2%)	1.42	20/1298 (1.5%)
2	I	1.32	14/1748 (0.8%)	2.41	83/2331 (3.6%)
2	J	1.39	20/1748 (1.1%)	2.56	104/2331 (4.5%)
2	L	1.15	7/966 (0.7%)	1.82	37/1298 (2.9%)
All	All	1.05	102/21430 (0.5%)	1.83	600/28824 (2.1%)

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	A	1	11
1	D	0	14
1	G	1	12
1	K	0	14
2	B	5	40
2	C	4	9
2	E	10	36
2	F	7	10
2	H	4	9
2	I	5	39
2	J	10	36
2	L	7	10
All	All	54	240

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	490	HIS	C-O	-16.99	0.91	1.23
2	I	490	HIS	C-O	-16.99	0.91	1.23
2	B	699	SER	CB-OG	-16.13	1.21	1.42
2	I	699	SER	CB-OG	-16.07	1.21	1.42
2	I	492	ASP	C-O	-14.57	0.95	1.23
2	B	492	ASP	C-O	-14.56	0.95	1.23
2	E	492	ASP	C-O	-14.26	0.96	1.23
2	J	492	ASP	C-O	-14.26	0.96	1.23
1	D	318	ARG	CB-CG	-13.80	1.15	1.52
1	K	318	ARG	CB-CG	-13.79	1.15	1.52
2	B	488	THR	C-O	-12.46	0.99	1.23
2	I	488	THR	C-O	-12.45	0.99	1.23
2	E	490	HIS	CG-CD2	-12.41	1.14	1.35
2	J	490	HIS	CG-CD2	-12.39	1.14	1.35
2	J	699	SER	CB-OG	-12.22	1.26	1.42
2	E	699	SER	CB-OG	-12.19	1.26	1.42
2	E	449	TYR	CA-CB	-11.52	1.28	1.53
2	J	449	TYR	CA-CB	-11.52	1.28	1.53
2	E	490	HIS	C-O	-11.35	1.01	1.23
2	J	490	HIS	C-O	-11.34	1.01	1.23
1	K	317	PHE	C-O	-10.57	1.03	1.23
1	D	317	PHE	C-O	-10.56	1.03	1.23
2	J	491	GLU	CB-CG	-10.44	1.32	1.52
2	E	491	GLU	CB-CG	-10.41	1.32	1.52
1	G	245	LYS	CA-CB	-9.84	1.32	1.53
1	A	245	LYS	CA-CB	-9.84	1.32	1.53
2	E	491	GLU	CA-CB	9.48	1.74	1.53
2	J	491	GLU	CA-CB	9.48	1.74	1.53
2	L	628	GLU	CA-CB	-8.93	1.34	1.53
2	F	628	GLU	CA-CB	-8.92	1.34	1.53
2	B	489	ASN	CA-C	-8.70	1.30	1.52
2	I	489	ASN	CA-C	-8.66	1.30	1.52
1	A	88	GLY	N-CA	-8.59	1.33	1.46
1	G	88	GLY	N-CA	-8.59	1.33	1.46
2	J	700	GLU	CB-CG	-8.30	1.36	1.52
2	E	700	GLU	CB-CG	-8.28	1.36	1.52
2	I	490	HIS	CA-C	-8.13	1.31	1.52
2	I	487	ASN	C-N	8.12	1.52	1.34
2	B	490	HIS	CA-C	-8.11	1.31	1.52
2	B	487	ASN	C-N	8.10	1.52	1.34
2	E	490	HIS	CA-C	-7.65	1.33	1.52
2	J	490	HIS	CA-C	-7.65	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	318	ARG	N-CA	-7.49	1.31	1.46
1	K	318	ARG	N-CA	-7.48	1.31	1.46
1	D	313	GLU	C-O	-7.47	1.09	1.23
1	K	313	GLU	C-O	-7.45	1.09	1.23
2	I	489	ASN	N-CA	-7.26	1.31	1.46
2	B	489	ASN	N-CA	-7.25	1.31	1.46
2	I	489	ASN	C-N	-7.23	1.17	1.34
2	B	489	ASN	C-N	-7.21	1.17	1.34
2	J	449	TYR	C-N	7.13	1.47	1.34
2	E	449	TYR	C-N	7.12	1.47	1.34
2	L	569	ASN	CA-CB	-6.86	1.35	1.53
2	F	569	ASN	CA-CB	-6.85	1.35	1.53
1	D	316	ASN	C-N	-6.84	1.18	1.34
1	K	316	ASN	C-N	-6.84	1.18	1.34
2	J	449	TYR	CB-CG	-6.66	1.41	1.51
2	E	449	TYR	CB-CG	-6.66	1.41	1.51
2	J	442	CYS	N-CA	-6.47	1.33	1.46
2	E	442	CYS	N-CA	-6.46	1.33	1.46
2	J	490	HIS	ND1-CE1	-6.45	1.18	1.34
2	E	490	HIS	ND1-CE1	-6.45	1.18	1.34
1	D	316	ASN	C-O	6.43	1.35	1.23
1	K	316	ASN	C-O	6.41	1.35	1.23
2	J	456	MET	CG-SD	-6.32	1.64	1.81
2	E	456	MET	CG-SD	-6.32	1.64	1.81
2	I	442	CYS	N-CA	-6.18	1.33	1.46
2	B	442	CYS	N-CA	-6.16	1.34	1.46
2	I	490	HIS	N-CA	-5.93	1.34	1.46
2	F	581	SER	N-CA	-5.93	1.34	1.46
2	L	581	SER	N-CA	-5.92	1.34	1.46
2	B	490	HIS	N-CA	-5.91	1.34	1.46
2	E	672	ILE	CB-CG1	-5.65	1.38	1.54
2	J	672	ILE	CB-CG1	-5.65	1.38	1.54
2	B	487	ASN	C-O	-5.64	1.12	1.23
2	I	487	ASN	C-O	-5.62	1.12	1.23
2	E	452	LEU	N-CA	-5.56	1.35	1.46
2	J	452	LEU	N-CA	-5.56	1.35	1.46
2	F	561	LYS	N-CA	-5.45	1.35	1.46
2	I	491	GLU	CA-C	-5.43	1.38	1.52
2	B	491	GLU	CA-C	-5.41	1.38	1.52
2	L	561	LYS	N-CA	-5.39	1.35	1.46
2	C	630	VAL	N-CA	-5.38	1.35	1.46
2	E	491	GLU	C-O	-5.37	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	630	VAL	N-CA	-5.37	1.35	1.46
2	J	491	GLU	C-O	-5.37	1.13	1.23
2	H	561	LYS	N-CA	-5.36	1.35	1.46
2	C	561	LYS	N-CA	-5.35	1.35	1.46
2	L	577	LYS	C-N	-5.26	1.23	1.33
2	F	577	LYS	C-N	-5.25	1.23	1.33
2	J	491	GLU	CG-CD	-5.24	1.44	1.51
2	E	491	GLU	CG-CD	-5.24	1.44	1.51
2	L	529	ASN	CA-CB	-5.22	1.39	1.53
2	F	529	ASN	CA-CB	-5.21	1.39	1.53
2	L	534	MET	N-CA	-5.20	1.35	1.46
2	F	534	MET	N-CA	-5.18	1.35	1.46
2	E	491	GLU	CA-C	-5.12	1.39	1.52
2	J	491	GLU	CA-C	-5.12	1.39	1.52
2	E	491	GLU	CD-OE2	-5.09	1.20	1.25
2	J	491	GLU	CD-OE2	-5.08	1.20	1.25
2	B	339	ASP	CA-CB	-5.05	1.42	1.53
2	I	339	ASP	CA-CB	-5.05	1.42	1.53

All (600) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	492	ASP	CB-CG-OD2	34.21	149.09	118.30
2	B	492	ASP	CB-CG-OD2	34.19	149.07	118.30
2	J	492	ASP	CB-CG-OD2	32.74	147.76	118.30
2	E	492	ASP	CB-CG-OD2	32.72	147.75	118.30
2	B	489	ASN	O-C-N	-30.67	73.63	122.70
2	I	489	ASN	O-C-N	-30.65	73.66	122.70
2	J	490	HIS	CG-ND1-CE1	25.62	144.07	108.20
2	E	490	HIS	CG-ND1-CE1	25.60	144.04	108.20
2	J	449	TYR	CA-CB-CG	24.77	160.47	113.40
2	E	449	TYR	CA-CB-CG	24.75	160.43	113.40
2	E	491	GLU	O-C-N	-24.50	83.49	122.70
2	J	491	GLU	O-C-N	-24.50	83.50	122.70
2	J	490	HIS	ND1-CG-CD2	-22.67	74.26	106.00
2	E	490	HIS	ND1-CG-CD2	-22.66	74.27	106.00
2	B	488	THR	C-N-CA	21.27	174.88	121.70
2	I	488	THR	C-N-CA	21.25	174.83	121.70
2	I	489	ASN	C-N-CA	20.45	172.83	121.70
2	B	489	ASN	C-N-CA	20.45	172.83	121.70
1	K	317	PHE	O-C-N	-18.48	93.14	122.70
1	D	317	PHE	O-C-N	-18.47	93.15	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	467	ARG	NE-CZ-NH2	17.72	129.16	120.30
2	I	467	ARG	NE-CZ-NH2	17.70	129.15	120.30
2	J	492	ASP	O-C-N	-17.37	94.91	122.70
2	E	492	ASP	O-C-N	-17.36	94.93	122.70
2	I	489	ASN	CA-C-N	17.09	154.81	117.20
2	B	489	ASN	CA-C-N	17.09	154.79	117.20
2	B	492	ASP	O-C-N	-16.94	95.60	122.70
2	I	492	ASP	O-C-N	-16.87	95.71	122.70
2	E	492	ASP	CA-C-N	16.53	153.56	117.20
2	J	492	ASP	CA-C-N	16.53	153.56	117.20
2	I	491	GLU	O-C-N	-16.22	96.75	122.70
2	B	491	GLU	O-C-N	-16.17	96.82	122.70
2	J	452	LEU	CB-CG-CD2	-16.15	83.55	111.00
2	E	452	LEU	CB-CG-CD2	-16.14	83.56	111.00
2	J	449	TYR	CB-CA-C	15.90	142.19	110.40
2	E	449	TYR	CB-CA-C	15.88	142.17	110.40
1	K	316	ASN	CB-CG-OD1	15.02	151.65	121.60
1	D	316	ASN	CB-CG-OD1	15.01	151.62	121.60
2	I	488	THR	CA-C-N	14.85	149.86	117.20
2	B	488	THR	CA-C-N	14.84	149.85	117.20
2	B	492	ASP	OD1-CG-OD2	-14.56	95.63	123.30
2	I	492	ASP	OD1-CG-OD2	-14.56	95.63	123.30
1	D	317	PHE	C-N-CA	14.17	157.12	121.70
1	K	317	PHE	C-N-CA	14.15	157.08	121.70
2	E	491	GLU	N-CA-C	14.13	149.15	111.00
2	J	491	GLU	N-CA-C	14.12	149.13	111.00
1	D	313	GLU	O-C-N	-13.62	100.91	122.70
1	K	313	GLU	O-C-N	-13.61	100.93	122.70
2	B	490	HIS	ND1-CE1-NE2	-13.12	81.04	109.90
2	I	490	HIS	ND1-CE1-NE2	-13.11	81.06	109.90
2	E	449	TYR	CB-CG-CD2	-12.85	113.29	121.00
2	J	449	TYR	CB-CG-CD2	-12.83	113.30	121.00
1	D	317	PHE	CA-C-N	12.79	145.34	117.20
1	K	317	PHE	CA-C-N	12.78	145.32	117.20
2	E	672	ILE	CB-CG1-CD1	12.68	149.40	113.90
2	J	672	ILE	CB-CG1-CD1	12.68	149.39	113.90
2	E	492	ASP	OD1-CG-OD2	-12.51	99.52	123.30
2	J	492	ASP	OD1-CG-OD2	-12.51	99.53	123.30
1	K	316	ASN	CA-C-N	12.46	144.61	117.20
1	D	316	ASN	CA-C-N	12.45	144.58	117.20
2	E	453	ARG	NE-CZ-NH1	12.28	126.44	120.30
2	J	453	ARG	NE-CZ-NH1	12.25	126.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	490	HIS	N-CA-CB	12.19	132.55	110.60
2	I	490	HIS	N-CA-CB	12.19	132.55	110.60
2	B	698	PHE	CB-CG-CD2	-12.16	112.28	120.80
2	I	698	PHE	CB-CG-CD2	-12.16	112.29	120.80
2	E	490	HIS	ND1-CE1-NE2	-12.08	83.32	109.90
2	J	490	HIS	ND1-CE1-NE2	-12.08	83.32	109.90
2	J	491	GLU	C-N-CA	12.01	151.72	121.70
2	E	491	GLU	C-N-CA	12.00	151.71	121.70
2	E	485	TYR	CG-CD2-CE2	-11.94	111.75	121.30
2	J	485	TYR	CG-CD2-CE2	-11.94	111.75	121.30
2	I	491	GLU	C-N-CA	11.67	150.87	121.70
2	B	491	GLU	C-N-CA	11.64	150.81	121.70
1	K	316	ASN	CB-CG-ND2	-11.58	88.91	116.70
1	D	316	ASN	CB-CG-ND2	-11.56	88.95	116.70
2	F	581	SER	N-CA-CB	11.54	127.80	110.50
2	L	581	SER	N-CA-CB	11.54	127.80	110.50
2	E	451	ARG	O-C-N	-11.51	104.28	122.70
2	E	456	MET	CA-CB-CG	11.50	132.85	113.30
2	J	451	ARG	O-C-N	-11.50	104.30	122.70
2	J	456	MET	CA-CB-CG	11.49	132.83	113.30
2	L	569	ASN	CA-CB-CG	11.47	138.64	113.40
2	B	449	TYR	CB-CG-CD2	-11.47	114.12	121.00
2	F	569	ASN	CA-CB-CG	11.47	138.63	113.40
2	L	628	GLU	CB-CA-C	11.47	133.33	110.40
2	F	628	GLU	CB-CA-C	11.44	133.28	110.40
2	I	449	TYR	CB-CG-CD2	-11.41	114.15	121.00
2	E	491	GLU	CA-C-N	11.34	142.16	117.20
2	J	491	GLU	CA-C-N	11.34	142.15	117.20
2	I	490	HIS	CA-C-N	11.27	141.99	117.20
2	B	490	HIS	CA-C-N	11.24	141.94	117.20
2	E	339	ASP	N-CA-CB	11.23	130.81	110.60
2	J	339	ASP	N-CA-CB	11.22	130.80	110.60
2	E	441	GLN	C-N-CA	11.19	149.68	121.70
2	J	441	GLN	C-N-CA	11.18	149.66	121.70
2	B	485	TYR	CG-CD2-CE2	-11.14	112.39	121.30
2	B	346	GLY	CA-C-O	11.12	140.61	120.60
2	I	346	GLY	CA-C-O	11.12	140.61	120.60
2	I	485	TYR	CG-CD2-CE2	-11.10	112.42	121.30
1	K	318	ARG	CB-CG-CD	11.10	140.46	111.60
2	I	339	ASP	N-CA-CB	11.09	130.56	110.60
2	B	339	ASP	N-CA-CB	11.09	130.55	110.60
1	D	318	ARG	CB-CG-CD	11.08	140.41	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	488	THR	O-C-N	-10.98	105.13	122.70
2	B	488	THR	O-C-N	-10.96	105.17	122.70
2	E	490	HIS	CG-CD2-NE2	10.94	129.99	109.20
2	I	441	GLN	C-N-CA	10.93	149.01	121.70
2	J	490	HIS	CG-CD2-NE2	10.93	129.96	109.20
2	B	441	GLN	C-N-CA	10.91	148.97	121.70
2	F	580	MET	C-N-CA	10.90	148.95	121.70
2	L	580	MET	C-N-CA	10.89	148.93	121.70
2	J	453	ARG	O-C-N	-10.85	105.35	122.70
2	E	453	ARG	O-C-N	-10.83	105.37	122.70
2	J	454	GLU	N-CA-CB	10.83	130.09	110.60
2	E	454	GLU	N-CA-CB	10.82	130.08	110.60
2	E	451	ARG	C-N-CA	10.81	148.73	121.70
2	J	451	ARG	C-N-CA	10.80	148.70	121.70
2	B	488	THR	CA-C-O	-10.80	97.42	120.10
2	I	488	THR	CA-C-O	-10.80	97.43	120.10
2	J	456	MET	CG-SD-CE	10.74	117.39	100.20
2	E	456	MET	CG-SD-CE	10.71	117.34	100.20
2	J	491	GLU	CB-CA-C	-10.65	89.09	110.40
2	E	491	GLU	CB-CA-C	-10.65	89.10	110.40
2	I	491	GLU	CA-C-N	10.61	140.53	117.20
2	B	491	GLU	CA-C-N	10.57	140.45	117.20
2	J	485	TYR	CD1-CE1-CZ	-10.15	110.66	119.80
2	I	490	HIS	O-C-N	-10.15	106.46	122.70
2	E	485	TYR	CD1-CE1-CZ	-10.13	110.68	119.80
2	B	490	HIS	O-C-N	-10.12	106.51	122.70
2	I	491	GLU	N-CA-C	10.12	138.31	111.00
2	B	491	GLU	N-CA-C	10.11	138.30	111.00
2	J	492	ASP	CB-CG-OD1	-10.11	109.20	118.30
2	E	492	ASP	CB-CG-OD1	-10.06	109.25	118.30
1	A	228	ARG	CB-CG-CD	9.92	137.38	111.60
1	G	228	ARG	CB-CG-CD	9.90	137.34	111.60
2	E	490	HIS	CB-CG-ND1	9.81	147.72	123.20
2	J	490	HIS	CB-CG-ND1	9.81	147.72	123.20
2	E	448	GLN	O-C-N	-9.77	107.07	122.70
2	E	492	ASP	C-N-CA	9.76	146.11	121.70
2	J	448	GLN	O-C-N	-9.76	107.09	122.70
2	J	492	ASP	C-N-CA	9.76	146.09	121.70
2	J	485	TYR	CG-CD1-CE1	-9.57	113.65	121.30
2	C	629	ARG	C-N-CA	9.55	145.58	121.70
1	K	314	TYR	O-C-N	-9.55	107.43	122.70
2	H	629	ARG	C-N-CA	9.54	145.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	314	TYR	O-C-N	-9.53	107.45	122.70
2	E	485	TYR	CG-CD1-CE1	-9.52	113.69	121.30
2	I	492	ASP	CA-C-N	9.42	137.93	117.20
2	B	492	ASP	CA-C-N	9.41	137.91	117.20
2	B	489	ASN	N-CA-C	9.41	136.41	111.00
2	I	489	ASN	N-CA-C	9.39	136.34	111.00
1	K	316	ASN	C-N-CA	9.37	145.11	121.70
1	D	316	ASN	C-N-CA	9.36	145.09	121.70
2	J	338	VAL	C-N-CA	9.30	144.96	121.70
2	E	338	VAL	C-N-CA	9.29	144.93	121.70
1	A	67	ARG	NE-CZ-NH2	9.27	124.93	120.30
1	G	67	ARG	NE-CZ-NH2	9.26	124.93	120.30
1	G	67	ARG	NE-CZ-NH1	-9.23	115.69	120.30
2	J	453	ARG	NH1-CZ-NH2	-9.23	109.25	119.40
2	E	453	ARG	NH1-CZ-NH2	-9.23	109.25	119.40
2	B	449	TYR	CB-CG-CD1	9.19	126.52	121.00
1	A	67	ARG	NE-CZ-NH1	-9.17	115.72	120.30
2	I	490	HIS	ND1-CG-CD2	-9.12	93.23	106.00
1	D	303	GLN	CA-CB-CG	9.11	133.45	113.40
1	K	303	GLN	CA-CB-CG	9.11	133.44	113.40
2	B	441	GLN	O-C-N	-9.09	108.16	122.70
2	I	449	TYR	CB-CG-CD1	9.09	126.45	121.00
2	I	441	GLN	O-C-N	-9.08	108.17	122.70
2	B	490	HIS	ND1-CG-CD2	-9.08	93.29	106.00
2	J	492	ASP	N-CA-CB	9.05	126.90	110.60
2	E	492	ASP	N-CA-CB	9.05	126.89	110.60
2	J	699	SER	N-CA-C	9.04	135.41	111.00
2	E	699	SER	N-CA-C	9.04	135.41	111.00
2	B	338	VAL	C-N-CA	8.95	144.09	121.70
2	F	573	ARG	NE-CZ-NH1	-8.94	115.83	120.30
2	I	338	VAL	C-N-CA	8.94	144.04	121.70
2	L	573	ARG	NE-CZ-NH1	-8.93	115.84	120.30
1	G	245	LYS	CA-CB-CG	8.83	132.82	113.40
1	A	245	LYS	CA-CB-CG	8.82	132.81	113.40
2	B	699	SER	N-CA-C	8.74	134.59	111.00
2	C	629	ARG	NE-CZ-NH1	-8.73	115.93	120.30
2	I	699	SER	N-CA-C	8.73	134.56	111.00
2	J	449	TYR	O-C-N	-8.71	104.54	121.10
2	E	449	TYR	O-C-N	-8.70	104.58	121.10
2	E	485	TYR	CB-CG-CD2	-8.69	115.79	121.00
2	E	452	LEU	CA-CB-CG	8.67	135.25	115.30
2	E	449	TYR	CB-CG-CD1	8.66	126.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	452	LEU	CA-CB-CG	8.66	135.21	115.30
2	J	485	TYR	CB-CG-CD2	-8.65	115.81	121.00
2	J	449	TYR	CB-CG-CD1	8.64	126.18	121.00
2	H	629	ARG	NE-CZ-NH1	-8.61	115.99	120.30
1	A	87	LYS	C-N-CA	8.48	140.11	122.30
1	G	87	LYS	C-N-CA	8.47	140.09	122.30
2	F	574	ASP	CB-CG-OD1	-8.38	110.76	118.30
2	H	577	LYS	C-N-CA	8.37	139.88	122.30
2	C	577	LYS	C-N-CA	8.36	139.85	122.30
2	E	339	ASP	O-C-N	-8.33	109.37	122.70
2	L	574	ASP	CB-CG-OD1	-8.33	110.80	118.30
1	D	317	PHE	N-CA-C	8.33	133.49	111.00
1	K	317	PHE	N-CA-C	8.32	133.47	111.00
2	J	339	ASP	O-C-N	-8.32	109.39	122.70
1	A	123	ARG	NE-CZ-NH1	-8.27	116.17	120.30
2	E	448	GLN	C-N-CA	8.22	142.26	121.70
1	G	123	ARG	NE-CZ-NH1	-8.22	116.19	120.30
2	J	448	GLN	C-N-CA	8.21	142.24	121.70
1	D	159	MET	CA-CB-CG	8.19	127.23	113.30
1	K	159	MET	CA-CB-CG	8.19	127.23	113.30
2	I	700	GLU	CA-CB-CG	8.17	131.37	113.40
2	B	700	GLU	CA-CB-CG	8.16	131.35	113.40
1	K	316	ASN	CA-C-O	-8.15	102.98	120.10
1	D	316	ASN	CA-C-O	-8.15	102.98	120.10
1	A	245	LYS	CB-CA-C	8.11	126.63	110.40
1	G	245	LYS	CB-CA-C	8.10	126.61	110.40
2	B	485	TYR	CB-CG-CD2	-8.05	116.17	121.00
2	B	492	ASP	CB-CG-OD1	-8.04	111.07	118.30
2	I	492	ASP	CB-CG-OD1	-8.03	111.07	118.30
2	J	453	ARG	NE-CZ-NH2	8.03	124.31	120.30
2	L	574	ASP	N-CA-CB	8.01	125.03	110.60
2	F	574	ASP	N-CA-CB	8.01	125.01	110.60
2	E	453	ARG	NE-CZ-NH2	7.99	124.29	120.30
2	E	450	PRO	CA-C-N	7.92	134.62	117.20
2	J	450	PRO	CA-C-N	7.91	134.61	117.20
2	E	450	PRO	O-C-N	-7.91	110.05	122.70
2	I	485	TYR	CB-CG-CD2	-7.90	116.26	121.00
2	J	450	PRO	O-C-N	-7.90	110.07	122.70
1	D	318	ARG	CA-C-O	-7.88	103.56	120.10
1	K	228	ARG	CB-CG-CD	7.87	132.07	111.60
1	D	228	ARG	CB-CG-CD	7.86	132.04	111.60
1	K	318	ARG	CA-C-O	-7.86	103.60	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	487	ASN	CA-C-N	7.82	134.40	117.20
2	B	487	ASN	CA-C-N	7.81	134.39	117.20
2	E	340	PHE	CB-CG-CD1	-7.72	115.40	120.80
2	E	452	LEU	N-CA-C	7.69	131.76	111.00
2	J	452	LEU	N-CA-C	7.69	131.77	111.00
2	I	414	LYS	N-CA-CB	7.67	124.41	110.60
2	B	414	LYS	N-CA-CB	7.67	124.41	110.60
1	G	88	GLY	N-CA-C	7.67	132.28	113.10
2	F	573	ARG	C-N-CA	7.67	140.87	121.70
1	A	88	GLY	N-CA-C	7.67	132.26	113.10
2	F	560	GLU	C-N-CA	7.66	140.85	121.70
2	L	573	ARG	C-N-CA	7.65	140.83	121.70
2	J	340	PHE	CB-CG-CD1	-7.65	115.45	120.80
2	F	601	ARG	C-N-CA	7.64	140.81	121.70
2	L	560	GLU	C-N-CA	7.64	140.80	121.70
2	L	601	ARG	C-N-CA	7.63	140.78	121.70
2	B	494	ILE	CA-CB-CG1	7.58	125.40	111.00
2	I	494	ILE	CA-CB-CG1	7.55	125.35	111.00
2	B	490	HIS	CG-ND1-CE1	7.54	118.75	108.20
2	I	490	HIS	CG-ND1-CE1	7.54	118.75	108.20
2	H	560	GLU	C-N-CA	7.53	140.52	121.70
2	C	560	GLU	C-N-CA	7.53	140.52	121.70
2	I	491	GLU	OE1-CD-OE2	7.45	132.24	123.30
1	K	317	PHE	CB-CG-CD1	7.43	126.00	120.80
2	J	450	PRO	CA-N-CD	-7.42	101.11	111.50
1	D	317	PHE	CB-CG-CD1	7.42	126.00	120.80
2	E	450	PRO	CA-N-CD	-7.42	101.11	111.50
2	B	491	GLU	OE1-CD-OE2	7.41	132.19	123.30
1	G	73	LEU	N-CA-CB	7.41	125.21	110.40
1	A	73	LEU	N-CA-CB	7.39	125.18	110.40
2	F	573	ARG	CD-NE-CZ	7.37	133.92	123.60
2	L	573	ARG	CD-NE-CZ	7.37	133.92	123.60
2	B	467	ARG	NH1-CZ-NH2	-7.35	111.32	119.40
2	I	467	ARG	NH1-CZ-NH2	-7.34	111.33	119.40
2	C	561	LYS	N-CA-CB	7.33	123.80	110.60
2	J	449	TYR	C-N-CD	-7.31	104.52	120.60
2	H	561	LYS	N-CA-CB	7.31	123.76	110.60
2	E	449	TYR	C-N-CD	-7.31	104.52	120.60
2	J	454	GLU	CA-CB-CG	7.29	129.44	113.40
2	E	454	GLU	CA-CB-CG	7.29	129.43	113.40
2	L	569	ASN	CB-CA-C	7.26	124.92	110.40
2	L	628	GLU	CA-CB-CG	7.26	129.37	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	669	TYR	CB-CG-CD2	7.25	125.35	121.00
2	F	628	GLU	CA-CB-CG	7.25	129.34	113.40
2	E	706	TYR	CB-CG-CD2	-7.24	116.65	121.00
2	J	706	TYR	CB-CG-CD2	-7.24	116.66	121.00
2	F	569	ASN	CB-CA-C	7.24	124.88	110.40
2	B	669	TYR	CB-CG-CD2	7.23	125.34	121.00
2	L	533	ILE	C-N-CA	7.23	139.77	121.70
2	E	672	ILE	CG1-CB-CG2	7.22	127.30	111.40
2	F	533	ILE	C-N-CA	7.22	139.76	121.70
1	G	87	LYS	CG-CD-CE	7.22	133.56	111.90
2	J	672	ILE	CG1-CB-CG2	7.22	127.28	111.40
1	A	87	LYS	CG-CD-CE	7.21	133.53	111.90
2	E	669	TYR	CB-CG-CD2	7.18	125.31	121.00
2	J	669	TYR	CB-CG-CD2	7.17	125.31	121.00
2	F	558	GLU	CA-CB-CG	7.14	129.12	113.40
2	I	702	LEU	CB-CG-CD2	7.13	123.12	111.00
2	H	534	MET	N-CA-CB	7.13	123.43	110.60
2	B	702	LEU	CB-CG-CD2	7.12	123.11	111.00
1	K	316	ASN	O-C-N	-7.12	111.31	122.70
2	L	558	GLU	CA-CB-CG	7.12	129.06	113.40
1	D	316	ASN	O-C-N	-7.11	111.32	122.70
2	C	534	MET	N-CA-CB	7.11	123.40	110.60
2	E	485	TYR	CB-CG-CD1	7.11	125.27	121.00
2	J	455	GLU	OE1-CD-OE2	-7.08	114.81	123.30
2	L	575	VAL	CG1-CB-CG2	7.08	122.22	110.90
2	E	455	GLU	OE1-CD-OE2	-7.07	114.82	123.30
2	F	575	VAL	CG1-CB-CG2	7.06	122.20	110.90
2	J	485	TYR	CB-CG-CD1	7.05	125.23	121.00
2	E	448	GLN	N-CA-CB	-7.02	97.96	110.60
2	I	414	LYS	CA-CB-CG	7.02	128.84	113.40
2	J	448	GLN	N-CA-CB	-7.01	97.97	110.60
2	B	414	LYS	CA-CB-CG	7.00	128.79	113.40
2	I	678	ARG	NE-CZ-NH2	6.97	123.78	120.30
2	L	569	ASN	CB-CG-OD1	6.95	135.51	121.60
2	F	569	ASN	CB-CG-OD1	6.95	135.50	121.60
2	L	581	SER	CA-CB-OG	-6.95	92.44	111.20
2	F	581	SER	CA-CB-OG	-6.95	92.45	111.20
2	B	696	PHE	CD1-CE1-CZ	-6.92	111.80	120.10
2	B	488	THR	OG1-CB-CG2	6.91	125.90	110.00
2	I	488	THR	OG1-CB-CG2	6.91	125.89	110.00
2	I	696	PHE	CD1-CE1-CZ	-6.91	111.81	120.10
2	I	675	LYS	N-CA-CB	6.88	122.98	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	675	LYS	N-CA-CB	6.87	122.97	110.60
2	B	678	ARG	NE-CZ-NH2	6.86	123.73	120.30
2	B	464	ILE	CB-CG1-CD1	6.81	132.98	113.90
2	I	464	ILE	CB-CG1-CD1	6.81	132.97	113.90
2	L	573	ARG	CG-CD-NE	-6.77	97.58	111.80
2	I	490	HIS	CA-C-O	-6.76	105.90	120.10
2	F	573	ARG	CG-CD-NE	-6.76	97.61	111.80
2	J	453	ARG	C-N-CA	6.75	138.59	121.70
2	B	413	VAL	CG1-CB-CG2	6.75	121.70	110.90
2	B	490	HIS	CA-C-O	-6.75	105.92	120.10
2	J	491	GLU	CA-C-O	6.75	134.28	120.10
2	E	491	GLU	CA-C-O	6.75	134.28	120.10
2	E	453	ARG	C-N-CA	6.75	138.57	121.70
2	I	413	VAL	CG1-CB-CG2	6.75	121.70	110.90
1	D	90	LYS	CB-CG-CD	6.74	129.12	111.60
2	B	707	SER	N-CA-CB	6.73	120.60	110.50
2	I	707	SER	N-CA-CB	6.73	120.59	110.50
1	K	90	LYS	CB-CG-CD	6.72	129.08	111.60
2	F	529	ASN	CA-CB-CG	6.70	128.15	113.40
2	F	569	ASN	CB-CG-ND2	-6.70	100.61	116.70
2	L	529	ASN	CA-CB-CG	6.70	128.14	113.40
2	L	569	ASN	CB-CG-ND2	-6.70	100.62	116.70
2	F	601	ARG	O-C-N	-6.63	112.09	122.70
2	L	601	ARG	O-C-N	-6.63	112.10	122.70
2	B	421	ARG	NE-CZ-NH2	-6.62	116.99	120.30
2	H	601	ARG	O-C-N	-6.62	112.11	122.70
2	B	707	SER	CB-CA-C	6.60	122.65	110.10
2	H	559	LYS	C-N-CA	6.60	138.21	121.70
2	I	707	SER	CB-CA-C	6.60	122.64	110.10
2	C	559	LYS	C-N-CA	6.60	138.20	121.70
1	K	316	ASN	N-CA-C	6.58	128.78	111.00
1	D	316	ASN	N-CA-C	6.58	128.77	111.00
2	I	421	ARG	NE-CZ-NH2	-6.56	117.02	120.30
2	C	601	ARG	O-C-N	-6.55	112.22	122.70
2	H	601	ARG	C-N-CA	6.54	138.04	121.70
2	C	601	ARG	C-N-CA	6.52	138.00	121.70
2	J	705	LEU	N-CA-CB	6.52	123.44	110.40
2	E	705	LEU	N-CA-CB	6.51	123.43	110.40
2	B	486	MET	O-C-N	-6.50	112.31	122.70
2	J	362	ILE	N-CA-C	-6.49	93.47	111.00
2	E	362	ILE	N-CA-C	-6.49	93.48	111.00
2	H	554	LYS	CB-CG-CD	6.48	128.45	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	486	MET	O-C-N	-6.48	112.34	122.70
2	C	554	LYS	CB-CG-CD	6.47	128.44	111.60
2	B	339	ASP	O-C-N	-6.43	112.41	122.70
2	I	339	ASP	O-C-N	-6.43	112.41	122.70
1	A	123	ARG	NE-CZ-NH2	-6.41	117.09	120.30
2	J	451	ARG	CA-CB-CG	6.40	127.49	113.40
2	E	451	ARG	CA-CB-CG	6.40	127.47	113.40
2	E	494	ILE	CA-CB-CG1	6.39	123.14	111.00
2	J	494	ILE	CA-CB-CG1	6.38	123.11	111.00
2	B	362	ILE	N-CA-C	-6.37	93.81	111.00
2	I	362	ILE	N-CA-C	-6.35	93.85	111.00
2	H	533	ILE	C-N-CA	6.32	137.49	121.70
2	C	533	ILE	C-N-CA	6.31	137.47	121.70
2	J	488	THR	O-C-N	-6.31	112.61	122.70
2	E	488	THR	O-C-N	-6.30	112.62	122.70
1	G	123	ARG	NE-CZ-NH2	-6.29	117.15	120.30
2	J	484	ALA	N-CA-CB	-6.29	101.29	110.10
1	K	310	GLU	O-C-N	-6.29	112.64	122.70
2	E	484	ALA	N-CA-CB	-6.28	101.31	110.10
2	E	696	PHE	CZ-CE2-CD2	-6.26	112.58	120.10
2	J	453	ARG	N-CA-CB	6.26	121.87	110.60
2	E	453	ARG	N-CA-CB	6.26	121.86	110.60
2	J	696	PHE	CZ-CE2-CD2	-6.26	112.59	120.10
1	D	310	GLU	O-C-N	-6.25	112.70	122.70
2	B	485	TYR	CB-CG-CD1	6.25	124.75	121.00
2	E	678	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	D	318	ARG	N-CA-CB	6.24	121.83	110.60
1	K	318	ARG	N-CA-CB	6.22	121.80	110.60
1	K	315	LYS	O-C-N	-6.21	112.77	122.70
2	J	678	ARG	NE-CZ-NH2	6.21	123.40	120.30
2	I	678	ARG	NH1-CZ-NH2	-6.19	112.59	119.40
2	F	561	LYS	N-CA-CB	6.18	121.72	110.60
1	D	315	LYS	O-C-N	-6.18	112.82	122.70
2	E	451	ARG	CA-C-N	6.18	130.79	117.20
2	J	451	ARG	CA-C-N	6.17	130.76	117.20
2	L	561	LYS	N-CA-CB	6.17	121.70	110.60
2	E	698	PHE	CG-CD2-CE2	-6.16	114.02	120.80
2	I	485	TYR	CB-CG-CD1	6.16	124.70	121.00
2	J	698	PHE	CG-CD2-CE2	-6.16	114.03	120.80
2	B	678	ARG	NH1-CZ-NH2	-6.16	112.63	119.40
2	E	441	GLN	O-C-N	-6.13	112.89	122.70
2	I	488	THR	N-CA-C	6.13	127.54	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	441	GLN	O-C-N	-6.13	112.90	122.70
2	B	488	THR	N-CA-C	6.12	127.52	111.00
2	L	522	ARG	NE-CZ-NH1	-6.11	117.24	120.30
2	F	522	ARG	NE-CZ-NH1	-6.10	117.25	120.30
2	L	534	MET	N-CA-CB	6.06	121.52	110.60
2	B	327	LYS	CB-CG-CD	6.05	127.34	111.60
2	I	327	LYS	CB-CG-CD	6.05	127.34	111.60
2	I	480	ASP	CB-CG-OD1	-6.05	112.85	118.30
2	B	700	GLU	N-CA-CB	6.05	121.48	110.60
2	C	630	VAL	CA-CB-CG1	-6.05	101.83	110.90
2	H	630	VAL	CA-CB-CG1	-6.05	101.83	110.90
2	I	700	GLU	N-CA-CB	6.05	121.48	110.60
2	F	534	MET	N-CA-CB	6.03	121.46	110.60
1	D	89	LYS	N-CA-CB	6.03	121.44	110.60
1	K	89	LYS	N-CA-CB	6.02	121.44	110.60
2	B	480	ASP	CB-CG-OD1	-6.02	112.88	118.30
2	J	491	GLU	N-CA-CB	5.97	121.35	110.60
2	J	701	LEU	CB-CG-CD2	-5.96	100.87	111.00
1	A	741	ILE	CA-CB-CG1	-5.96	99.68	111.00
2	E	701	LEU	CB-CG-CD2	-5.96	100.87	111.00
2	E	491	GLU	N-CA-CB	5.96	121.32	110.60
1	G	741	ILE	CA-CB-CG1	-5.96	99.69	111.00
1	K	256	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	D	256	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	D	315	LYS	CA-C-N	5.93	130.24	117.20
1	K	315	LYS	CA-C-N	5.92	130.24	117.20
2	E	492	ASP	N-CA-C	5.92	126.98	111.00
2	J	492	ASP	N-CA-C	5.92	126.97	111.00
2	C	577	LYS	O-C-N	-5.91	113.15	123.20
2	H	577	LYS	O-C-N	-5.91	113.15	123.20
2	F	529	ASN	N-CA-CB	5.91	121.24	110.60
2	I	676	THR	CA-CB-CG2	5.90	120.66	112.40
2	L	529	ASN	N-CA-CB	5.89	121.21	110.60
2	B	676	THR	CA-CB-CG2	5.87	120.62	112.40
2	B	442	CYS	N-CA-C	5.85	126.80	111.00
2	I	442	CYS	N-CA-C	5.84	126.77	111.00
1	K	318	ARG	NH1-CZ-NH2	-5.83	112.98	119.40
2	L	575	VAL	C-N-CA	5.83	136.27	121.70
1	D	318	ARG	NH1-CZ-NH2	-5.82	113.00	119.40
2	F	575	VAL	C-N-CA	5.82	136.24	121.70
2	J	456	MET	CB-CG-SD	-5.78	95.06	112.40
2	E	456	MET	CB-CG-SD	-5.77	95.08	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	314	TYR	CA-C-O	5.77	132.22	120.10
1	K	314	TYR	CA-C-O	5.77	132.22	120.10
2	L	559	LYS	C-N-CA	5.76	136.10	121.70
1	A	223	LYS	CB-CG-CD	5.75	126.56	111.60
2	F	559	LYS	C-N-CA	5.75	136.07	121.70
1	G	741	ILE	CB-CG1-CD1	-5.74	97.83	113.90
2	L	573	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	A	741	ILE	CB-CG1-CD1	-5.73	97.85	113.90
1	G	223	LYS	CB-CG-CD	5.73	126.50	111.60
2	C	630	VAL	N-CA-CB	5.72	124.09	111.50
2	E	698	PHE	CB-CG-CD2	-5.72	116.80	120.80
2	J	698	PHE	CB-CG-CD2	-5.72	116.79	120.80
2	H	630	VAL	N-CA-CB	5.72	124.09	111.50
2	J	672	ILE	CA-CB-CG1	5.71	121.85	111.00
2	H	629	ARG	O-C-N	-5.71	113.57	122.70
2	E	672	ILE	CA-CB-CG1	5.70	121.83	111.00
2	I	338	VAL	CA-CB-CG1	5.70	119.45	110.90
2	C	629	ARG	O-C-N	-5.70	113.58	122.70
2	I	485	TYR	CZ-CE2-CD2	-5.70	114.67	119.80
2	J	669	TYR	O-C-N	-5.69	113.59	122.70
2	E	669	TYR	O-C-N	-5.69	113.59	122.70
2	B	338	VAL	CA-CB-CG1	5.69	119.43	110.90
2	E	491	GLU	OE1-CD-OE2	-5.67	116.49	123.30
2	E	494	ILE	CA-C-N	5.67	127.54	116.20
2	J	491	GLU	OE1-CD-OE2	-5.67	116.50	123.30
2	J	494	ILE	CA-C-N	5.66	127.52	116.20
2	B	485	TYR	CZ-CE2-CD2	-5.66	114.71	119.80
2	F	573	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	D	159	MET	CB-CG-SD	5.66	129.37	112.40
1	K	159	MET	CB-CG-SD	5.66	129.37	112.40
1	D	136	ASP	CB-CG-OD2	-5.65	113.22	118.30
2	L	575	VAL	N-CA-CB	5.62	123.86	111.50
2	E	490	HIS	CA-C-O	-5.62	108.30	120.10
2	J	490	HIS	CA-C-O	-5.62	108.30	120.10
2	F	575	VAL	N-CA-CB	5.61	123.85	111.50
1	K	136	ASP	CB-CG-OD2	-5.59	113.27	118.30
2	J	449	TYR	N-CA-CB	-5.59	100.54	110.60
2	E	449	TYR	N-CA-CB	-5.57	100.57	110.60
2	J	455	GLU	C-N-CA	5.56	135.60	121.70
2	E	455	GLU	C-N-CA	5.55	135.57	121.70
2	I	467	ARG	CA-CB-CG	-5.54	101.22	113.40
1	D	315	LYS	C-N-CA	5.53	135.53	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	315	LYS	C-N-CA	5.53	135.54	121.70
1	A	270	ASP	C-N-CA	5.52	135.50	121.70
2	B	467	ARG	CA-CB-CG	-5.52	101.26	113.40
2	I	391	ALA	CB-CA-C	5.51	118.37	110.10
1	G	270	ASP	C-N-CA	5.50	135.46	121.70
2	B	391	ALA	CB-CA-C	5.49	118.33	110.10
2	B	670	MET	O-C-N	-5.44	113.99	122.70
2	I	456	MET	CG-SD-CE	5.44	108.90	100.20
2	I	487	ASN	O-C-N	-5.44	114.00	122.70
2	F	580	MET	O-C-N	-5.43	114.02	122.70
2	B	456	MET	CG-SD-CE	5.42	108.87	100.20
2	B	487	ASN	O-C-N	-5.41	114.05	122.70
2	I	670	MET	O-C-N	-5.40	114.05	122.70
2	L	580	MET	O-C-N	-5.40	114.05	122.70
2	C	600	TYR	N-CA-C	5.40	125.58	111.00
1	A	189	VAL	CA-CB-CG2	-5.40	102.80	110.90
2	I	449	TYR	CA-CB-CG	5.40	123.65	113.40
2	E	702	LEU	CB-CG-CD2	5.40	120.17	111.00
1	G	189	VAL	CA-CB-CG2	-5.40	102.81	110.90
2	H	600	TYR	N-CA-C	5.40	125.57	111.00
2	B	449	TYR	CA-CB-CG	5.39	123.65	113.40
2	J	702	LEU	CB-CG-CD2	5.39	120.17	111.00
1	D	178	ASN	C-N-CA	5.39	135.18	121.70
1	A	73	LEU	CB-CG-CD1	-5.39	101.84	111.00
2	B	489	ASN	CA-C-O	5.39	131.41	120.10
2	J	494	ILE	N-CA-CB	5.39	123.19	110.80
1	G	73	LEU	CB-CG-CD1	-5.38	101.84	111.00
2	E	450	PRO	CA-CB-CG	-5.38	93.78	104.00
2	J	450	PRO	CA-CB-CG	-5.38	93.78	104.00
1	K	178	ASN	C-N-CA	5.38	135.15	121.70
2	E	494	ILE	N-CA-CB	5.38	123.17	110.80
2	J	669	TYR	CG-CD2-CE2	5.37	125.60	121.30
1	D	318	ARG	NE-CZ-NH2	-5.37	117.62	120.30
2	I	489	ASN	CA-C-O	5.37	131.37	120.10
2	E	669	TYR	CG-CD2-CE2	5.37	125.59	121.30
2	E	452	LEU	C-N-CA	5.36	135.11	121.70
2	J	452	LEU	C-N-CA	5.36	135.09	121.70
2	I	674	ASN	O-C-N	-5.35	114.14	122.70
2	B	674	ASN	O-C-N	-5.35	114.15	122.70
2	L	600	TYR	N-CA-C	5.35	125.44	111.00
2	I	669	TYR	CG-CD1-CE1	-5.34	117.03	121.30
2	F	600	TYR	N-CA-C	5.34	125.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	318	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	J	490	HIS	N-CA-C	5.34	125.42	111.00
2	H	584	HIS	N-CA-CB	5.34	120.21	110.60
2	C	584	HIS	N-CA-CB	5.34	120.20	110.60
2	E	490	HIS	N-CA-C	5.33	125.39	111.00
2	J	491	GLU	CB-CG-CD	5.29	128.47	114.20
2	B	669	TYR	CG-CD1-CE1	-5.28	117.07	121.30
2	E	491	GLU	CB-CG-CD	5.28	128.46	114.20
2	E	343	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	B	413	VAL	C-N-CA	5.28	134.89	121.70
2	I	413	VAL	C-N-CA	5.27	134.88	121.70
2	C	576	GLU	C-N-CA	5.27	134.88	121.70
2	B	675	LYS	CA-CB-CG	5.26	124.98	113.40
2	I	675	LYS	CA-CB-CG	5.26	124.98	113.40
2	H	576	GLU	C-N-CA	5.26	134.86	121.70
2	B	487	ASN	CA-C-O	-5.25	109.08	120.10
2	E	493	PHE	C-N-CA	5.25	134.82	121.70
2	J	493	PHE	C-N-CA	5.25	134.82	121.70
2	B	492	ASP	N-CA-CB	5.24	120.03	110.60
2	I	492	ASP	N-CA-CB	5.24	120.03	110.60
2	J	445	LYS	CA-CB-CG	5.24	124.92	113.40
2	I	487	ASN	CA-C-O	-5.23	109.11	120.10
2	E	445	LYS	CA-CB-CG	5.23	124.91	113.40
2	J	343	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	E	338	VAL	O-C-N	-5.22	114.35	122.70
2	L	574	ASP	CA-C-N	5.22	128.68	117.20
2	J	338	VAL	O-C-N	-5.22	114.35	122.70
2	F	560	GLU	N-CA-C	5.21	125.08	111.00
2	F	574	ASP	CA-C-N	5.21	128.66	117.20
2	I	340	PHE	N-CA-C	5.21	125.06	111.00
2	L	560	GLU	N-CA-C	5.20	125.05	111.00
2	B	340	PHE	N-CA-C	5.20	125.04	111.00
2	J	452	LEU	CB-CG-CD1	5.19	119.82	111.00
2	J	489	ASN	CB-CA-C	5.19	120.78	110.40
2	E	489	ASN	CB-CA-C	5.19	120.78	110.40
2	C	560	GLU	N-CA-C	5.19	125.00	111.00
2	J	490	HIS	CA-CB-CG	-5.19	104.78	113.60
2	L	604	GLU	CA-CB-CG	5.19	124.81	113.40
2	E	452	LEU	CB-CG-CD1	5.18	119.81	111.00
2	H	560	GLU	N-CA-C	5.18	125.00	111.00
2	E	490	HIS	CA-CB-CG	-5.18	104.79	113.60
2	J	451	ARG	N-CA-CB	5.18	119.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	604	GLU	CA-CB-CG	5.17	124.77	113.40
2	H	577	LYS	CA-C-N	5.17	126.53	116.20
2	E	451	ARG	N-CA-CB	5.17	119.90	110.60
2	L	533	ILE	O-C-N	-5.16	114.44	122.70
2	F	533	ILE	O-C-N	-5.16	114.45	122.70
1	G	244	GLY	O-C-N	-5.15	114.46	122.70
1	D	726	ASP	O-C-N	-5.15	114.47	122.70
1	A	244	GLY	O-C-N	-5.14	114.48	122.70
2	C	577	LYS	CA-C-N	5.14	126.48	116.20
2	E	494	ILE	CA-C-O	-5.13	109.33	120.10
1	K	726	ASP	O-C-N	-5.12	114.50	122.70
2	J	494	ILE	CA-C-O	-5.12	109.35	120.10
1	D	131	ASN	C-N-CA	5.12	134.50	121.70
1	K	131	ASN	C-N-CA	5.12	134.50	121.70
1	K	299	LYS	CA-CB-CG	5.11	124.65	113.40
1	A	85	HIS	O-C-N	-5.11	114.52	122.70
2	J	340	PHE	N-CA-C	5.11	124.80	111.00
2	E	340	PHE	N-CA-C	5.10	124.78	111.00
1	D	299	LYS	CA-CB-CG	5.10	124.62	113.40
1	G	85	HIS	O-C-N	-5.08	114.56	122.70
1	D	317	PHE	CB-CG-CD2	-5.05	117.26	120.80
1	K	317	PHE	CB-CG-CD2	-5.05	117.27	120.80
2	E	487	ASN	O-C-N	-5.03	114.66	122.70
2	B	703	ALA	N-CA-CB	-5.03	103.06	110.10
2	J	487	ASN	O-C-N	-5.03	114.66	122.70
2	E	443	THR	N-CA-CB	5.02	119.84	110.30
2	J	443	THR	N-CA-CB	5.02	119.83	110.30
2	E	441	GLN	CA-C-N	5.01	128.22	117.20
2	B	669	TYR	CD1-CE1-CZ	-5.01	115.29	119.80
2	J	441	GLN	CA-C-N	5.01	128.22	117.20
2	L	577	LYS	C-N-CA	5.01	132.81	122.30
2	I	669	TYR	CD1-CE1-CZ	-5.00	115.30	119.80
2	F	577	LYS	C-N-CA	5.00	132.81	122.30
2	I	703	ALA	N-CA-CB	-5.00	103.09	110.10

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	726	ASP	CA
2	B	339	ASP	CA
2	B	442	CYS	CA
2	B	489	ASN	CA

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Mol	Chain	Res	Type	Atom
2	B	490	HIS	CA
2	B	707	SER	CA
2	C	534	MET	CA
2	C	560	GLU	CA
2	C	563	TYR	CA
2	C	630	VAL	CA
2	E	339	ASP	CA
2	E	442	CYS	CA
2	E	445	LYS	CA
2	E	452	LEU	CA
2	E	454	GLU	CA
2	E	490	HIS	CA
2	E	491	GLU	CA
2	E	492	ASP	CA
2	E	494	ILE	CB
2	E	672	ILE	CB
2	F	529	ASN	CA
2	F	534	MET	CA
2	F	560	GLU	CA
2	F	574	ASP	CA
2	F	575	VAL	CA
2	F	581	SER	CA
2	F	627	PRO	CA
1	G	726	ASP	CA
2	H	534	MET	CA
2	H	560	GLU	CA
2	H	563	TYR	CA
2	H	630	VAL	CA
2	I	339	ASP	CA
2	I	442	CYS	CA
2	I	489	ASN	CA
2	I	490	HIS	CA
2	I	707	SER	CA
2	J	339	ASP	CA
2	J	442	CYS	CA
2	J	445	LYS	CA
2	J	452	LEU	CA
2	J	454	GLU	CA
2	J	490	HIS	CA
2	J	491	GLU	CA
2	J	492	ASP	CA
2	J	494	ILE	CB

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Mol	Chain	Res	Type	Atom
2	J	672	ILE	CB
2	L	529	ASN	CA
2	L	534	MET	CA
2	L	560	GLU	CA
2	L	574	ASP	CA
2	L	575	VAL	CA
2	L	581	SER	CA
2	L	627	PRO	CA

All (240) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	THR	Mainchain
1	A	123	ARG	Sidechain
1	A	177	ALA	Mainchain
1	A	206	LYS	Mainchain
1	A	228	ARG	Sidechain
1	A	233	GLY	Mainchain
1	A	237	ARG	Sidechain
1	A	28	ASP	Mainchain
1	A	41	SER	Mainchain
1	A	50	ASN	Sidechain
1	A	727	GLU	Mainchain
2	B	336	PHE	Sidechain
2	B	337	ALA	Mainchain
2	B	339	ASP	Mainchain
2	B	340	PHE	Sidechain,Mainchain
2	B	341	GLU	Mainchain
2	B	358	GLY	Mainchain
2	B	361	ARG	Mainchain
2	B	362	ILE	Mainchain
2	B	371	PRO	Mainchain
2	B	391	ALA	Mainchain
2	B	409	PHE	Sidechain
2	B	414	LYS	Mainchain
2	B	440	ARG	Sidechain,Mainchain
2	B	441	GLN	Mainchain
2	B	461	THR	Peptide
2	B	467	ARG	Sidechain,Mainchain
2	B	470	ARG	Sidechain
2	B	483	LEU	Mainchain
2	B	485	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	486	MET	Peptide
2	B	487	ASN	Mainchain
2	B	488	THR	Mainchain,Peptide
2	B	490	HIS	Sidechain,Mainchain
2	B	491	GLU	Mainchain
2	B	492	ASP	Mainchain
2	B	654	GLN	Mainchain
2	B	669	TYR	Sidechain
2	B	678	ARG	Sidechain,Mainchain
2	B	696	PHE	Sidechain
2	B	698	PHE	Sidechain
2	B	699	SER	Mainchain
2	B	700	GLU	Mainchain
2	B	702	LEU	Peptide
2	B	706	TYR	Sidechain
2	C	532	GLY	Mainchain
2	C	564	MET	Mainchain
2	C	569	ASN	Mainchain
2	C	576	GLU	Mainchain
2	C	579	PHE	Sidechain
2	C	584	HIS	Sidechain
2	C	594	ARG	Sidechain
2	C	607	CYS	Mainchain
2	C	629	ARG	Sidechain
1	D	125	TYR	Sidechain
1	D	177	ALA	Mainchain
1	D	206	LYS	Mainchain
1	D	221	GLU	Mainchain
1	D	237	ARG	Sidechain
1	D	313	GLU	Mainchain
1	D	316	ASN	Mainchain
1	D	318	ARG	Sidechain,Mainchain
1	D	41	SER	Mainchain
1	D	43	GLY	Mainchain
1	D	50	ASN	Sidechain
1	D	62	GLY	Mainchain
1	D	82	GLU	Mainchain
2	E	339	ASP	Mainchain
2	E	340	PHE	Sidechain,Mainchain
2	E	358	GLY	Mainchain
2	E	361	ARG	Mainchain
2	E	370	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	E	371	PRO	Mainchain
2	E	378	GLU	Mainchain
2	E	381	GLU	Peptide
2	E	414	LYS	Mainchain
2	E	440	ARG	Sidechain
2	E	448	GLN	Mainchain
2	E	449	TYR	Sidechain,Mainchain
2	E	451	ARG	Sidechain
2	E	453	ARG	Mainchain
2	E	455	GLU	Sidechain
2	E	457	GLU	Sidechain
2	E	467	ARG	Mainchain
2	E	469	GLY	Mainchain
2	E	470	ARG	Sidechain
2	E	482	GLU	Mainchain
2	E	485	TYR	Sidechain
2	E	489	ASN	Mainchain,Peptide
2	E	490	HIS	Sidechain,Mainchain
2	E	491	GLU	Peptide
2	E	492	ASP	Peptide
2	E	494	ILE	Mainchain
2	E	653	PRO	Mainchain
2	E	654	GLN	Mainchain
2	E	670	MET	Mainchain
2	E	678	ARG	Mainchain
2	E	696	PHE	Sidechain
2	E	698	PHE	Sidechain
2	F	522	ARG	Sidechain
2	F	532	GLY	Mainchain
2	F	563	TYR	Sidechain,Mainchain
2	F	569	ASN	Sidechain,Mainchain
2	F	576	GLU	Mainchain
2	F	581	SER	Mainchain
2	F	594	ARG	Sidechain
2	F	607	CYS	Mainchain
1	G	105	THR	Mainchain
1	G	123	ARG	Sidechain
1	G	177	ALA	Mainchain
1	G	197	GLY	Mainchain
1	G	206	LYS	Mainchain
1	G	228	ARG	Sidechain
1	G	233	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	G	237	ARG	Sidechain
1	G	28	ASP	Mainchain
1	G	41	SER	Mainchain
1	G	50	ASN	Sidechain
1	G	727	GLU	Mainchain
2	H	532	GLY	Mainchain
2	H	564	MET	Mainchain
2	H	569	ASN	Mainchain
2	H	576	GLU	Mainchain
2	H	579	PHE	Sidechain
2	H	584	HIS	Sidechain
2	H	594	ARG	Sidechain
2	H	607	CYS	Mainchain
2	H	629	ARG	Sidechain
2	I	336	PHE	Sidechain
2	I	337	ALA	Mainchain
2	I	339	ASP	Mainchain
2	I	340	PHE	Sidechain,Mainchain
2	I	358	GLY	Mainchain
2	I	361	ARG	Mainchain
2	I	362	ILE	Mainchain
2	I	371	PRO	Mainchain
2	I	391	ALA	Mainchain
2	I	409	PHE	Sidechain
2	I	414	LYS	Mainchain
2	I	440	ARG	Sidechain,Mainchain
2	I	441	GLN	Mainchain
2	I	461	THR	Peptide
2	I	467	ARG	Sidechain,Mainchain
2	I	470	ARG	Sidechain
2	I	483	LEU	Mainchain
2	I	485	TYR	Sidechain
2	I	486	MET	Peptide
2	I	487	ASN	Mainchain
2	I	488	THR	Mainchain,Peptide
2	I	490	HIS	Sidechain,Mainchain
2	I	491	GLU	Mainchain
2	I	492	ASP	Mainchain
2	I	654	GLN	Mainchain
2	I	669	TYR	Sidechain
2	I	678	ARG	Sidechain,Mainchain
2	I	696	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	I	698	PHE	Sidechain
2	I	699	SER	Mainchain
2	I	700	GLU	Mainchain
2	I	702	LEU	Peptide
2	I	706	TYR	Sidechain
2	J	339	ASP	Mainchain
2	J	340	PHE	Sidechain,Mainchain
2	J	358	GLY	Mainchain
2	J	361	ARG	Mainchain
2	J	362	ILE	Mainchain
2	J	370	PHE	Sidechain
2	J	371	PRO	Mainchain
2	J	378	GLU	Mainchain
2	J	381	GLU	Peptide
2	J	414	LYS	Mainchain
2	J	440	ARG	Sidechain
2	J	448	GLN	Mainchain
2	J	449	TYR	Sidechain,Mainchain
2	J	451	ARG	Sidechain
2	J	453	ARG	Mainchain
2	J	455	GLU	Sidechain
2	J	457	GLU	Sidechain
2	J	467	ARG	Mainchain
2	J	469	GLY	Mainchain
2	J	470	ARG	Sidechain
2	J	485	TYR	Sidechain
2	J	489	ASN	Mainchain,Peptide
2	J	490	HIS	Sidechain,Mainchain
2	J	491	GLU	Peptide
2	J	492	ASP	Peptide
2	J	494	ILE	Mainchain
2	J	653	PRO	Mainchain
2	J	654	GLN	Mainchain
2	J	670	MET	Mainchain
2	J	678	ARG	Mainchain
2	J	696	PHE	Sidechain
2	J	698	PHE	Sidechain
1	K	125	TYR	Sidechain
1	K	177	ALA	Mainchain
1	K	206	LYS	Mainchain
1	K	221	GLU	Mainchain
1	K	237	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	K	313	GLU	Mainchain
1	K	316	ASN	Mainchain
1	K	318	ARG	Sidechain,Mainchain
1	K	41	SER	Mainchain
1	K	43	GLY	Mainchain
1	K	50	ASN	Sidechain
1	K	62	GLY	Mainchain
1	K	82	GLU	Mainchain
2	L	522	ARG	Sidechain
2	L	532	GLY	Mainchain
2	L	563	TYR	Sidechain,Mainchain
2	L	569	ASN	Sidechain,Mainchain
2	L	576	GLU	Mainchain
2	L	581	SER	Mainchain
2	L	594	ARG	Sidechain
2	L	607	CYS	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2567	0	2629	78	0
1	D	2643	0	2693	164	0
1	G	2567	0	2629	75	0
1	K	2643	0	2693	167	0
2	B	1728	0	1777	198	0
2	C	946	0	937	29	0
2	E	1728	0	1777	285	0
2	F	946	0	935	28	0
2	H	946	0	937	29	0
2	I	1728	0	1777	98	0
2	J	1728	0	1777	193	0
2	L	946	0	935	26	0
All	All	21116	0	21496	1076	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 25.

All (1076) 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:J:491:GLU:CB	2:J:491:GLU:CA	1.74	1.58
2:E:491:GLU:CB	2:E:491:GLU:CA	1.74	1.57
2:B:338:VAL:HG13	2:E:687:HIS:CE1	1.40	1.54
2:J:453:ARG:HG2	1:K:318:ARG:N	1.17	1.44
1:D:318:ARG:N	2:E:453:ARG:HG2	1.17	1.44
2:J:455:GLU:N	1:K:318:ARG:NH2	1.64	1.41
2:B:463:HIS:HE1	2:E:334:GLN:CD	1.19	1.41
1:D:318:ARG:NH2	2:E:455:GLU:N	1.64	1.40
2:B:463:HIS:CE1	2:E:334:GLN:NE2	1.91	1.39
2:B:698:PHE:CG	2:E:695:GLU:HG3	1.55	1.38
2:J:453:ARG:HG2	1:K:318:ARG:CA	1.56	1.35
1:D:318:ARG:CA	2:E:453:ARG:HG2	1.56	1.35
2:B:707:SER:CA	2:E:704:ASN:HD21	1.31	1.34
2:B:703:ALA:CB	2:E:700:GLU:HA	1.55	1.33
2:J:449:TYR:CG	1:K:316:ASN:N	1.68	1.30
1:D:318:ARG:N	2:E:453:ARG:CG	1.94	1.28
2:J:453:ARG:CG	1:K:318:ARG:N	1.94	1.28
1:D:316:ASN:N	2:E:449:TYR:CG	1.68	1.27
2:J:454:GLU:N	1:K:318:ARG:HB2	1.48	1.26
1:D:318:ARG:HB2	2:E:454:GLU:N	1.48	1.26
2:B:338:VAL:CG1	2:E:687:HIS:CE1	2.19	1.25
2:B:707:SER:C	2:E:704:ASN:HD21	1.38	1.24
2:B:330:LEU:HD21	2:E:466:GLU:OE1	1.30	1.24
2:B:463:HIS:CE1	2:E:334:GLN:CD	2.08	1.22
2:B:463:HIS:CE1	2:E:334:GLN:OE1	1.96	1.18
2:B:463:HIS:HE1	2:E:334:GLN:OE1	1.23	1.17
2:J:449:TYR:CD1	1:K:316:ASN:N	2.12	1.17
1:D:316:ASN:N	2:E:449:TYR:CD1	2.12	1.17
2:B:467:ARG:HH21	2:E:334:GLN:HG2	1.06	1.16
2:B:330:LEU:HD11	2:E:466:GLU:HB3	1.26	1.15
2:B:342:LYS:CE	2:I:392:ILE:O	1.95	1.15
1:D:317:PHE:HB3	2:E:453:ARG:HD2	1.17	1.14
2:J:455:GLU:N	1:K:318:ARG:CZ	2.10	1.13
1:D:318:ARG:CZ	2:E:455:GLU:N	2.10	1.13
2:B:703:ALA:HB2	2:E:700:GLU:HA	1.17	1.12
2:J:453:ARG:HD2	1:K:317:PHE:HB3	1.17	1.11
2:B:698:PHE:CB	2:E:695:GLU:HG3	1.81	1.10
2:B:330:LEU:HD13	2:E:467:ARG:NH1	1.67	1.10
2:B:463:HIS:CE1	2:E:334:GLN:HE22	1.54	1.10
2:B:707:SER:CA	2:E:704:ASN:ND2	2.02	1.09
2:J:453:ARG:HB3	1:K:317:PHE:CA	1.83	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:LEU:HD11	2:E:466:GLU:CB	1.83	1.08
2:J:491:GLU:CB	2:J:491:GLU:C	2.21	1.08
2:E:491:GLU:C	2:E:491:GLU:CB	2.21	1.08
1:D:317:PHE:CA	2:E:453:ARG:HB3	1.83	1.07
2:B:706:TYR:CE2	2:E:700:GLU:OE1	2.08	1.07
2:J:443:THR:O	1:K:317:PHE:CE1	2.08	1.06
1:D:317:PHE:CE1	2:E:443:THR:O	2.08	1.06
2:B:698:PHE:CD1	2:E:695:GLU:HG3	1.90	1.06
2:B:330:LEU:CD1	2:E:466:GLU:HB3	1.84	1.06
2:B:698:PHE:HB3	2:E:695:GLU:HB3	1.32	1.04
1:D:222:ASN:O	1:K:319:PRO:HB2	1.58	1.03
2:J:449:TYR:CE1	1:K:316:ASN:HB2	1.93	1.02
1:D:316:ASN:HB2	2:E:449:TYR:CE1	1.93	1.02
1:D:318:ARG:CB	2:E:454:GLU:N	2.23	1.01
2:B:704:ASN:OD1	2:E:704:ASN:HA	1.61	1.01
2:J:454:GLU:N	1:K:318:ARG:CB	2.23	1.01
2:B:702:LEU:HB2	2:E:700:GLU:CD	1.80	1.00
2:B:698:PHE:HB3	2:E:695:GLU:CB	1.91	0.99
2:B:330:LEU:CD1	2:E:467:ARG:HH12	1.74	0.98
1:D:314:TYR:OH	2:E:450:PRO:CB	2.03	0.98
1:D:318:ARG:NH2	2:E:455:GLU:CA	2.26	0.98
1:D:314:TYR:OH	2:E:450:PRO:HB2	1.61	0.97
2:J:450:PRO:HB2	1:K:314:TYR:OH	1.61	0.97
2:B:330:LEU:HD13	2:E:467:ARG:HH12	0.82	0.97
2:J:455:GLU:CA	1:K:318:ARG:NH2	2.26	0.97
2:J:450:PRO:CB	1:K:314:TYR:OH	2.03	0.96
2:B:702:LEU:HB2	2:E:700:GLU:OE2	1.66	0.96
2:B:330:LEU:HD11	2:E:466:GLU:CG	1.96	0.95
2:B:467:ARG:NH2	2:E:334:GLN:HG2	1.81	0.94
2:B:703:ALA:CB	2:E:700:GLU:CA	2.45	0.94
2:B:330:LEU:CD2	2:E:466:GLU:OE1	2.16	0.94
2:J:471:THR:HG21	2:J:689:MET:HG2	1.50	0.93
2:E:471:THR:HG21	2:E:689:MET:HG2	1.50	0.92
1:D:318:ARG:HB2	2:E:453:ARG:C	1.88	0.92
2:B:414:LYS:HD2	2:B:483:LEU:HB3	1.52	0.92
2:I:414:LYS:HD2	2:I:483:LEU:HB3	1.52	0.92
1:G:12:LEU:HB3	1:G:745:ILE:HG12	1.52	0.92
1:D:317:PHE:HA	2:E:453:ARG:HB3	1.51	0.92
2:J:453:ARG:CG	1:K:317:PHE:C	2.37	0.91
2:J:453:ARG:HB3	1:K:317:PHE:C	1.91	0.91
2:J:453:ARG:C	1:K:318:ARG:HB2	1.88	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:PHE:C	2:E:453:ARG:CG	2.37	0.91
1:A:12:LEU:HB3	1:A:745:ILE:HG12	1.52	0.91
1:A:207:LEU:HB2	1:A:235:VAL:HG22	1.52	0.91
2:B:463:HIS:ND1	2:E:334:GLN:NE2	2.19	0.91
2:B:695:GLU:OE1	2:E:694:LYS:NZ	2.03	0.91
2:J:328:ALA:HB2	1:K:316:ASN:CG	1.91	0.91
1:D:316:ASN:CG	2:E:328:ALA:HB2	1.91	0.91
2:J:453:ARG:HB3	1:K:317:PHE:HA	1.51	0.91
1:D:317:PHE:C	2:E:453:ARG:HB3	1.91	0.91
2:B:707:SER:C	2:E:704:ASN:ND2	2.19	0.91
1:G:207:LEU:HB2	1:G:235:VAL:HG22	1.52	0.90
2:B:342:LYS:NZ	2:I:392:ILE:O	2.04	0.90
2:J:453:ARG:CB	1:K:318:ARG:N	2.35	0.90
2:J:453:ARG:CA	1:K:318:ARG:HB2	2.01	0.89
1:D:318:ARG:N	2:E:453:ARG:CB	2.35	0.89
1:D:318:ARG:HB2	2:E:453:ARG:CA	2.01	0.89
2:B:707:SER:N	2:E:704:ASN:ND2	2.20	0.89
2:B:703:ALA:HB1	2:E:700:GLU:HA	1.55	0.88
1:G:67:ARG:HD3	1:G:105:THR:HA	1.54	0.87
2:B:698:PHE:CB	2:E:695:GLU:CG	2.53	0.87
1:A:67:ARG:HD3	1:A:105:THR:HA	1.54	0.87
2:B:338:VAL:HG13	2:E:687:HIS:HE1	1.08	0.86
2:B:698:PHE:HB3	2:E:695:GLU:CG	2.05	0.86
1:D:316:ASN:CA	2:E:449:TYR:CD1	2.58	0.86
2:J:452:LEU:O	1:K:318:ARG:NE	2.09	0.86
2:J:449:TYR:CD1	1:K:316:ASN:CA	2.58	0.86
2:L:561:LYS:HD2	2:L:564:MET:HB2	1.58	0.86
2:F:561:LYS:HD2	2:F:564:MET:HB2	1.58	0.86
1:D:235:VAL:HB	1:D:255:GLU:HA	1.57	0.86
1:D:318:ARG:NE	2:E:452:LEU:O	2.08	0.86
1:K:235:VAL:HB	1:K:255:GLU:HA	1.57	0.86
2:B:345:GLU:HA	2:B:345:GLU:OE1	1.76	0.85
2:I:345:GLU:HA	2:I:345:GLU:OE1	1.76	0.85
1:K:9:LEU:HD11	1:K:289:ILE:HD12	1.55	0.85
1:D:9:LEU:HD11	1:D:289:ILE:HD12	1.55	0.85
1:D:34:ILE:HD13	1:D:170:LEU:HD23	1.58	0.85
2:J:453:ARG:CB	1:K:317:PHE:C	2.45	0.85
1:D:317:PHE:C	2:E:453:ARG:CB	2.45	0.85
1:K:34:ILE:HD13	1:K:170:LEU:HD23	1.58	0.85
1:A:31:LEU:HG	1:A:285:LEU:HD22	1.58	0.84
1:G:31:LEU:HG	1:G:285:LEU:HD22	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:700:GLU:HB3	2:E:699:SER:HB2	1.60	0.84
2:B:330:LEU:O	2:E:470:ARG:NH2	2.11	0.84
2:J:451:ARG:O	1:K:318:ARG:HD3	1.79	0.83
2:B:672:ILE:HD11	2:J:489:ASN:HA	1.61	0.83
2:I:391:ALA:HB1	2:I:408:ALA:HB1	1.59	0.83
1:K:137:LEU:HB3	1:K:160:LEU:HD22	1.61	0.82
1:D:137:LEU:HB3	1:D:160:LEU:HD22	1.61	0.82
1:D:170:LEU:HD21	1:D:281:LEU:HD22	1.60	0.82
1:D:318:ARG:HD3	2:E:451:ARG:O	1.79	0.82
2:B:391:ALA:HB1	2:B:408:ALA:HB1	1.59	0.82
2:E:489:ASN:HA	2:I:672:ILE:HD11	1.61	0.82
1:K:170:LEU:HD21	1:K:281:LEU:HD22	1.60	0.81
2:B:342:LYS:HE2	2:I:392:ILE:O	1.80	0.81
2:J:345:GLU:OE1	2:J:345:GLU:HA	1.81	0.80
2:J:454:GLU:CA	1:K:318:ARG:CZ	2.60	0.80
1:D:318:ARG:CZ	2:E:454:GLU:CA	2.60	0.80
1:D:317:PHE:CD1	2:E:443:THR:O	2.34	0.80
2:J:443:THR:O	1:K:317:PHE:CD1	2.34	0.79
2:E:421:ARG:HG2	2:E:479:ILE:HD13	1.62	0.79
2:E:345:GLU:OE1	2:E:345:GLU:HA	1.81	0.79
2:B:698:PHE:HB3	2:E:695:GLU:HG3	1.64	0.79
2:J:445:LYS:HA	1:K:317:PHE:CE2	2.19	0.78
1:D:318:ARG:NH2	2:E:455:GLU:HB2	1.98	0.78
1:D:317:PHE:CE2	2:E:445:LYS:HA	2.19	0.78
2:B:698:PHE:CD1	2:E:695:GLU:CG	2.67	0.78
2:J:421:ARG:HG2	2:J:479:ILE:HD13	1.62	0.78
1:D:222:ASN:O	1:K:319:PRO:CB	2.32	0.78
2:J:422:GLU:HB3	2:J:423:PRO:HD3	1.64	0.78
2:J:455:GLU:HB2	1:K:318:ARG:NH2	1.98	0.78
2:B:698:PHE:CD2	2:E:695:GLU:HG3	2.18	0.78
1:G:59:ARG:HB3	1:G:242:ILE:HG23	1.67	0.77
1:D:16:LEU:HD23	1:D:29:LEU:HD11	1.66	0.77
2:E:422:GLU:HB3	2:E:423:PRO:HD3	1.64	0.77
2:B:346:GLY:HA3	2:I:654:GLN:H	1.49	0.77
1:A:206:LYS:HE2	1:A:238:SER:HA	1.66	0.77
2:B:491:GLU:HG3	2:J:494:ILE:HB	1.66	0.77
1:A:59:ARG:HB3	1:A:242:ILE:HG23	1.67	0.76
2:B:695:GLU:CD	2:E:694:LYS:NZ	2.39	0.76
2:B:698:PHE:CG	2:E:695:GLU:CG	2.52	0.76
1:G:206:LYS:HE2	1:G:238:SER:HA	1.66	0.76
1:K:16:LEU:HD23	1:K:29:LEU:HD11	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:422:GLU:HB3	2:I:423:PRO:HD3	1.68	0.76
2:B:422:GLU:HB3	2:B:423:PRO:HD3	1.68	0.76
1:D:317:PHE:CB	2:E:453:ARG:HD2	2.09	0.75
1:K:40:GLN:HB2	1:K:141:THR:HG22	1.68	0.75
2:J:455:GLU:CB	1:K:318:ARG:NH2	2.49	0.75
2:J:453:ARG:CG	1:K:318:ARG:CA	2.52	0.75
2:B:707:SER:N	2:E:704:ASN:HD21	1.81	0.75
2:E:494:ILE:HB	2:I:491:GLU:HG3	1.66	0.75
1:A:191:LYS:HA	1:A:195:PRO:HA	1.69	0.75
1:G:191:LYS:HA	1:G:195:PRO:HA	1.69	0.74
1:A:27:ALA:HB1	1:A:296:LEU:HD12	1.68	0.74
1:D:40:GLN:HB2	1:D:141:THR:HG22	1.68	0.74
2:I:702:LEU:CD2	2:I:702:LEU:H	1.99	0.74
1:D:318:ARG:NH2	2:E:455:GLU:CB	2.49	0.74
1:G:27:ALA:HB1	1:G:296:LEU:HD12	1.68	0.74
2:L:573:ARG:HD2	2:L:575:VAL:HG12	1.70	0.74
2:J:453:ARG:HD2	1:K:317:PHE:CB	2.09	0.74
1:D:317:PHE:CD1	2:E:444:LYS:HA	2.23	0.73
2:B:702:LEU:CD2	2:B:702:LEU:H	1.99	0.73
2:B:374:LEU:HD13	2:B:423:PRO:HB2	1.71	0.73
2:B:699:SER:HB2	2:E:696:PHE:HA	1.69	0.73
2:I:374:LEU:HD13	2:I:423:PRO:HB2	1.71	0.73
1:K:161:MET:HA	1:K:164:VAL:HG22	1.69	0.73
1:D:161:MET:HA	1:D:164:VAL:HG22	1.69	0.73
2:J:444:LYS:HA	1:K:317:PHE:CD1	2.23	0.73
2:B:695:GLU:HG3	2:E:698:PHE:CE1	2.24	0.72
2:B:702:LEU:CB	2:E:700:GLU:OE2	2.38	0.72
1:G:83:PHE:HZ	1:G:97:VAL:HG13	1.55	0.72
1:A:83:PHE:HZ	1:A:97:VAL:HG13	1.55	0.72
2:F:573:ARG:HD2	2:F:575:VAL:HG12	1.70	0.71
2:B:330:LEU:HD11	2:E:466:GLU:HG2	1.71	0.71
1:D:81:ALA:HB1	1:D:122:LEU:HD11	1.72	0.71
1:K:81:ALA:HB1	1:K:122:LEU:HD11	1.72	0.71
2:J:450:PRO:HD2	1:K:314:TYR:CE2	2.13	0.71
1:G:48:LEU:HG	1:G:134:LEU:HD23	1.72	0.71
2:J:444:LYS:HA	1:K:317:PHE:CG	2.26	0.70
1:D:83:PHE:HB2	1:D:86:CYS:HB2	1.72	0.70
2:E:688:LEU:N	2:E:688:LEU:HD23	2.07	0.70
2:J:453:ARG:CD	1:K:317:PHE:O	2.40	0.70
1:D:317:PHE:CG	2:E:444:LYS:HA	2.26	0.70
1:D:314:TYR:CE2	2:E:450:PRO:HD2	2.13	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:ALA:HB1	2:E:700:GLU:CA	2.19	0.70
1:A:48:LEU:HG	1:A:134:LEU:HD23	1.72	0.70
2:E:702:LEU:H	2:E:702:LEU:HD23	1.55	0.70
2:J:688:LEU:HD23	2:J:688:LEU:N	2.07	0.70
2:J:453:ARG:CD	1:K:317:PHE:HB3	2.11	0.70
2:J:702:LEU:H	2:J:702:LEU:HD23	1.55	0.70
2:I:687:HIS:CD2	2:I:688:LEU:CD2	2.75	0.69
1:K:83:PHE:HB2	1:K:86:CYS:HB2	1.72	0.69
2:L:518:ILE:HG13	2:L:519:LEU:H	1.57	0.69
1:D:317:PHE:CB	2:E:453:ARG:HB3	2.22	0.69
2:I:688:LEU:N	2:I:688:LEU:HD23	2.07	0.69
1:K:36:VAL:HG22	1:K:48:LEU:HD22	1.74	0.69
1:D:317:PHE:O	2:E:453:ARG:CD	2.40	0.69
2:B:346:GLY:HA3	2:I:654:GLN:N	2.06	0.69
1:D:36:VAL:HG22	1:D:48:LEU:HD22	1.74	0.69
2:B:338:VAL:CG1	2:E:687:HIS:NE2	2.55	0.69
2:J:453:ARG:HB3	1:K:317:PHE:CB	2.22	0.69
2:B:687:HIS:CD2	2:B:688:LEU:CD2	2.75	0.69
2:J:687:HIS:CD2	2:J:688:LEU:CD2	2.75	0.69
1:A:29:LEU:HD23	1:A:289:ILE:HG12	1.74	0.69
1:G:29:LEU:HD23	1:G:289:ILE:HG12	1.74	0.69
1:A:57:LEU:HD22	1:A:136:ASP:HB2	1.74	0.69
2:B:699:SER:OG	2:E:695:GLU:O	2.10	0.69
2:B:698:PHE:HE1	2:E:692:ASN:HA	1.57	0.69
2:I:687:HIS:CD2	2:I:688:LEU:HD21	2.27	0.69
2:B:687:HIS:CD2	2:B:688:LEU:HD21	2.28	0.69
2:E:412:ILE:HG21	2:E:666:VAL:HG11	1.74	0.69
2:E:687:HIS:CD2	2:E:688:LEU:CD2	2.75	0.69
1:A:12:LEU:HD13	1:A:745:ILE:HA	1.75	0.69
2:B:688:LEU:N	2:B:688:LEU:HD23	2.07	0.68
2:B:692:ASN:HA	2:E:341:GLU:OE2	1.93	0.68
2:E:410:GLU:HG3	2:E:486:MET:HE1	1.76	0.68
1:G:57:LEU:HD22	1:G:136:ASP:HB2	1.74	0.68
1:G:12:LEU:HD13	1:G:745:ILE:HA	1.75	0.68
2:J:412:ILE:HG21	2:J:666:VAL:HG11	1.74	0.68
2:E:687:HIS:CD2	2:E:688:LEU:HD21	2.28	0.68
2:J:687:HIS:CD2	2:J:688:LEU:HD21	2.28	0.68
1:K:85:HIS:HE1	1:K:120:ILE:HG23	1.59	0.68
1:D:317:PHE:C	2:E:453:ARG:CD	2.62	0.68
2:F:518:ILE:HG13	2:F:519:LEU:H	1.57	0.68
2:J:453:ARG:CD	1:K:317:PHE:C	2.62	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:ARG:HG2	1:D:115:ILE:HG22	1.75	0.68
2:H:565:LEU:HD11	2:H:596:VAL:HG22	1.76	0.67
1:K:303:GLN:HG2	1:K:735:LEU:HD11	1.76	0.67
1:K:66:ARG:HG2	1:K:115:ILE:HG22	1.76	0.67
2:C:565:LEU:HD11	2:C:596:VAL:HG22	1.76	0.67
1:D:303:GLN:HG2	1:D:735:LEU:HD11	1.76	0.67
2:B:695:GLU:HA	2:E:695:GLU:OE1	1.94	0.67
1:D:318:ARG:CA	2:E:453:ARG:CG	2.52	0.67
2:J:449:TYR:CE1	1:K:316:ASN:CB	2.76	0.67
2:C:518:ILE:HG13	2:C:519:LEU:H	1.59	0.67
2:B:338:VAL:CG1	2:E:687:HIS:HE1	1.83	0.67
2:H:518:ILE:HG13	2:H:519:LEU:H	1.59	0.66
2:B:341:GLU:OE1	2:E:691:ASN:ND2	2.27	0.66
2:B:346:GLY:C	2:I:654:GLN:HB3	2.16	0.66
1:D:60:GLY:H	1:D:64:VAL:HG13	1.60	0.66
1:K:60:GLY:H	1:K:64:VAL:HG13	1.61	0.66
2:C:522:ARG:HH12	2:C:615:SER:HB2	1.61	0.66
1:D:85:HIS:HE1	1:D:120:ILE:HG23	1.59	0.66
1:D:317:PHE:HB3	2:E:453:ARG:CD	2.11	0.66
2:B:341:GLU:HG3	2:B:698:PHE:HE2	1.61	0.66
2:H:522:ARG:HH12	2:H:615:SER:HB2	1.61	0.66
2:I:341:GLU:HG3	2:I:698:PHE:HE2	1.61	0.65
2:J:445:LYS:HA	1:K:317:PHE:HE2	1.62	0.65
1:D:318:ARG:CZ	2:E:454:GLU:C	2.64	0.65
2:B:692:ASN:C	2:B:692:ASN:HD22	2.00	0.65
2:B:706:TYR:HE2	2:E:700:GLU:OE1	1.78	0.65
1:K:17:GLN:HG3	1:K:29:LEU:HD12	1.77	0.65
1:D:17:GLN:HG3	1:D:29:LEU:HD12	1.77	0.65
2:J:454:GLU:C	1:K:318:ARG:CZ	2.64	0.65
1:D:316:ASN:CG	2:E:328:ALA:CB	2.66	0.65
2:I:692:ASN:HD22	2:I:692:ASN:C	2.00	0.65
2:B:699:SER:CB	2:E:696:PHE:HA	2.26	0.65
2:J:328:ALA:CB	1:K:316:ASN:CG	2.66	0.65
2:C:578:GLY:HA3	2:C:585:ILE:HD12	1.78	0.65
2:B:330:LEU:HD21	2:E:466:GLU:CD	2.14	0.64
2:J:690:ILE:HG22	2:J:691:ASN:N	2.11	0.64
2:H:578:GLY:HA3	2:H:585:ILE:HD12	1.78	0.64
1:K:98:ARG:HH22	1:K:245:LYS:HD2	1.63	0.64
2:B:338:VAL:HG11	2:E:687:HIS:NE2	2.12	0.64
2:B:342:LYS:HE3	2:I:392:ILE:O	1.93	0.64
1:A:56:PHE:HB3	1:A:94:PHE:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:690:ILE:HG22	2:E:691:ASN:N	2.11	0.64
2:J:448:GLN:HB3	1:K:313:GLU:HB2	1.80	0.64
1:D:316:ASN:CB	2:E:449:TYR:CE1	2.77	0.64
2:J:410:GLU:HG3	2:J:486:MET:HE1	1.78	0.64
2:B:702:LEU:HG	2:E:700:GLU:OE2	1.98	0.64
1:D:98:ARG:HH22	1:D:245:LYS:HD2	1.63	0.64
2:J:692:ASN:C	2:J:692:ASN:HD22	2.00	0.64
1:D:313:GLU:HB2	2:E:448:GLN:HB3	1.79	0.64
2:E:435:LEU:HD11	2:E:693:THR:HB	1.79	0.64
1:G:56:PHE:HB3	1:G:94:PHE:HB3	1.78	0.64
2:B:703:ALA:HA	2:E:700:GLU:HB3	1.79	0.64
2:J:428:VAL:HG13	2:J:689:MET:HE3	1.80	0.64
1:G:176:PRO:HB3	1:G:206:LYS:HD2	1.80	0.63
1:D:317:PHE:HE2	2:E:445:LYS:HA	1.62	0.63
1:G:217:ARG:HG3	1:G:265:TYR:HE1	1.62	0.63
2:I:452:LEU:C	2:I:452:LEU:HD13	2.19	0.63
2:B:452:LEU:C	2:B:452:LEU:HD13	2.19	0.63
2:E:692:ASN:HD22	2:E:692:ASN:C	2.00	0.63
2:B:690:ILE:HG22	2:B:691:ASN:N	2.14	0.63
2:J:435:LEU:HD11	2:J:693:THR:HB	1.79	0.63
1:D:20:PHE:HB3	1:D:27:ALA:HA	1.80	0.62
1:A:217:ARG:HG3	1:A:265:TYR:HE1	1.62	0.62
1:K:20:PHE:HB3	1:K:27:ALA:HA	1.80	0.62
2:E:428:VAL:HG13	2:E:689:MET:HE3	1.81	0.62
2:I:690:ILE:HG22	2:I:691:ASN:N	2.14	0.62
2:B:680:LEU:HD21	2:J:406:ASP:HB3	1.81	0.62
2:E:491:GLU:C	2:E:491:GLU:CG	2.68	0.62
2:J:681:MET:HB2	2:J:682:PRO:HD3	1.81	0.62
1:G:161:MET:HA	1:G:164:VAL:HG22	1.82	0.62
1:A:161:MET:HA	1:A:164:VAL:HG22	1.82	0.62
2:J:495:GLY:HA2	2:J:664:ASN:HB3	1.81	0.62
2:E:406:ASP:HB3	2:I:680:LEU:HD21	1.81	0.62
1:A:176:PRO:HB3	1:A:206:LYS:HD2	1.81	0.62
2:J:495:GLY:O	2:J:496:PHE:HB2	2.00	0.62
2:J:491:GLU:CG	2:J:491:GLU:C	2.68	0.61
2:E:495:GLY:HA2	2:E:664:ASN:HB3	1.81	0.61
2:E:681:MET:HB2	2:E:682:PRO:HD3	1.81	0.61
1:D:318:ARG:N	2:E:453:ARG:CA	2.63	0.61
2:B:698:PHE:CE1	2:E:692:ASN:HA	2.36	0.61
2:B:703:ALA:CA	2:E:700:GLU:HA	2.29	0.61
2:I:681:MET:HB2	2:I:682:PRO:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:681:MET:HB2	2:B:682:PRO:HD3	1.83	0.61
1:G:209:LEU:HD11	1:G:238:SER:HB3	1.83	0.61
2:B:496:PHE:HA	2:B:660:GLU:HG3	1.83	0.61
2:B:333:VAL:O	2:B:333:VAL:HG12	2.01	0.61
2:I:496:PHE:HA	2:I:660:GLU:HG3	1.83	0.61
2:J:453:ARG:CA	1:K:318:ARG:N	2.63	0.61
1:K:256:ARG:HH12	1:K:269:ALA:HB1	1.65	0.61
2:C:567:VAL:HA	2:C:570:LEU:HD12	1.82	0.61
2:E:495:GLY:O	2:E:496:PHE:HB2	2.00	0.61
2:J:340:PHE:HE2	2:J:694:LYS:HA	1.65	0.61
1:D:29:LEU:HD22	1:D:289:ILE:HG23	1.83	0.60
1:D:10:ILE:HB	1:D:11:PRO:HD3	1.82	0.60
2:F:518:ILE:HG13	2:F:519:LEU:N	2.16	0.60
2:H:567:VAL:HA	2:H:570:LEU:HD12	1.82	0.60
1:D:256:ARG:HH12	1:D:269:ALA:HB1	1.65	0.60
1:D:318:ARG:CB	2:E:453:ARG:HG2	2.30	0.60
1:K:29:LEU:HD22	1:K:289:ILE:HG23	1.83	0.60
2:E:340:PHE:HE2	2:E:694:LYS:HA	1.65	0.60
2:L:518:ILE:HG13	2:L:519:LEU:N	2.16	0.60
1:G:87:LYS:HE2	1:G:88:GLY:HA3	1.83	0.60
1:G:232:ILE:HG21	1:G:277:LEU:HA	1.82	0.60
1:A:232:ILE:HG21	1:A:277:LEU:HA	1.82	0.60
2:B:706:TYR:CD2	2:E:700:GLU:OE1	2.55	0.60
1:A:87:LYS:HE2	1:A:88:GLY:HA3	1.83	0.60
1:A:23:ILE:HG22	1:A:25:GLN:HG2	1.83	0.60
1:K:290:ARG:HD3	1:K:745:ILE:HG22	1.84	0.60
1:A:209:LEU:HD11	1:A:238:SER:HB3	1.83	0.60
1:K:10:ILE:HB	1:K:11:PRO:HD3	1.82	0.60
2:L:565:LEU:HD21	2:L:570:LEU:HD21	1.83	0.60
2:C:518:ILE:HG13	2:C:519:LEU:N	2.16	0.59
2:E:660:GLU:HA	2:E:663:ARG:HH12	1.67	0.59
2:H:518:ILE:HG13	2:H:519:LEU:N	2.16	0.59
2:F:565:LEU:HD21	2:F:570:LEU:HD21	1.84	0.59
2:J:374:LEU:HD13	2:J:423:PRO:HB2	1.83	0.59
2:L:573:ARG:HA	2:L:630:VAL:HA	1.85	0.59
1:G:23:ILE:HG22	1:G:25:GLN:HG2	1.83	0.59
2:I:333:VAL:HG12	2:I:333:VAL:O	2.01	0.59
2:F:573:ARG:HA	2:F:630:VAL:HA	1.85	0.59
2:C:607:CYS:HB2	2:C:613:VAL:HG23	1.85	0.59
1:D:300:LEU:HB2	1:D:739:LEU:HD21	1.85	0.59
2:E:491:GLU:CG	2:E:491:GLU:CA	2.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:ALA:HA	2:E:700:GLU:CB	2.32	0.59
1:G:94:PHE:HZ	1:G:124:VAL:HG11	1.68	0.59
2:C:579:PHE:N	2:C:579:PHE:CD1	2.70	0.59
2:E:374:LEU:HD13	2:E:423:PRO:HB2	1.83	0.58
2:J:660:GLU:HA	2:J:663:ARG:HH12	1.67	0.58
2:H:607:CYS:HB2	2:H:613:VAL:HG23	1.84	0.58
2:J:450:PRO:HD3	1:K:314:TYR:O	2.03	0.58
2:B:495:GLY:O	2:B:496:PHE:HB2	2.04	0.58
2:I:495:GLY:O	2:I:496:PHE:HB2	2.04	0.58
1:A:70:VAL:HG23	1:A:119:PRO:HB3	1.85	0.58
2:B:388:ILE:HD12	2:B:412:ILE:HD12	1.86	0.58
2:J:491:GLU:OE1	2:J:492:ASP:N	2.37	0.58
1:D:314:TYR:O	2:E:450:PRO:HD3	2.03	0.58
1:D:290:ARG:HD3	1:D:745:ILE:HG22	1.84	0.58
1:G:70:VAL:HG23	1:G:119:PRO:HB3	1.85	0.58
2:J:333:VAL:HG12	2:J:333:VAL:O	2.03	0.58
2:E:491:GLU:OE1	2:E:492:ASP:N	2.37	0.58
2:B:702:LEU:N	2:B:702:LEU:CD2	2.67	0.58
2:I:428:VAL:HG11	2:I:472:LYS:HG3	1.86	0.58
1:A:94:PHE:HZ	1:A:124:VAL:HG11	1.68	0.58
1:K:43:GLY:HA3	1:K:236:ASN:HD22	1.68	0.58
2:I:388:ILE:HD12	2:I:412:ILE:HD12	1.86	0.58
2:J:344:ILE:HD12	2:J:694:LYS:HG3	1.86	0.58
2:E:702:LEU:CD2	2:E:702:LEU:N	2.67	0.58
2:J:702:LEU:N	2:J:702:LEU:CD2	2.67	0.57
1:K:300:LEU:HB2	1:K:739:LEU:HD21	1.85	0.57
2:J:450:PRO:CD	1:K:314:TYR:O	2.53	0.57
1:D:43:GLY:HA3	1:D:236:ASN:HD22	1.68	0.57
1:D:314:TYR:O	2:E:450:PRO:CD	2.53	0.57
2:B:428:VAL:HG11	2:B:472:LYS:HG3	1.86	0.57
2:E:333:VAL:HG12	2:E:333:VAL:O	2.02	0.57
2:J:471:THR:HG22	2:J:688:LEU:HB2	1.87	0.57
2:E:471:THR:HG22	2:E:688:LEU:HB2	1.87	0.57
1:G:235:VAL:HB	1:G:255:GLU:HB2	1.87	0.57
2:F:579:PHE:HD1	2:F:579:PHE:N	2.02	0.57
2:H:583:LYS:HD2	2:H:606:ALA:HB1	1.87	0.57
1:K:87:LYS:H	1:K:87:LYS:HD3	1.70	0.57
2:B:388:ILE:HG12	2:B:666:VAL:HG21	1.87	0.57
2:J:491:GLU:CG	2:J:491:GLU:CA	2.67	0.57
2:E:344:ILE:HD12	2:E:694:LYS:HG3	1.86	0.57
1:A:69:LEU:HD13	1:A:101:ILE:HG12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:PHE:CG	2:E:444:LYS:CA	2.87	0.56
1:D:316:ASN:N	2:E:449:TYR:CB	2.58	0.56
2:F:579:PHE:N	2:F:579:PHE:CD1	2.72	0.56
1:D:241:ASP:HB3	1:D:246:LYS:HD2	1.85	0.56
2:J:453:ARG:HG2	1:K:318:ARG:CB	2.29	0.56
2:I:392:ILE:HG13	2:I:393:LYS:HG2	1.86	0.56
1:A:13:VAL:HG11	1:A:289:ILE:HD13	1.87	0.56
1:G:13:VAL:HG11	1:G:289:ILE:HD13	1.87	0.56
2:I:388:ILE:HG12	2:I:666:VAL:HG21	1.87	0.56
2:J:392:ILE:HG13	2:J:393:LYS:HG2	1.88	0.56
2:E:392:ILE:HG13	2:E:393:LYS:HG2	1.88	0.56
2:E:489:ASN:N	2:E:489:ASN:OD1	2.38	0.56
2:J:702:LEU:H	2:J:702:LEU:CD2	2.18	0.56
1:K:252:LEU:HD21	1:K:274:THR:HB	1.88	0.56
1:D:157:ARG:HH22	1:D:188:LYS:HD3	1.71	0.56
1:K:241:ASP:HB3	1:K:246:LYS:HD2	1.86	0.56
2:C:583:LYS:HD2	2:C:606:ALA:HB1	1.87	0.56
2:L:579:PHE:CD1	2:L:579:PHE:N	2.72	0.56
1:K:157:ARG:HH22	1:K:188:LYS:HD3	1.71	0.56
2:B:345:GLU:CA	2:B:345:GLU:OE1	2.52	0.56
2:B:687:HIS:CG	2:B:688:LEU:HD23	2.41	0.56
1:G:69:LEU:HD13	1:G:101:ILE:HG12	1.86	0.56
2:E:491:GLU:OE1	2:E:492:ASP:HA	2.06	0.56
2:L:579:PHE:HD1	2:L:579:PHE:N	2.02	0.56
2:B:392:ILE:HG13	2:B:393:LYS:HG2	1.86	0.56
2:J:470:ARG:HG3	2:J:470:ARG:HH11	1.71	0.56
2:J:489:ASN:OD1	2:J:489:ASN:N	2.38	0.56
2:I:470:ARG:HG3	2:I:470:ARG:HH11	1.71	0.56
2:C:571:LYS:HD3	2:C:591:THR:HG21	1.87	0.56
2:E:470:ARG:HG3	2:E:470:ARG:HH11	1.71	0.55
1:A:235:VAL:HB	1:A:255:GLU:HB2	1.87	0.55
2:I:687:HIS:CG	2:I:688:LEU:HD23	2.41	0.55
1:G:66:ARG:HB2	1:G:105:THR:HG21	1.88	0.55
2:H:579:PHE:CD1	2:H:579:PHE:N	2.70	0.55
1:G:15:ARG:HG3	1:G:15:ARG:HH11	1.71	0.55
1:A:66:ARG:HB2	1:A:105:THR:HG21	1.88	0.55
2:B:495:GLY:HA2	2:B:664:ASN:HB2	1.89	0.55
1:K:218:ASP:HB3	1:K:224:LEU:HB2	1.88	0.55
1:D:87:LYS:H	1:D:87:LYS:HD3	1.70	0.55
2:H:571:LYS:HD3	2:H:591:THR:HG21	1.87	0.55
2:B:695:GLU:OE2	2:E:694:LYS:NZ	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:491:GLU:OE2	2:I:492:ASP:N	2.39	0.55
1:D:56:PHE:HA	1:D:98:ARG:HB2	1.89	0.55
2:F:562:LYS:O	2:F:563:TYR:HB2	2.07	0.55
1:K:56:PHE:HA	1:K:98:ARG:HB2	1.89	0.55
2:I:495:GLY:HA2	2:I:664:ASN:HB2	1.89	0.55
2:L:562:LYS:O	2:L:563:TYR:HB2	2.07	0.55
1:D:65:THR:HB	1:D:138:PRO:HA	1.88	0.55
2:B:491:GLU:OE2	2:B:492:ASP:N	2.39	0.55
2:I:702:LEU:CD2	2:I:702:LEU:N	2.67	0.55
1:K:65:THR:HB	1:K:138:PRO:HA	1.88	0.55
2:B:428:VAL:HG13	2:B:689:MET:HE1	1.89	0.55
2:C:579:PHE:N	2:C:579:PHE:HD1	2.03	0.55
1:D:318:ARG:CD	2:E:452:LEU:O	2.54	0.55
1:K:229:ARG:HD2	1:K:280:VAL:HG22	1.89	0.55
1:D:229:ARG:HD2	1:D:280:VAL:HG22	1.89	0.55
1:D:252:LEU:HD21	1:D:274:THR:HB	1.88	0.55
2:I:345:GLU:OE1	2:I:345:GLU:CA	2.52	0.55
2:I:428:VAL:HG13	2:I:689:MET:HE1	1.89	0.55
2:J:491:GLU:OE1	2:J:492:ASP:HA	2.06	0.54
2:J:452:LEU:O	1:K:318:ARG:CD	2.54	0.54
1:D:317:PHE:O	2:E:453:ARG:HD3	2.07	0.54
2:E:388:ILE:HD11	2:E:666:VAL:HG11	1.89	0.54
2:J:388:ILE:HD11	2:J:666:VAL:HG11	1.89	0.54
1:D:218:ASP:HB3	1:D:224:LEU:HB2	1.89	0.54
2:J:453:ARG:HD3	1:K:317:PHE:O	2.07	0.54
2:E:409:PHE:HE2	2:E:486:MET:HB3	1.72	0.54
2:H:579:PHE:HD1	2:H:579:PHE:N	2.03	0.54
1:K:57:LEU:HD22	1:K:136:ASP:HB2	1.89	0.54
2:E:702:LEU:H	2:E:702:LEU:CD2	2.18	0.54
2:J:409:PHE:HE2	2:J:486:MET:HB3	1.72	0.54
2:J:362:ILE:CG2	2:J:363:ASN:N	2.70	0.54
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.71	0.54
1:D:57:LEU:HD22	1:D:136:ASP:HB2	1.89	0.54
2:B:470:ARG:HG3	2:B:470:ARG:HH11	1.71	0.54
2:L:570:LEU:HD13	2:L:588:LEU:HD13	1.90	0.54
2:F:570:LEU:HD13	2:F:588:LEU:HD13	1.90	0.54
2:E:491:GLU:CB	2:E:491:GLU:O	2.55	0.53
2:E:687:HIS:CG	2:E:688:LEU:HD23	2.42	0.53
2:B:695:GLU:HG3	2:E:698:PHE:CZ	2.43	0.53
2:J:687:HIS:CG	2:J:688:LEU:HD23	2.42	0.53
1:G:274:THR:HB	1:G:275:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:362:ILE:CG2	2:E:363:ASN:N	2.70	0.53
2:B:695:GLU:CD	2:E:694:LYS:HZ2	1.95	0.53
1:A:274:THR:HB	1:A:275:PRO:HD3	1.90	0.53
2:B:346:GLY:HA3	2:I:654:GLN:CB	2.39	0.53
2:E:436:ILE:HG13	2:E:464:ILE:HG21	1.90	0.53
2:I:702:LEU:HD22	2:I:702:LEU:H	1.74	0.53
2:H:577:LYS:HE3	2:H:577:LYS:H	1.73	0.53
1:D:6:MET:HE2	1:D:282:ASN:HB3	1.91	0.53
2:B:362:ILE:CG2	2:B:363:ASN:N	2.72	0.53
2:B:346:GLY:CA	2:I:654:GLN:HB3	2.39	0.53
1:K:36:VAL:HG13	1:K:48:LEU:HD13	1.91	0.53
1:D:36:VAL:HG13	1:D:48:LEU:HD13	1.91	0.53
1:K:307:ILE:HB	1:K:728:MET:HG3	1.91	0.53
2:C:577:LYS:HE3	2:C:577:LYS:H	1.73	0.53
2:J:491:GLU:CB	2:J:491:GLU:O	2.55	0.53
2:B:340:PHE:O	2:B:341:GLU:C	2.43	0.53
2:B:702:LEU:HD22	2:B:702:LEU:H	1.74	0.53
2:B:485:TYR:HB3	2:J:485:TYR:CE2	2.44	0.53
2:E:485:TYR:CE2	2:I:485:TYR:HB3	2.44	0.53
2:J:436:ILE:HG13	2:J:464:ILE:HG21	1.90	0.53
2:I:362:ILE:CG2	2:I:363:ASN:N	2.72	0.53
2:J:688:LEU:O	2:J:689:MET:C	2.46	0.52
2:J:370:PHE:N	2:J:371:PRO:HD2	2.24	0.52
2:J:370:PHE:CE1	2:J:427:CYS:HB2	2.44	0.52
2:I:702:LEU:N	2:I:702:LEU:HD22	2.24	0.52
1:A:33:GLN:HB2	1:A:133:THR:HB	1.90	0.52
2:C:574:ASP:H	2:C:630:VAL:HG21	1.74	0.52
2:J:417:VAL:HG21	2:J:482:GLU:HB2	1.90	0.52
2:I:459:ILE:HD13	2:I:704:ASN:HB3	1.90	0.52
2:L:577:LYS:HE3	2:L:577:LYS:H	1.74	0.52
2:J:451:ARG:O	1:K:318:ARG:CD	2.55	0.52
1:D:318:ARG:HB2	2:E:453:ARG:N	2.24	0.52
2:H:574:ASP:H	2:H:630:VAL:HG21	1.74	0.52
2:J:453:ARG:N	1:K:318:ARG:HB2	2.24	0.52
1:D:318:ARG:CD	2:E:451:ARG:O	2.55	0.52
2:B:459:ILE:HD13	2:B:704:ASN:HB3	1.90	0.52
1:G:33:GLN:HB2	1:G:133:THR:HB	1.90	0.52
2:E:370:PHE:N	2:E:371:PRO:HD2	2.24	0.52
2:B:702:LEU:N	2:B:702:LEU:HD22	2.24	0.52
2:E:370:PHE:CE1	2:E:427:CYS:HB2	2.44	0.52
2:I:688:LEU:O	2:I:689:MET:C	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:490:HIS:CD2	2:I:490:HIS:HA	2.45	0.52
2:J:453:ARG:CA	1:K:318:ARG:CB	2.84	0.52
1:G:31:LEU:HD21	1:G:130:LEU:HD12	1.92	0.52
2:E:417:VAL:HG21	2:E:482:GLU:HB2	1.90	0.52
2:F:577:LYS:HE3	2:F:577:LYS:H	1.75	0.52
2:B:688:LEU:O	2:B:689:MET:C	2.45	0.52
2:I:340:PHE:O	2:I:341:GLU:C	2.43	0.52
2:J:371:PRO:HA	2:J:374:LEU:HD23	1.92	0.51
2:E:371:PRO:HA	2:E:374:LEU:HD23	1.92	0.51
2:B:384:LEU:HD22	2:B:670:MET:HG2	1.92	0.51
1:K:232:ILE:HD11	1:K:276:TYR:HD2	1.75	0.51
2:J:445:LYS:CA	1:K:317:PHE:CE2	2.93	0.51
1:A:31:LEU:HD21	1:A:130:LEU:HD12	1.92	0.51
1:D:307:ILE:HB	1:D:728:MET:HG3	1.91	0.51
2:B:490:HIS:HA	2:J:490:HIS:CD2	2.45	0.51
2:J:453:ARG:HG2	1:K:318:ARG:O	2.11	0.51
1:D:318:ARG:HB3	2:E:454:GLU:N	2.22	0.51
2:E:340:PHE:O	2:E:341:GLU:C	2.48	0.51
2:I:337:ALA:HB1	2:I:698:PHE:CD1	2.46	0.51
2:L:579:PHE:HD1	2:L:579:PHE:H	1.59	0.51
2:C:587:ALA:HB1	2:C:602:GLN:HB2	1.93	0.51
2:C:545:LEU:HD13	2:C:550:LEU:HD13	1.93	0.51
1:D:232:ILE:HD11	1:D:276:TYR:HD2	1.76	0.51
2:B:337:ALA:HB1	2:B:698:PHE:CD1	2.46	0.51
1:K:66:ARG:O	1:K:67:ARG:HG3	2.11	0.51
1:G:300:LEU:HB3	1:G:735:LEU:HD22	1.92	0.51
1:K:74:VAL:HG21	1:K:123:ARG:HH21	1.76	0.51
1:K:221:GLU:HG2	1:K:268:LEU:HD11	1.92	0.51
2:I:384:LEU:HD22	2:I:670:MET:HG2	1.92	0.51
2:H:587:ALA:HB1	2:H:602:GLN:HB2	1.93	0.51
1:D:318:ARG:O	2:E:453:ARG:HG2	2.11	0.50
2:B:491:GLU:HG2	2:B:491:GLU:O	2.10	0.50
1:A:83:PHE:HB2	1:A:86:CYS:HB2	1.94	0.50
2:J:340:PHE:O	2:J:341:GLU:C	2.48	0.50
2:J:454:GLU:N	1:K:318:ARG:HB3	2.22	0.50
1:G:83:PHE:HB2	1:G:86:CYS:HB2	1.94	0.50
2:H:545:LEU:HD13	2:H:550:LEU:HD13	1.93	0.50
2:J:450:PRO:HB2	1:K:314:TYR:HH	1.75	0.50
2:I:491:GLU:O	2:I:491:GLU:HG2	2.10	0.50
2:E:478:LEU:HA	2:E:481:ILE:HD12	1.94	0.50
2:L:545:LEU:HD13	2:L:550:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HB3	1:A:735:LEU:HD22	1.92	0.50
2:I:329:LEU:HD23	2:I:706:TYR:CE1	2.47	0.50
1:D:66:ARG:O	1:D:67:ARG:HG3	2.11	0.50
2:H:526:LEU:HB2	2:H:543:PHE:CE1	2.46	0.50
2:C:526:LEU:HB2	2:C:543:PHE:CE1	2.46	0.50
2:B:329:LEU:HD23	2:B:706:TYR:CE1	2.47	0.50
2:B:700:GLU:N	2:E:699:SER:OG	2.44	0.50
2:E:345:GLU:OE1	2:E:345:GLU:CA	2.57	0.50
2:L:596:VAL:HG11	2:L:603:LEU:HB2	1.93	0.50
1:D:317:PHE:CE2	2:E:445:LYS:CA	2.93	0.50
2:E:387:GLU:HB2	2:E:412:ILE:HG23	1.94	0.50
2:F:579:PHE:HD1	2:F:579:PHE:H	1.59	0.50
2:F:545:LEU:HD13	2:F:550:LEU:HD13	1.94	0.50
1:D:221:GLU:HG2	1:D:268:LEU:HD11	1.92	0.50
2:B:707:SER:H	2:E:704:ASN:ND2	2.07	0.50
1:K:303:GLN:HE21	1:K:735:LEU:HD21	1.77	0.50
2:J:340:PHE:CE2	2:J:694:LYS:HA	2.45	0.50
2:J:478:LEU:HA	2:J:481:ILE:HD12	1.94	0.50
2:J:453:ARG:N	1:K:318:ARG:N	2.60	0.49
2:J:345:GLU:OE1	2:J:345:GLU:CA	2.57	0.49
1:D:74:VAL:HG21	1:D:123:ARG:HH21	1.76	0.49
2:C:553:TYR:CG	2:C:558:GLU:HG2	2.47	0.49
2:J:387:GLU:HB2	2:J:412:ILE:HG23	1.94	0.49
1:G:140:MET:HE2	1:G:160:LEU:HD21	1.92	0.49
2:F:596:VAL:HG11	2:F:603:LEU:HB2	1.93	0.49
2:J:362:ILE:HG23	2:J:363:ASN:N	2.27	0.49
1:K:6:MET:HE2	1:K:282:ASN:HB3	1.95	0.49
2:E:688:LEU:O	2:E:689:MET:C	2.46	0.49
1:D:303:GLN:HE21	1:D:735:LEU:HD21	1.77	0.49
2:B:334:GLN:NE2	2:E:692:ASN:HD21	2.11	0.49
2:E:370:PHE:CE2	2:E:374:LEU:HD21	2.48	0.49
2:C:579:PHE:HD1	2:C:579:PHE:H	1.59	0.49
1:G:37:VAL:HG22	1:G:171:ILE:HG23	1.94	0.49
2:H:553:TYR:CG	2:H:558:GLU:HG2	2.47	0.49
1:D:318:ARG:N	2:E:453:ARG:N	2.60	0.49
2:B:467:ARG:HE	2:E:334:GLN:HG3	1.77	0.49
1:K:135:VAL:HG12	1:K:137:LEU:HG	1.94	0.49
1:A:83:PHE:CZ	1:A:97:VAL:HG13	2.43	0.49
2:I:384:LEU:HD11	2:I:412:ILE:HG22	1.94	0.49
2:F:525:TRP:HB3	2:F:540:GLU:HG2	1.95	0.49
1:D:135:VAL:HG12	1:D:137:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HD2	1:A:264:SER:HB3	1.94	0.49
2:L:525:TRP:HB3	2:L:540:GLU:HG2	1.95	0.49
2:J:328:ALA:HB2	1:K:316:ASN:ND2	2.27	0.49
1:A:140:MET:HE2	1:A:160:LEU:HD21	1.93	0.49
2:J:332:MET:SD	1:K:317:PHE:CE2	3.06	0.49
2:E:676:THR:HG22	2:E:680:LEU:HD22	1.93	0.49
2:I:377:MET:HG3	2:I:422:GLU:HG2	1.95	0.48
1:D:229:ARG:HG3	1:D:280:VAL:CG1	2.43	0.48
1:A:37:VAL:HG22	1:A:171:ILE:HG23	1.94	0.48
1:A:40:GLN:O	1:A:41:SER:HB3	2.13	0.48
1:D:317:PHE:CE2	2:E:332:MET:SD	3.06	0.48
2:J:370:PHE:CE2	2:J:374:LEU:HD21	2.48	0.48
1:G:217:ARG:HD2	1:G:264:SER:HB3	1.94	0.48
2:H:579:PHE:HD1	2:H:579:PHE:H	1.59	0.48
2:J:676:THR:HG22	2:J:680:LEU:HD22	1.93	0.48
2:B:703:ALA:HB1	2:E:700:GLU:C	2.33	0.48
2:I:370:PHE:N	2:I:371:PRO:HD2	2.28	0.48
2:B:461:THR:HB	2:B:465:ARG:HE	1.79	0.48
2:E:340:PHE:CE2	2:E:694:LYS:HA	2.45	0.48
2:B:370:PHE:N	2:B:371:PRO:HD2	2.28	0.48
2:J:370:PHE:CZ	2:J:374:LEU:HD21	2.49	0.48
2:B:377:MET:HG3	2:B:422:GLU:HG2	1.95	0.48
1:A:33:GLN:CB	1:A:133:THR:HB	2.43	0.48
1:D:221:GLU:CG	1:D:268:LEU:HD11	2.44	0.48
2:B:384:LEU:HD11	2:B:412:ILE:HG22	1.94	0.48
1:K:229:ARG:HG3	1:K:280:VAL:CG1	2.43	0.48
1:G:33:GLN:CB	1:G:133:THR:HB	2.43	0.48
2:E:370:PHE:CZ	2:E:374:LEU:HD21	2.49	0.48
2:E:362:ILE:HG23	2:E:363:ASN:N	2.27	0.48
2:B:362:ILE:HG23	2:B:363:ASN:N	2.29	0.48
1:K:221:GLU:CG	1:K:268:LEU:HD11	2.44	0.48
1:G:40:GLN:O	1:G:41:SER:HB3	2.13	0.48
1:D:318:ARG:N	2:E:453:ARG:H	2.11	0.48
2:B:371:PRO:HA	2:B:374:LEU:HD23	1.96	0.48
2:I:461:THR:HB	2:I:465:ARG:HE	1.78	0.48
2:B:370:PHE:CE1	2:B:427:CYS:HB2	2.49	0.48
2:I:361:ARG:O	2:I:362:ILE:C	2.52	0.48
2:I:362:ILE:HG23	2:I:363:ASN:N	2.29	0.48
2:J:449:TYR:CB	1:K:316:ASN:N	2.58	0.47
2:B:687:HIS:HD2	2:B:688:LEU:HD21	1.77	0.47
2:B:452:LEU:HD11	2:B:456:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:384:LEU:HD22	2:J:670:MET:HB2	1.96	0.47
2:B:485:TYR:CD1	2:J:481:ILE:HG21	2.49	0.47
1:G:173:ALA:HB1	1:G:187:LEU:HD23	1.97	0.47
2:I:428:VAL:HG22	2:I:689:MET:HE2	1.97	0.47
2:B:409:PHE:CE2	2:B:486:MET:HE3	2.49	0.47
1:A:173:ALA:HB1	1:A:187:LEU:HD23	1.96	0.47
2:I:409:PHE:CE2	2:I:486:MET:HE3	2.49	0.47
2:J:453:ARG:H	1:K:318:ARG:N	2.11	0.47
2:E:702:LEU:N	2:E:702:LEU:HD23	2.25	0.47
1:K:12:LEU:HG	1:K:745:ILE:HG12	1.96	0.47
1:D:12:LEU:HG	1:D:745:ILE:HG12	1.96	0.47
2:B:361:ARG:O	2:B:362:ILE:C	2.52	0.47
1:K:201:ILE:HD12	1:K:277:LEU:HD12	1.95	0.47
1:G:9:LEU:HG	1:G:286:THR:HG23	1.95	0.47
1:A:9:LEU:HG	1:A:286:THR:HG23	1.95	0.47
2:B:380:ASP:N	2:B:380:ASP:OD1	2.48	0.47
1:D:42:ALA:HB1	1:D:174:VAL:HB	1.97	0.47
2:E:384:LEU:HD11	2:E:412:ILE:HG22	1.96	0.47
2:J:384:LEU:HD11	2:J:412:ILE:HG22	1.96	0.47
2:H:567:VAL:HA	2:H:570:LEU:CD1	2.45	0.47
2:E:481:ILE:HG21	2:I:485:TYR:CD1	2.49	0.47
1:D:201:ILE:HD12	1:D:277:LEU:HD12	1.95	0.47
2:J:452:LEU:C	1:K:318:ARG:CD	2.83	0.47
2:B:346:GLY:HA3	2:I:654:GLN:HB3	1.96	0.47
2:I:374:LEU:HD13	2:I:423:PRO:CB	2.44	0.47
2:E:384:LEU:HD22	2:E:670:MET:HB2	1.97	0.47
1:K:60:GLY:N	1:K:64:VAL:HG13	2.30	0.47
2:I:452:LEU:HD13	2:I:452:LEU:O	2.15	0.47
2:C:567:VAL:HA	2:C:570:LEU:CD1	2.45	0.47
1:K:42:ALA:HB1	1:K:174:VAL:HB	1.97	0.47
2:E:428:VAL:HG13	2:E:689:MET:CE	2.45	0.47
2:J:444:LYS:CA	1:K:317:PHE:CG	2.87	0.47
1:D:317:PHE:O	2:E:453:ARG:CG	2.60	0.47
2:B:707:SER:C	2:E:458:ARG:HH22	2.18	0.47
2:B:414:LYS:HB3	2:B:483:LEU:HD23	1.97	0.47
2:I:702:LEU:HD23	2:I:702:LEU:H	1.76	0.47
2:B:374:LEU:HD13	2:B:423:PRO:CB	2.44	0.47
2:I:687:HIS:HD2	2:I:688:LEU:HD21	1.77	0.47
1:K:67:ARG:HH21	1:K:120:ILE:HG12	1.80	0.47
1:D:67:ARG:HH21	1:D:120:ILE:HG12	1.80	0.47
2:I:380:ASP:OD1	2:I:380:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:452:LEU:O	2:B:452:LEU:HD13	2.15	0.47
2:L:589:PHE:CE2	2:L:591:THR:HG22	2.50	0.47
2:I:370:PHE:CE1	2:I:427:CYS:HB2	2.49	0.46
2:J:361:ARG:O	2:J:362:ILE:C	2.51	0.46
1:G:205:THR:HG22	1:G:236:ASN:HD22	1.81	0.46
1:A:205:THR:HG22	1:A:236:ASN:HD22	1.81	0.46
1:D:318:ARG:CB	2:E:453:ARG:CA	2.84	0.46
2:E:460:VAL:HA	2:E:696:PHE:CE1	2.50	0.46
1:K:16:LEU:HD11	1:K:20:PHE:HE1	1.80	0.46
2:H:600:TYR:O	2:H:601:ARG:HB2	2.15	0.46
2:F:589:PHE:CE2	2:F:591:THR:HG22	2.50	0.46
2:F:600:TYR:O	2:F:601:ARG:HB2	2.15	0.46
2:I:414:LYS:HB3	2:I:483:LEU:HD23	1.97	0.46
2:H:586:PHE:CD1	2:H:613:VAL:HG13	2.51	0.46
2:B:485:TYR:CD1	2:J:481:ILE:HD13	2.51	0.46
2:E:481:ILE:HD13	2:I:485:TYR:CD1	2.51	0.46
2:J:391:ALA:HB1	2:J:408:ALA:HA	1.96	0.46
2:B:703:ALA:CA	2:E:700:GLU:CA	2.92	0.46
2:B:428:VAL:HG22	2:B:689:MET:HE2	1.96	0.46
2:E:435:LEU:HD11	2:E:693:THR:CB	2.45	0.46
2:E:391:ALA:HB1	2:E:408:ALA:HA	1.96	0.46
1:D:318:ARG:CD	2:E:452:LEU:C	2.83	0.46
2:I:371:PRO:HA	2:I:374:LEU:HD23	1.96	0.46
2:F:572:LEU:CD2	2:F:617:LYS:HE2	2.45	0.46
2:E:489:ASN:HB2	2:I:669:TYR:CZ	2.51	0.46
2:C:600:TYR:O	2:C:601:ARG:HB2	2.16	0.46
2:J:455:GLU:N	1:K:318:ARG:NE	2.61	0.46
2:J:452:LEU:HD11	2:J:456:MET:HE3	1.98	0.46
2:B:702:LEU:HD23	2:B:702:LEU:H	1.76	0.46
1:D:316:ASN:ND2	2:E:328:ALA:HB2	2.27	0.46
2:B:669:TYR:CZ	2:J:489:ASN:HB2	2.51	0.46
2:C:586:PHE:CD1	2:C:613:VAL:HG13	2.50	0.46
2:L:600:TYR:O	2:L:601:ARG:HB2	2.15	0.46
1:D:39:GLY:N	1:D:186:ALA:HB2	2.31	0.46
2:J:460:VAL:HA	2:J:696:PHE:CE1	2.50	0.46
2:B:692:ASN:CA	2:E:341:GLU:OE2	2.62	0.46
1:K:12:LEU:CG	1:K:745:ILE:HG12	2.45	0.46
1:G:259:PHE:HB3	1:G:272:MET:HB3	1.98	0.46
1:A:170:LEU:HD22	1:A:201:ILE:CG1	2.46	0.46
2:B:338:VAL:CB	2:E:687:HIS:HE1	2.29	0.46
1:K:63:ILE:CD1	1:K:115:ILE:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:406:ASP:OD1	2:E:407:MET:N	2.49	0.46
2:E:361:ARG:O	2:E:362:ILE:C	2.51	0.46
2:I:369:ARG:CD	2:I:369:ARG:C	2.84	0.46
2:L:572:LEU:CD2	2:L:617:LYS:HE2	2.45	0.46
1:K:39:GLY:N	1:K:186:ALA:HB2	2.31	0.46
2:E:428:VAL:HG11	2:E:472:LYS:HG3	1.98	0.46
2:B:467:ARG:CZ	2:E:334:GLN:HG2	2.42	0.46
2:E:346:GLY:HA3	2:E:360:ALA:HB2	1.98	0.46
2:J:346:GLY:HA3	2:J:360:ALA:HB2	1.98	0.46
1:G:170:LEU:HD22	1:G:201:ILE:CG1	2.46	0.46
2:B:702:LEU:CG	2:E:700:GLU:OE2	2.64	0.45
1:D:170:LEU:HD11	1:D:199:ARG:HB2	1.98	0.45
1:A:29:LEU:HD12	1:A:29:LEU:N	2.31	0.45
1:D:63:ILE:CD1	1:D:115:ILE:HG21	2.46	0.45
1:A:80:TYR:HB2	1:A:90:LYS:HB3	1.98	0.45
1:G:80:TYR:HB2	1:G:90:LYS:HB3	1.98	0.45
1:D:16:LEU:HD11	1:D:20:PHE:HE1	1.80	0.45
2:J:409:PHE:CE2	2:J:486:MET:HB3	2.51	0.45
2:B:369:ARG:C	2:B:369:ARG:CD	2.84	0.45
2:F:523:LYS:HE2	2:F:544:VAL:HG13	1.97	0.45
1:K:20:PHE:CB	1:K:27:ALA:HA	2.47	0.45
1:D:20:PHE:CB	1:D:27:ALA:HA	2.46	0.45
2:J:369:ARG:CD	2:J:369:ARG:C	2.85	0.45
2:E:369:ARG:C	2:E:369:ARG:CD	2.85	0.45
2:J:428:VAL:HG11	2:J:472:LYS:HG3	1.98	0.45
1:G:309:LYS:HB3	1:G:309:LYS:NZ	2.31	0.45
2:L:523:LYS:HE2	2:L:544:VAL:HG13	1.97	0.45
1:G:29:LEU:N	1:G:29:LEU:HD12	2.31	0.45
2:E:435:LEU:HD21	2:E:693:THR:HG21	1.99	0.45
2:J:435:LEU:HD11	2:J:693:THR:CB	2.45	0.45
1:A:51:PHE:CD1	1:A:281:LEU:HD12	2.51	0.45
2:E:684:THR:HG22	2:E:685:ILE:N	2.32	0.45
2:J:459:ILE:HD11	2:J:704:ASN:HD22	1.82	0.45
2:B:375:VAL:HG13	2:B:629:ARG:NH1	2.32	0.45
2:J:380:ASP:OD1	2:J:380:ASP:N	2.49	0.45
2:J:452:LEU:C	1:K:318:ARG:HD3	2.37	0.45
1:D:318:ARG:HB3	2:E:454:GLU:HA	1.99	0.45
1:D:318:ARG:O	2:E:453:ARG:CG	2.65	0.45
2:E:459:ILE:HD11	2:E:704:ASN:HD22	1.82	0.45
2:E:384:LEU:HD22	2:E:670:MET:CG	2.46	0.45
1:D:12:LEU:CG	1:D:745:ILE:HG12	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PHE:HB3	1:A:272:MET:HB3	1.98	0.45
1:G:51:PHE:CD1	1:G:281:LEU:HD12	2.51	0.45
1:D:318:ARG:HD3	2:E:452:LEU:C	2.37	0.45
2:J:435:LEU:HD21	2:J:693:THR:HG21	1.99	0.45
1:K:290:ARG:HD3	1:K:745:ILE:CG2	2.46	0.45
1:G:9:LEU:HD23	1:G:290:ARG:CZ	2.46	0.45
2:F:571:LYS:HD3	2:F:591:THR:HG21	1.99	0.45
2:E:380:ASP:N	2:E:380:ASP:OD1	2.49	0.45
2:J:454:GLU:HA	1:K:318:ARG:HB3	1.98	0.45
1:K:170:LEU:HD11	1:K:199:ARG:HB2	1.98	0.45
2:J:384:LEU:HD22	2:J:670:MET:CG	2.46	0.45
1:D:63:ILE:HD13	1:D:115:ILE:HG21	1.98	0.45
1:K:42:ALA:HB1	1:K:174:VAL:CG1	2.47	0.45
2:I:375:VAL:HG13	2:I:629:ARG:NH1	2.32	0.45
2:J:453:ARG:CG	1:K:318:ARG:O	2.65	0.45
1:D:317:PHE:HE2	2:E:332:MET:SD	2.40	0.45
2:J:687:HIS:HD2	2:J:688:LEU:HD21	1.79	0.45
1:K:55:ASP:HB3	1:K:98:ARG:HD3	1.98	0.45
2:J:406:ASP:OD1	2:J:407:MET:N	2.49	0.45
1:A:9:LEU:HD23	1:A:290:ARG:CZ	2.46	0.45
1:A:309:LYS:HB3	1:A:309:LYS:NZ	2.31	0.45
2:I:370:PHE:CZ	2:I:374:LEU:HD21	2.52	0.45
2:E:409:PHE:CE2	2:E:486:MET:HB3	2.51	0.45
2:B:684:THR:HG22	2:B:685:ILE:N	2.31	0.45
2:L:571:LYS:HD3	2:L:591:THR:HG21	1.99	0.45
2:I:684:THR:HG22	2:I:685:ILE:N	2.31	0.45
2:E:373:GLU:HG2	2:E:426:LYS:HD3	1.99	0.45
2:E:329:LEU:HA	2:E:329:LEU:HD12	1.87	0.45
2:J:456:MET:HE2	2:J:456:MET:HB2	1.75	0.44
1:D:318:ARG:NE	2:E:455:GLU:N	2.61	0.44
2:E:692:ASN:C	2:E:692:ASN:ND2	2.70	0.44
1:D:313:GLU:HB2	2:E:448:GLN:CB	2.42	0.44
1:D:9:LEU:HD22	1:D:286:THR:HA	1.99	0.44
1:G:176:PRO:CB	1:G:206:LYS:HD2	2.46	0.44
1:K:303:GLN:NE2	1:K:735:LEU:HD21	2.32	0.44
1:D:55:ASP:HB3	1:D:98:ARG:HD3	1.98	0.44
2:C:613:VAL:HG12	2:C:617:LYS:HE2	1.98	0.44
1:D:12:LEU:HD23	1:D:745:ILE:HG23	1.99	0.44
1:K:307:ILE:CB	1:K:728:MET:HG3	2.47	0.44
1:D:307:ILE:CB	1:D:728:MET:HG3	2.47	0.44
2:J:684:THR:HG22	2:J:685:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:373:GLU:HG2	2:J:426:LYS:HD3	1.99	0.44
1:G:46:SER:HA	1:G:237:ARG:HH21	1.82	0.44
2:C:572:LEU:HB2	2:C:625:VAL:HG12	2.00	0.44
1:D:318:ARG:C	2:E:453:ARG:HG2	2.31	0.44
2:E:340:PHE:CZ	2:E:439:VAL:HG12	2.53	0.44
2:B:698:PHE:HB2	2:E:695:GLU:OE1	2.18	0.44
1:K:9:LEU:HD22	1:K:286:THR:HA	2.00	0.44
1:A:209:LEU:HD11	1:A:238:SER:CB	2.47	0.44
2:J:340:PHE:CZ	2:J:439:VAL:HG12	2.53	0.44
1:K:12:LEU:HD23	1:K:745:ILE:HG23	1.99	0.44
1:D:290:ARG:HD3	1:D:745:ILE:CG2	2.46	0.44
2:J:449:TYR:CD1	1:K:316:ASN:CB	3.00	0.44
2:B:370:PHE:CZ	2:B:374:LEU:HD21	2.52	0.44
2:B:664:ASN:HA	2:B:664:ASN:HD22	1.60	0.44
2:I:388:ILE:CG1	2:I:666:VAL:HG21	2.48	0.44
2:H:572:LEU:HB2	2:H:625:VAL:HG12	2.00	0.44
1:G:31:LEU:CD2	1:G:130:LEU:HD12	2.48	0.44
1:K:63:ILE:HD13	1:K:115:ILE:HG21	1.98	0.44
2:H:613:VAL:HG12	2:H:617:LYS:HE2	1.98	0.44
2:B:388:ILE:CG1	2:B:666:VAL:HG21	2.48	0.44
2:E:687:HIS:HD2	2:E:688:LEU:HD21	1.79	0.44
1:D:12:LEU:HD23	1:D:745:ILE:HG12	2.00	0.44
1:K:140:MET:SD	1:K:157:ARG:HG3	2.57	0.44
2:J:391:ALA:HB1	2:J:408:ALA:CA	2.48	0.44
1:D:177:ALA:HB1	1:D:210:MET:SD	2.58	0.44
1:G:83:PHE:CZ	1:G:97:VAL:HG13	2.43	0.44
1:A:83:PHE:CZ	1:A:122:LEU:HD22	2.53	0.44
1:D:303:GLN:NE2	1:D:735:LEU:HD21	2.32	0.44
2:H:526:LEU:HB2	2:H:543:PHE:CD1	2.53	0.44
1:K:282:ASN:HA	1:K:282:ASN:HD22	1.66	0.44
1:A:46:SER:HA	1:A:237:ARG:HH21	1.82	0.44
2:J:453:ARG:CG	1:K:317:PHE:O	2.60	0.44
2:B:341:GLU:CD	2:E:691:ASN:HD22	2.19	0.44
2:I:672:ILE:C	2:I:672:ILE:HD12	2.38	0.44
1:A:176:PRO:CB	1:A:206:LYS:HD2	2.46	0.44
1:A:98:ARG:HA	1:A:101:ILE:HD12	1.99	0.44
1:D:42:ALA:HB1	1:D:174:VAL:CG1	2.47	0.44
2:E:391:ALA:HB1	2:E:408:ALA:CA	2.48	0.44
2:B:330:LEU:HA	2:E:467:ARG:HH22	1.82	0.44
1:G:209:LEU:HD11	1:G:238:SER:CB	2.47	0.44
2:I:494:ILE:HG22	2:I:495:GLY:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:87:LYS:N	1:K:87:LYS:HD3	2.33	0.44
1:D:140:MET:SD	1:D:157:ARG:HG3	2.57	0.44
2:J:332:MET:SD	1:K:317:PHE:HE2	2.40	0.43
2:J:453:ARG:CB	1:K:317:PHE:HA	2.35	0.43
2:B:672:ILE:HD12	2:B:672:ILE:C	2.38	0.43
2:J:475:VAL:HG22	2:J:681:MET:SD	2.58	0.43
2:E:475:VAL:HG22	2:E:681:MET:SD	2.58	0.43
1:G:57:LEU:HA	1:G:58:PRO:HD3	1.90	0.43
1:D:87:LYS:N	1:D:87:LYS:HD3	2.33	0.43
2:L:572:LEU:HD22	2:L:617:LYS:HE2	2.01	0.43
2:E:688:LEU:CD2	2:E:688:LEU:N	2.77	0.43
2:B:707:SER:O	2:E:458:ARG:NH2	2.47	0.43
1:G:83:PHE:CZ	1:G:122:LEU:HD22	2.53	0.43
1:A:234:VAL:CG1	1:A:277:LEU:HD22	2.48	0.43
2:F:572:LEU:HD22	2:F:617:LYS:HE2	2.00	0.43
2:I:435:LEU:HD21	2:I:693:THR:HG21	2.00	0.43
2:E:697:ILE:HD13	2:E:697:ILE:O	2.18	0.43
1:G:56:PHE:CB	1:G:94:PHE:HB3	2.48	0.43
1:G:234:VAL:CG1	1:G:277:LEU:HD22	2.47	0.43
2:J:385:ARG:NH1	2:J:663:ARG:HD2	2.33	0.43
2:B:435:LEU:HD21	2:B:693:THR:HG21	2.00	0.43
1:K:208:ASP:HB3	1:K:258:PHE:CD1	2.54	0.43
2:I:697:ILE:HD13	2:I:697:ILE:O	2.18	0.43
2:I:406:ASP:OD1	2:I:407:MET:N	2.51	0.43
1:G:16:LEU:HD21	1:G:742:ILE:HG12	2.01	0.43
2:B:338:VAL:CG2	2:E:687:HIS:CE1	3.01	0.43
2:J:450:PRO:HD3	1:K:314:TYR:CG	2.27	0.43
1:K:87:LYS:HZ3	1:K:87:LYS:HB2	1.83	0.43
2:C:526:LEU:HB2	2:C:543:PHE:CD1	2.53	0.43
1:A:232:ILE:CG1	1:A:280:VAL:HG21	2.48	0.43
1:K:12:LEU:HD23	1:K:745:ILE:HG12	2.00	0.43
1:D:208:ASP:HB3	1:D:258:PHE:CD1	2.54	0.43
1:D:318:ARG:CZ	2:E:454:GLU:CB	2.97	0.43
1:K:157:ARG:NH2	1:K:188:LYS:HD3	2.33	0.43
1:G:98:ARG:HA	1:G:101:ILE:HD12	1.99	0.43
2:B:406:ASP:OD1	2:B:407:MET:N	2.51	0.43
1:A:16:LEU:HD21	1:A:742:ILE:HG12	2.01	0.43
2:B:697:ILE:O	2:B:697:ILE:HD13	2.18	0.43
1:A:31:LEU:CD2	1:A:130:LEU:HD12	2.48	0.43
2:E:407:MET:CE	2:I:474:GLN:HG2	2.49	0.43
2:B:494:ILE:HG22	2:B:495:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:ASP:HB3	2:J:680:LEU:HD11	2.01	0.43
1:D:316:ASN:CB	2:E:449:TYR:CD1	3.00	0.43
2:J:428:VAL:HG13	2:J:689:MET:CE	2.45	0.43
1:G:232:ILE:CG1	1:G:280:VAL:HG21	2.49	0.43
1:K:39:GLY:H	1:K:186:ALA:HB2	1.84	0.43
2:I:464:ILE:HD13	2:I:696:PHE:HD2	1.84	0.43
1:K:177:ALA:HB1	1:K:210:MET:SD	2.58	0.43
2:J:449:TYR:HB3	1:K:313:GLU:O	2.19	0.43
2:L:596:VAL:HG13	2:L:597:TYR:HD1	1.84	0.43
1:D:318:ARG:NH2	2:E:454:GLU:C	2.56	0.42
2:E:385:ARG:NH1	2:E:663:ARG:HD2	2.33	0.42
2:I:384:LEU:HD22	2:I:670:MET:CG	2.49	0.42
2:J:436:ILE:CD1	2:J:464:ILE:HG21	2.49	0.42
2:F:596:VAL:HG13	2:F:597:TYR:HD1	1.84	0.42
2:E:680:LEU:HD11	2:I:406:ASP:HB3	2.00	0.42
1:D:39:GLY:H	1:D:186:ALA:HB2	1.84	0.42
2:F:520:VAL:HG11	2:F:523:LYS:HG3	2.01	0.42
2:J:454:GLU:CB	1:K:318:ARG:CZ	2.97	0.42
1:A:66:ARG:HB2	1:A:105:THR:CG2	2.48	0.42
2:E:436:ILE:CD1	2:E:464:ILE:HG21	2.49	0.42
2:L:520:VAL:HG11	2:L:523:LYS:HG3	2.01	0.42
1:G:63:ILE:HG21	1:G:148:GLN:HE22	1.84	0.42
1:D:313:GLU:O	2:E:449:TYR:HB3	2.19	0.42
2:J:692:ASN:ND2	2:J:692:ASN:C	2.70	0.42
1:A:9:LEU:CD1	1:A:286:THR:HG23	2.49	0.42
2:J:697:ILE:O	2:J:697:ILE:HD13	2.18	0.42
2:B:707:SER:N	2:E:704:ASN:CG	2.69	0.42
1:A:167:GLU:O	1:A:168:ASN:HB2	2.19	0.42
2:B:692:ASN:C	2:B:692:ASN:ND2	2.70	0.42
1:K:67:ARG:NH2	1:K:120:ILE:HG12	2.33	0.42
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.91	0.42
1:G:9:LEU:CD1	1:G:286:THR:HG23	2.49	0.42
2:B:341:GLU:OE2	2:E:691:ASN:CB	2.68	0.42
2:J:449:TYR:CE1	1:K:316:ASN:N	2.82	0.42
2:J:687:HIS:CD2	2:J:688:LEU:HD23	2.54	0.42
2:E:370:PHE:CD1	2:E:427:CYS:HB2	2.55	0.42
1:D:60:GLY:N	1:D:64:VAL:HG13	2.30	0.42
1:A:56:PHE:CB	1:A:94:PHE:HB3	2.48	0.42
1:D:87:LYS:HB2	1:D:87:LYS:HZ3	1.84	0.42
2:B:464:ILE:HD13	2:B:696:PHE:HD2	1.84	0.42
1:D:316:ASN:HB2	2:E:449:TYR:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:ARG:HB2	1:G:105:THR:CG2	2.48	0.42
1:D:67:ARG:NH2	1:D:120:ILE:HG12	2.33	0.42
2:I:388:ILE:N	2:I:388:ILE:HD12	2.35	0.42
2:J:485:TYR:CZ	2:J:487:ASN:HB3	2.55	0.42
1:G:167:GLU:O	1:G:168:ASN:HB2	2.19	0.42
1:A:63:ILE:HG21	1:A:148:GLN:HE22	1.84	0.42
1:A:67:ARG:HH22	1:A:107:ARG:HH21	1.67	0.42
1:K:81:ALA:HB1	1:K:122:LEU:CD1	2.47	0.42
2:C:526:LEU:HD13	2:C:605:LEU:HD22	2.01	0.42
2:L:539:LYS:NZ	2:L:554:LYS:HE2	2.34	0.42
1:D:78:THR:HB	1:D:80:TYR:CE1	2.54	0.42
2:I:489:ASN:OD1	2:I:489:ASN:N	2.51	0.42
2:E:687:HIS:C	2:E:688:LEU:HD23	2.39	0.42
2:B:687:HIS:CD2	2:B:688:LEU:HD23	2.53	0.42
2:J:664:ASN:HA	2:J:664:ASN:HD22	1.64	0.42
2:H:526:LEU:HD13	2:H:605:LEU:HD22	2.01	0.42
1:K:68:PRO:HD2	1:K:119:PRO:HA	2.01	0.42
2:B:654:GLN:O	2:B:654:GLN:HG2	2.20	0.42
2:J:629:ARG:HD2	2:J:629:ARG:HA	1.81	0.42
1:G:67:ARG:HH22	1:G:107:ARG:HH21	1.67	0.42
2:B:680:LEU:HA	2:B:680:LEU:HD12	1.88	0.42
2:I:629:ARG:HD2	2:I:629:ARG:HA	1.83	0.42
1:D:304:LEU:HD11	1:D:736:LYS:NZ	2.35	0.42
1:K:78:THR:HB	1:K:80:TYR:CE1	2.54	0.42
2:J:453:ARG:N	1:K:318:ARG:CB	2.83	0.41
2:B:672:ILE:HG13	2:B:673:VAL:N	2.35	0.41
2:J:370:PHE:CD1	2:J:427:CYS:HB2	2.55	0.41
2:E:494:ILE:HD12	2:E:494:ILE:HG21	1.91	0.41
1:G:170:LEU:HD22	1:G:201:ILE:HG12	2.02	0.41
1:K:304:LEU:HD11	1:K:736:LYS:NZ	2.35	0.41
2:I:654:GLN:O	2:I:654:GLN:HG2	2.20	0.41
2:B:474:GLN:HG2	2:J:407:MET:CE	2.49	0.41
1:D:157:ARG:NH2	1:D:188:LYS:HD3	2.33	0.41
2:E:672:ILE:CG2	2:I:489:ASN:HB2	2.50	0.41
1:D:68:PRO:HD2	1:D:119:PRO:HA	2.01	0.41
2:I:672:ILE:HG13	2:I:673:VAL:N	2.35	0.41
2:C:550:LEU:HD22	2:C:620:PHE:CE1	2.55	0.41
2:E:669:TYR:HA	2:E:672:ILE:HG13	2.02	0.41
2:B:699:SER:HG	2:E:695:GLU:C	2.18	0.41
2:J:687:HIS:C	2:J:688:LEU:HD23	2.39	0.41
2:C:607:CYS:HB3	2:C:612:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:LEU:HD22	2:B:670:MET:CG	2.49	0.41
2:B:486:MET:HB2	2:B:486:MET:HE2	1.93	0.41
2:J:669:TYR:HA	2:J:672:ILE:HG13	2.02	0.41
1:D:113:LYS:N	1:D:113:LYS:HD2	2.36	0.41
1:K:262:HIS:CE1	1:K:264:SER:HB2	2.56	0.41
1:D:316:ASN:N	2:E:449:TYR:CE1	2.82	0.41
1:A:23:ILE:HG12	1:A:734:ALA:HB1	2.02	0.41
2:B:388:ILE:N	2:B:388:ILE:HD12	2.35	0.41
1:A:170:LEU:HD22	1:A:201:ILE:HG12	2.02	0.41
2:B:489:ASN:OD1	2:B:489:ASN:N	2.51	0.41
1:A:135:VAL:HG12	1:A:137:LEU:HG	2.02	0.41
2:J:449:TYR:HA	2:J:450:PRO:HD3	1.81	0.41
1:G:23:ILE:HG12	1:G:734:ALA:HB1	2.02	0.41
2:J:362:ILE:CG2	2:J:363:ASN:H	2.34	0.41
2:I:435:LEU:HD23	2:I:436:ILE:N	2.35	0.41
1:K:262:HIS:HA	1:K:263:PRO:HD2	1.94	0.41
2:B:341:GLU:OE2	2:E:691:ASN:HB2	2.21	0.41
2:I:452:LEU:HD11	2:I:456:MET:HE3	2.03	0.41
2:E:485:TYR:CZ	2:E:487:ASN:HB3	2.55	0.41
2:B:629:ARG:HA	2:B:629:ARG:HD2	1.83	0.41
1:D:262:HIS:CE1	1:D:264:SER:HB2	2.56	0.41
1:K:113:LYS:HD2	1:K:113:LYS:N	2.36	0.41
2:J:444:LYS:CA	1:K:317:PHE:CD1	2.98	0.41
2:H:550:LEU:HD22	2:H:620:PHE:CE1	2.55	0.41
1:A:140:MET:CE	1:A:160:LEU:HD21	2.50	0.41
2:F:539:LYS:NZ	2:F:554:LYS:HE2	2.34	0.41
1:G:135:VAL:HG12	1:G:137:LEU:HG	2.02	0.41
2:J:445:LYS:HB3	2:J:445:LYS:NZ	2.36	0.41
1:D:318:ARG:CB	2:E:453:ARG:N	2.83	0.41
2:E:445:LYS:NZ	2:E:445:LYS:HB3	2.36	0.41
2:J:449:TYR:CD1	1:K:316:ASN:HB2	2.49	0.41
2:I:370:PHE:HZ	2:I:681:MET:HG3	1.86	0.41
2:I:687:HIS:C	2:I:688:LEU:HD23	2.40	0.41
2:J:388:ILE:HD11	2:J:666:VAL:CG1	2.51	0.41
1:G:140:MET:CE	1:G:160:LEU:HD21	2.50	0.41
2:H:535:LYS:HG2	2:H:535:LYS:O	2.21	0.41
2:J:630:VAL:CG2	2:J:671:ALA:HB1	2.51	0.41
2:B:481:ILE:HG22	2:B:482:GLU:OE1	2.21	0.41
2:J:654:GLN:O	2:J:654:GLN:HG2	2.21	0.41
2:J:491:GLU:CD	2:J:491:GLU:C	2.80	0.41
2:H:607:CYS:HB3	2:H:612:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:363:ASN:HD21	2:B:685:ILE:HG21	1.85	0.41
1:D:38:GLY:HA2	1:D:186:ALA:CB	2.51	0.41
1:G:63:ILE:HG21	1:G:148:GLN:NE2	2.36	0.41
2:E:491:GLU:C	2:E:491:GLU:CD	2.80	0.40
1:D:13:VAL:HG13	1:D:29:LEU:HD13	2.02	0.40
2:J:370:PHE:CE2	2:J:681:MET:HB2	2.56	0.40
2:F:570:LEU:HA	2:F:570:LEU:HD23	1.92	0.40
1:K:229:ARG:HG3	1:K:280:VAL:HG11	2.02	0.40
2:L:525:TRP:CE3	2:L:540:GLU:HG2	2.57	0.40
2:B:489:ASN:HB2	2:J:672:ILE:CG2	2.50	0.40
2:E:629:ARG:HD2	2:E:629:ARG:HA	1.81	0.40
2:C:535:LYS:O	2:C:535:LYS:HG2	2.21	0.40
1:D:317:PHE:CD1	2:E:444:LYS:CA	2.98	0.40
2:E:370:PHE:CE2	2:E:681:MET:HB2	2.57	0.40
2:B:346:GLY:C	2:I:654:GLN:CB	2.88	0.40
1:G:134:LEU:N	1:G:134:LEU:HD12	2.36	0.40
2:B:452:LEU:HD11	2:B:456:MET:CE	2.51	0.40
1:G:164:VAL:HG21	1:G:193:VAL:HG11	2.04	0.40
1:A:164:VAL:HG21	1:A:193:VAL:HG11	2.04	0.40
2:J:660:GLU:HA	2:J:663:ARG:NH1	2.35	0.40
2:B:435:LEU:HD23	2:B:436:ILE:N	2.35	0.40
1:A:63:ILE:HG21	1:A:148:GLN:NE2	2.36	0.40
2:L:624:GLY:HA2	2:L:626:TYR:CE1	2.56	0.40
1:G:307:ILE:HG21	1:G:728:MET:HB3	2.03	0.40
2:C:573:ARG:HB2	2:C:630:VAL:CG1	2.51	0.40
1:K:38:GLY:HA2	1:K:186:ALA:CB	2.51	0.40
1:A:307:ILE:HG21	1:A:728:MET:HB3	2.03	0.40
2:J:454:GLU:C	1:K:318:ARG:NH2	2.55	0.40
1:K:13:VAL:HG13	1:K:29:LEU:HD13	2.02	0.40
2:J:494:ILE:HG21	2:J:494:ILE:HD12	1.91	0.40
1:A:59:ARG:HB3	1:A:242:ILE:CG2	2.45	0.40
2:E:388:ILE:HD11	2:E:666:VAL:CG1	2.51	0.40
2:E:664:ASN:HA	2:E:664:ASN:HD22	1.64	0.40
2:E:660:GLU:HA	2:E:663:ARG:NH1	2.35	0.40
2:H:573:ARG:HB2	2:H:630:VAL:CG1	2.51	0.40
1:D:221:GLU:HA	1:D:268:LEU:HD11	2.04	0.40
2:F:525:TRP:CE3	2:F:540:GLU:HG2	2.57	0.40
2:J:669:TYR:CD1	2:J:672:ILE:HD11	2.57	0.40
2:E:630:VAL:CG2	2:E:671:ALA:HB1	2.51	0.40
1:A:301:GLN:HA	1:A:301:GLN:HE21	1.86	0.40
1:A:746:ASN:HD22	1:A:746:ASN:HA	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PRO:HG2	1:A:159:MET:SD	2.62	0.40
2:I:481:ILE:HG22	2:I:482:GLU:OE1	2.21	0.40
1:D:317:PHE:HB3	2:E:453:ARG:HB3	2.02	0.40
2:F:573:ARG:HD2	2:F:575:VAL:CG1	2.47	0.40
1:G:232:ILE:HG12	1:G:280:VAL:HG21	2.04	0.40
1:A:232:ILE:HG12	1:A:280:VAL:HG21	2.03	0.40
1:A:87:LYS:O	1:A:87:LYS:HG3	2.20	0.40
1:G:301:GLN:HA	1:G:301:GLN:HE21	1.85	0.40
2:F:535:LYS:O	2:F:535:LYS:HG2	2.21	0.40
2:E:654:GLN:HG2	2:E:654:GLN:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	325/864 (38%)	313 (96%)	10 (3%)	2 (1%)	30	74
1	D	333/864 (38%)	317 (95%)	14 (4%)	2 (1%)	30	74
1	G	325/864 (38%)	313 (96%)	10 (3%)	2 (1%)	30	74
1	K	333/864 (38%)	317 (95%)	14 (4%)	2 (1%)	30	74
2	B	196/864 (23%)	165 (84%)	22 (11%)	9 (5%)	3	33
2	C	111/864 (13%)	93 (84%)	13 (12%)	5 (4%)	3	33
2	E	196/864 (23%)	161 (82%)	27 (14%)	8 (4%)	3	35
2	F	111/864 (13%)	93 (84%)	12 (11%)	6 (5%)	2	29
2	H	111/864 (13%)	93 (84%)	13 (12%)	5 (4%)	3	33
2	I	196/864 (23%)	165 (84%)	22 (11%)	9 (5%)	3	33
2	J	196/864 (23%)	161 (82%)	27 (14%)	8 (4%)	3	35
2	L	111/864 (13%)	93 (84%)	12 (11%)	6 (5%)	2	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2544/10368 (24%)	2284 (90%)	196 (8%)	64 (2%)	11 46

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	GLY
2	B	489	ASN
2	B	490	HIS
2	B	492	ASP
2	C	534	MET
2	C	576	GLU
2	E	449	TYR
2	E	450	PRO
2	E	490	HIS
2	E	492	ASP
2	F	534	MET
2	F	574	ASP
2	F	627	PRO
1	G	88	GLY
2	H	534	MET
2	H	576	GLU
2	I	489	ASN
2	I	490	HIS
2	I	492	ASP
2	J	449	TYR
2	J	450	PRO
2	J	490	HIS
2	J	492	ASP
2	L	534	MET
2	L	574	ASP
2	L	627	PRO
2	B	414	LYS
2	B	487	ASN
2	B	690	ILE
2	C	577	LYS
2	E	454	GLU
2	F	576	GLU
2	H	577	LYS
2	I	414	LYS
2	I	487	ASN
2	I	690	ILE
2	L	576	GLU

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Mol	Chain	Res	Type
2	B	696	PHE
1	D	79	GLU
2	E	452	LEU
2	I	696	PHE
2	J	452	LEU
2	J	454	GLU
1	K	79	GLU
2	B	689	MET
2	E	453	ARG
2	I	689	MET
2	J	453	ARG
2	C	563	TYR
2	E	689	MET
2	F	577	LYS
2	H	563	TYR
2	J	689	MET
2	L	577	LYS
1	A	87	LYS
1	D	41	SER
1	G	87	LYS
1	K	41	SER
2	B	412	ILE
2	F	575	VAL
2	I	412	ILE
2	L	575	VAL
2	C	532	GLY
2	H	532	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	287/761 (38%)	275 (96%)	12 (4%)	36 70
1	D	295/761 (39%)	281 (95%)	14 (5%)	32 68
1	G	287/761 (38%)	275 (96%)	12 (4%)	36 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	295/761 (39%)	281 (95%)	14 (5%)	32 68
2	B	194/761 (26%)	155 (80%)	39 (20%)	1 11
2	C	102/761 (13%)	94 (92%)	8 (8%)	16 51
2	E	194/761 (26%)	153 (79%)	41 (21%)	1 9
2	F	102/761 (13%)	89 (87%)	13 (13%)	5 29
2	H	102/761 (13%)	94 (92%)	8 (8%)	16 51
2	I	194/761 (26%)	155 (80%)	39 (20%)	1 11
2	J	194/761 (26%)	152 (78%)	42 (22%)	1 9
2	L	102/761 (13%)	89 (87%)	13 (13%)	5 29
All	All	2348/9132 (26%)	2093 (89%)	255 (11%)	12 35

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	69	LEU
1	A	73	LEU
1	A	79	GLU
1	A	87	LYS
1	A	121	ASN
1	A	175	SER
1	A	228	ARG
1	A	240	LYS
1	A	245	LYS
1	A	301	GLN
1	A	727	GLU
2	B	327	LYS
2	B	329	LEU
2	B	330	LEU
2	B	339	ASP
2	B	340	PHE
2	B	345	GLU
2	B	357	SER
2	B	367	HIS
2	B	368	GLU
2	B	369	ARG
2	B	380	ASP
2	B	416	GLN
2	B	445	LYS

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Mol	Chain	Res	Type
2	B	449	TYR
2	B	451	ARG
2	B	467	ARG
2	B	468	GLU
2	B	489	ASN
2	B	490	HIS
2	B	491	GLU
2	B	492	ASP
2	B	493	PHE
2	B	494	ILE
2	B	628	GLU
2	B	664	ASN
2	B	667	ASP
2	B	672	ILE
2	B	676	THR
2	B	678	ARG
2	B	679	ASP
2	B	682	PRO
2	B	685	ILE
2	B	688	LEU
2	B	692	ASN
2	B	697	ILE
2	B	698	PHE
2	B	702	LEU
2	B	705	LEU
2	B	707	SER
2	C	534	MET
2	C	560	GLU
2	C	563	TYR
2	C	577	LYS
2	C	579	PHE
2	C	584	HIS
2	C	594	ARG
2	C	603	LEU
1	D	34	ILE
1	D	78	THR
1	D	87	LYS
1	D	99	LEU
1	D	113	LYS
1	D	123	ARG
1	D	159	MET
1	D	166	LYS

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Mol	Chain	Res	Type
1	D	171	ILE
1	D	228	ARG
1	D	248	ILE
1	D	290	ARG
1	D	304	LEU
1	D	318	ARG
2	E	327	LYS
2	E	329	LEU
2	E	330	LEU
2	E	339	ASP
2	E	340	PHE
2	E	345	GLU
2	E	357	SER
2	E	367	HIS
2	E	368	GLU
2	E	369	ARG
2	E	380	ASP
2	E	416	GLN
2	E	418	LYS
2	E	443	THR
2	E	445	LYS
2	E	449	TYR
2	E	450	PRO
2	E	451	ARG
2	E	452	LEU
2	E	454	GLU
2	E	456	MET
2	E	468	GLU
2	E	480	ASP
2	E	482	GLU
2	E	489	ASN
2	E	490	HIS
2	E	491	GLU
2	E	492	ASP
2	E	493	PHE
2	E	494	ILE
2	E	628	GLU
2	E	664	ASN
2	E	672	ILE
2	E	676	THR
2	E	678	ARG
2	E	679	ASP

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Mol	Chain	Res	Type
2	E	688	LEU
2	E	692	ASN
2	E	697	ILE
2	E	698	PHE
2	E	702	LEU
2	F	529	ASN
2	F	534	MET
2	F	551	SER
2	F	558	GLU
2	F	560	GLU
2	F	569	ASN
2	F	571	LYS
2	F	573	ARG
2	F	577	LYS
2	F	579	PHE
2	F	594	ARG
2	F	603	LEU
2	F	604	GLU
1	G	54	ARG
1	G	69	LEU
1	G	73	LEU
1	G	79	GLU
1	G	87	LYS
1	G	121	ASN
1	G	175	SER
1	G	228	ARG
1	G	240	LYS
1	G	245	LYS
1	G	301	GLN
1	G	727	GLU
2	H	534	MET
2	H	560	GLU
2	H	563	TYR
2	H	577	LYS
2	H	579	PHE
2	H	584	HIS
2	H	594	ARG
2	H	603	LEU
2	I	327	LYS
2	I	329	LEU
2	I	330	LEU
2	I	339	ASP

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Mol	Chain	Res	Type
2	I	340	PHE
2	I	345	GLU
2	I	357	SER
2	I	367	HIS
2	I	368	GLU
2	I	369	ARG
2	I	380	ASP
2	I	416	GLN
2	I	445	LYS
2	I	449	TYR
2	I	451	ARG
2	I	467	ARG
2	I	468	GLU
2	I	489	ASN
2	I	490	HIS
2	I	491	GLU
2	I	492	ASP
2	I	493	PHE
2	I	494	ILE
2	I	628	GLU
2	I	664	ASN
2	I	667	ASP
2	I	672	ILE
2	I	676	THR
2	I	678	ARG
2	I	679	ASP
2	I	682	PRO
2	I	685	ILE
2	I	688	LEU
2	I	692	ASN
2	I	697	ILE
2	I	698	PHE
2	I	702	LEU
2	I	705	LEU
2	I	707	SER
2	J	327	LYS
2	J	329	LEU
2	J	330	LEU
2	J	339	ASP
2	J	340	PHE
2	J	345	GLU
2	J	357	SER

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Mol	Chain	Res	Type
2	J	367	HIS
2	J	368	GLU
2	J	369	ARG
2	J	380	ASP
2	J	416	GLN
2	J	418	LYS
2	J	443	THR
2	J	445	LYS
2	J	449	TYR
2	J	450	PRO
2	J	451	ARG
2	J	452	LEU
2	J	454	GLU
2	J	456	MET
2	J	468	GLU
2	J	480	ASP
2	J	482	GLU
2	J	489	ASN
2	J	490	HIS
2	J	491	GLU
2	J	492	ASP
2	J	493	PHE
2	J	494	ILE
2	J	628	GLU
2	J	664	ASN
2	J	672	ILE
2	J	676	THR
2	J	678	ARG
2	J	679	ASP
2	J	682	PRO
2	J	688	LEU
2	J	692	ASN
2	J	697	ILE
2	J	698	PHE
2	J	702	LEU
1	K	34	ILE
1	K	78	THR
1	K	87	LYS
1	K	99	LEU
1	K	113	LYS
1	K	123	ARG
1	K	159	MET

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Mol	Chain	Res	Type
1	K	166	LYS
1	K	171	ILE
1	K	228	ARG
1	K	248	ILE
1	K	290	ARG
1	K	304	LEU
1	K	318	ARG
2	L	529	ASN
2	L	534	MET
2	L	551	SER
2	L	558	GLU
2	L	560	GLU
2	L	569	ASN
2	L	571	LYS
2	L	573	ARG
2	L	577	LYS
2	L	579	PHE
2	L	594	ARG
2	L	603	LEU
2	L	604	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	168	ASN
1	A	236	ASN
1	A	301	GLN
1	A	746	ASN
2	B	334	GLN
2	B	335	GLN
2	B	363	ASN
2	B	367	HIS
2	B	463	HIS
2	B	658	GLN
2	B	664	ASN
2	B	687	HIS
2	B	692	ASN
2	C	529	ASN
2	C	602	GLN
1	D	25	GLN
1	D	85	HIS

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Mol	Chain	Res	Type
1	D	148	GLN
1	D	155	GLN
1	D	236	ASN
1	D	239	GLN
1	D	282	ASN
1	D	303	GLN
2	E	335	GLN
2	E	363	ASN
2	E	664	ASN
2	E	687	HIS
2	E	704	ASN
2	F	602	GLN
1	G	25	GLN
1	G	168	ASN
1	G	236	ASN
1	G	301	GLN
1	G	746	ASN
2	H	529	ASN
2	H	602	GLN
2	I	335	GLN
2	I	363	ASN
2	I	367	HIS
2	I	658	GLN
2	I	664	ASN
2	I	687	HIS
2	I	692	ASN
2	I	704	ASN
2	J	335	GLN
2	J	363	ASN
2	J	664	ASN
2	J	687	HIS
2	J	692	ASN
2	J	704	ASN
1	K	25	GLN
1	K	85	HIS
1	K	148	GLN
1	K	155	GLN
1	K	236	ASN
1	K	239	GLN
1	K	282	ASN
1	K	303	GLN
2	L	602	GLN

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.