wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:03 PM BST

PDB ID	:	4UUD
EMDB ID:	:	EMD-2701
Title	:	Human dynamin 1 K44A superconstricted polymer stabilized with GTP
Authors	:	Sundborger, A.C.; Fang, S.; Heymann, J.A.; Ray, P.; Chappie, J.S.; Hinshaw, J.E.
Deposited on	:	2014-07-25
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

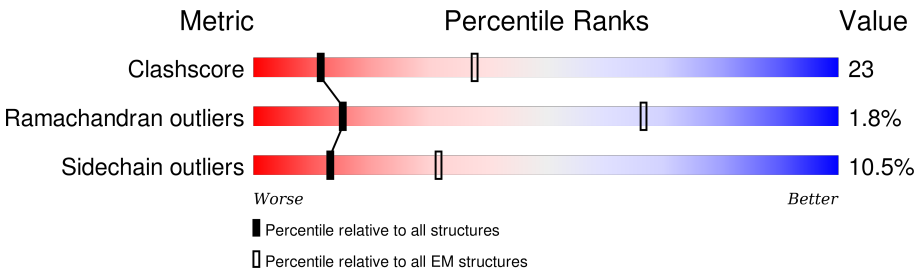
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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	25% 11% • • 61%
1	G	864	24% 13% • 62%
1	K	864	25% 11% • • 61%
2	B	864	9% 9% • • 76%
2	C	864	7% • • 87%
2	E	864	7% 10% • • 76%
2	F	864	7% • • • 87%
2	H	864	7% • • 87%

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

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20992 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
			Total	C	N	O	S		
1	A	329	2567	1615	453	489	10	0	0
1	D	337	2643	1664	466	503	10	0	0
1	G	329	2567	1615	453	489	10	0	0
1	K	337	2643	1664	466	503	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
			Total	C	N	O	S		
2	B	204	1697	1079	297	307	14	0	0
2	C	113	946	609	158	175	4	0	0
2	E	204	1697	1079	297	307	14	0	0
2	F	113	946	609	158	175	4	0	0
2	H	113	946	609	158	175	4	0	0
2	I	204	1697	1079	297	307	14	0	0
2	J	204	1697	1079	297	307	14	0	0

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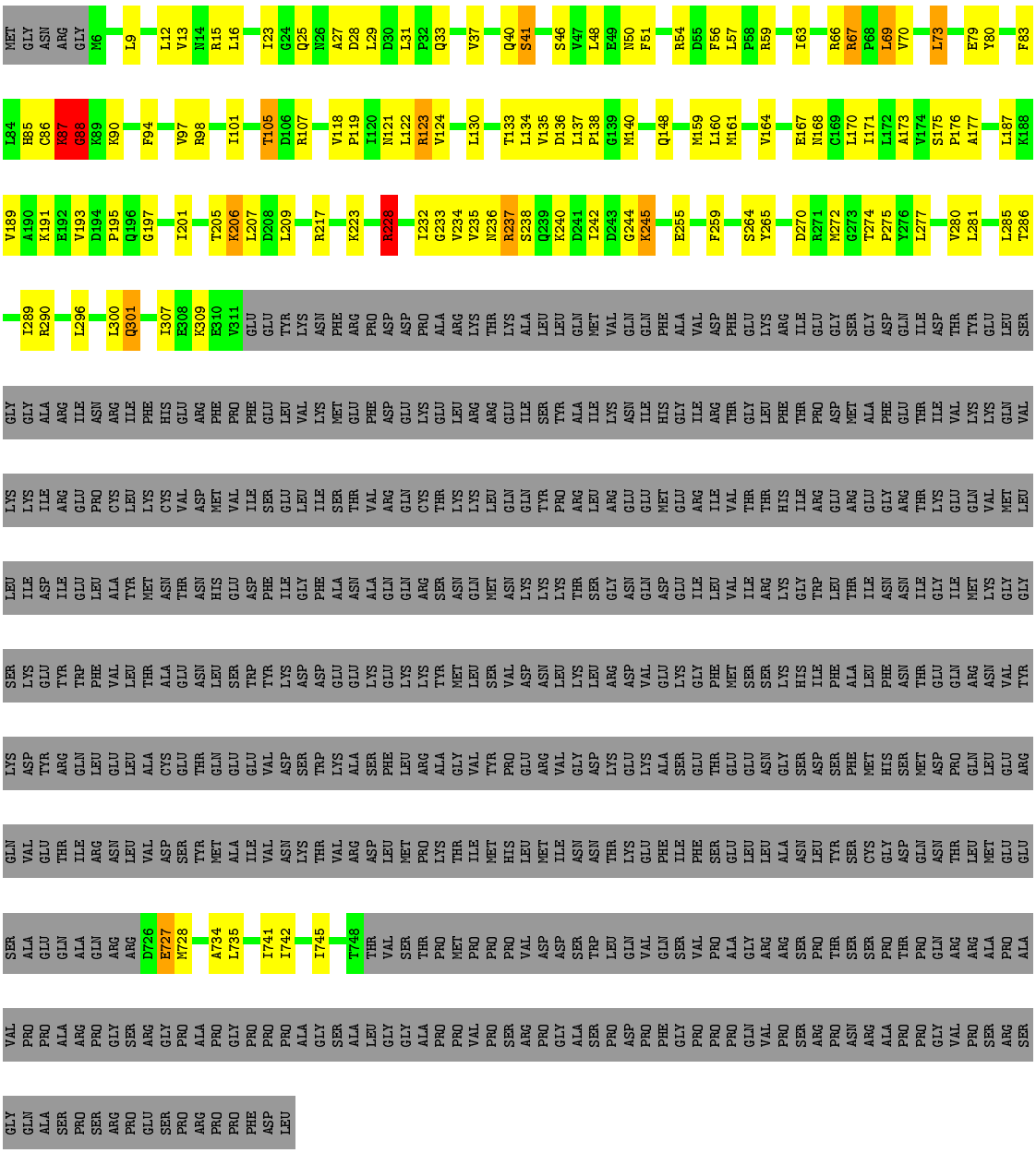
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	113	946	609	158	175	4	0	0

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.

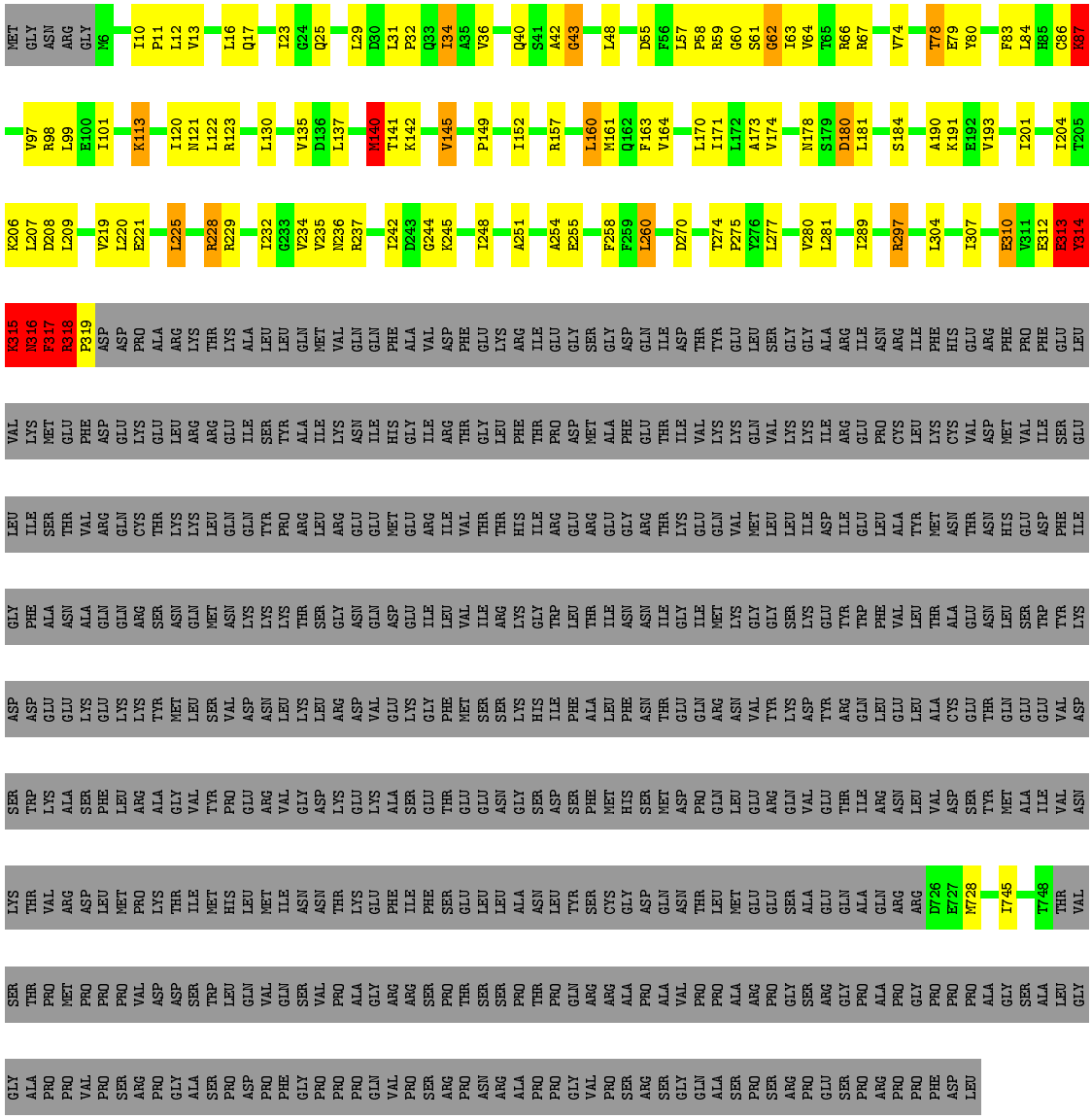
- Molecule 1: DYNAMIN-1

Chain A: 24% 13% • 62%



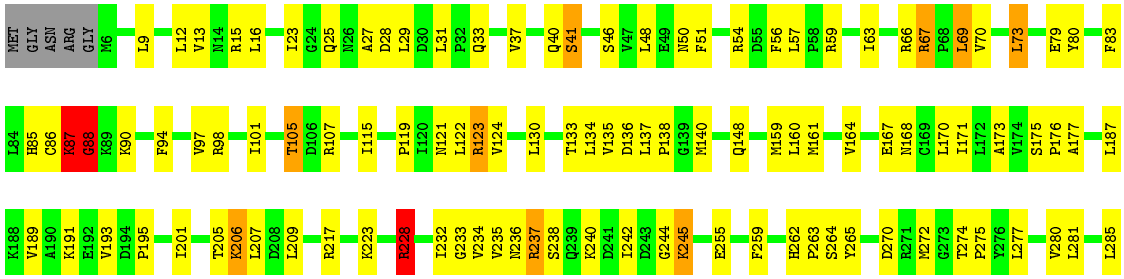
- Molecule 1: DYNAMIN-1

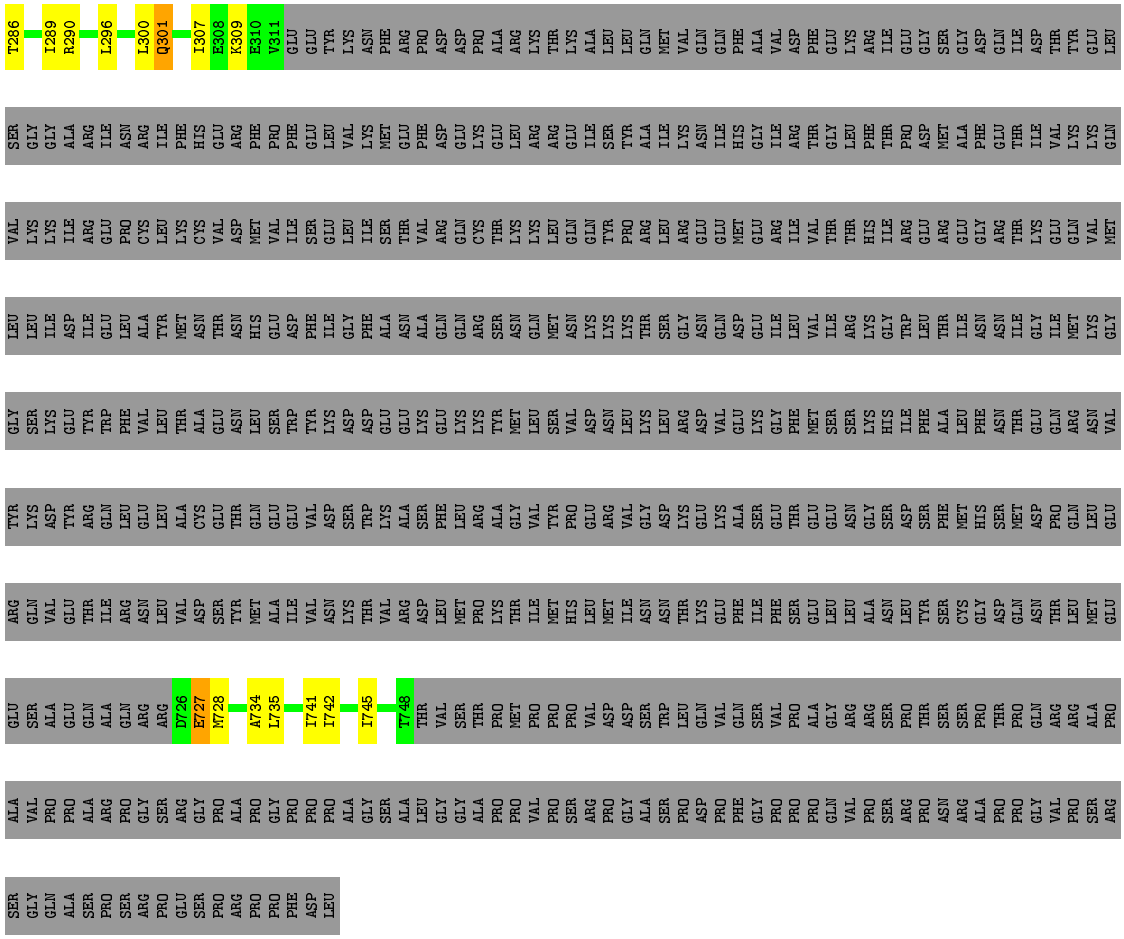
Chain D:



- Molecule 1: DYNAMIN-1

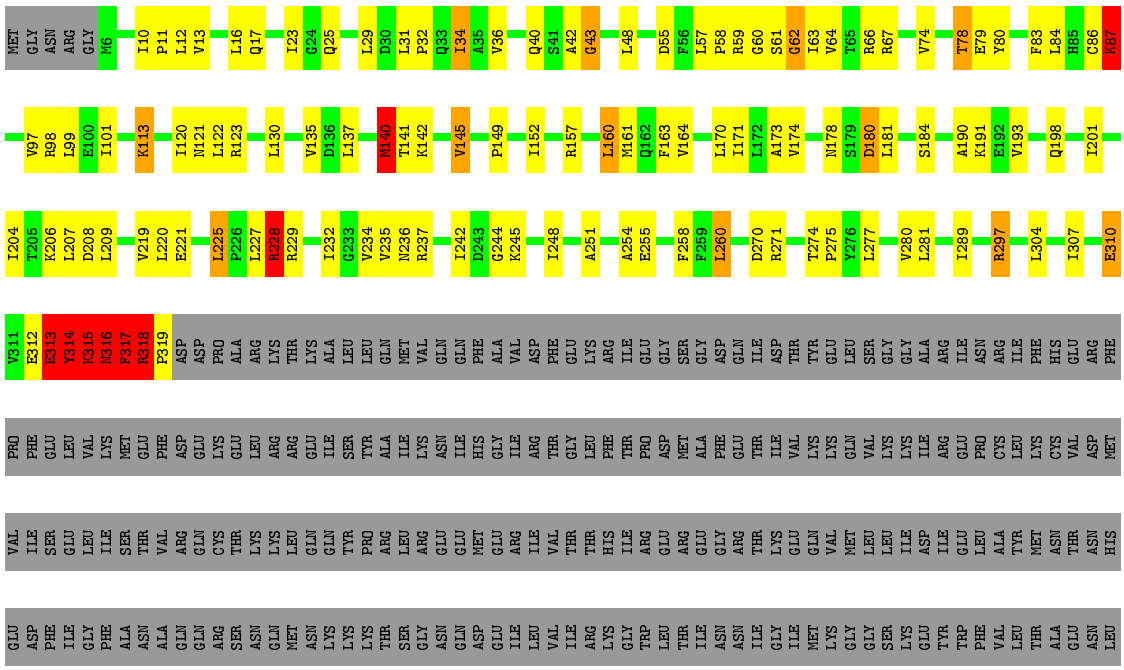
Chain G:

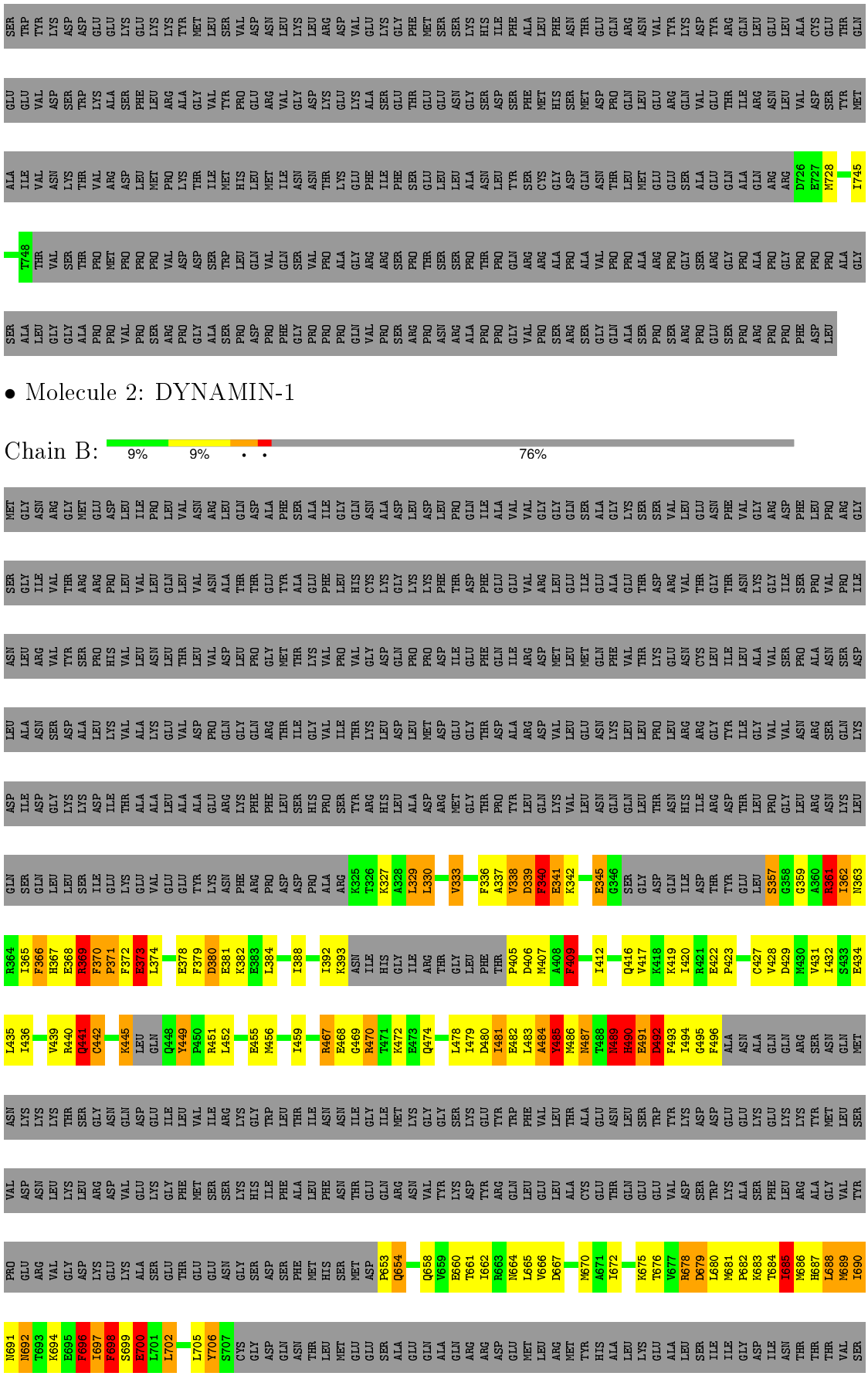




- Molecule 1: DYNAMIN-1

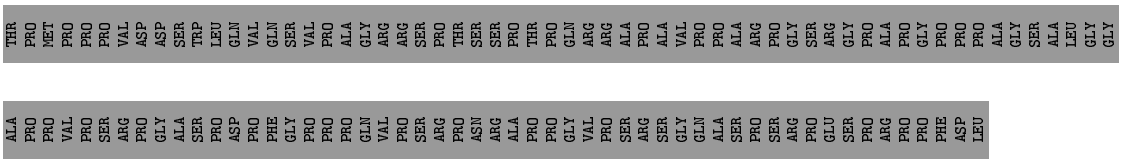
Chain K:





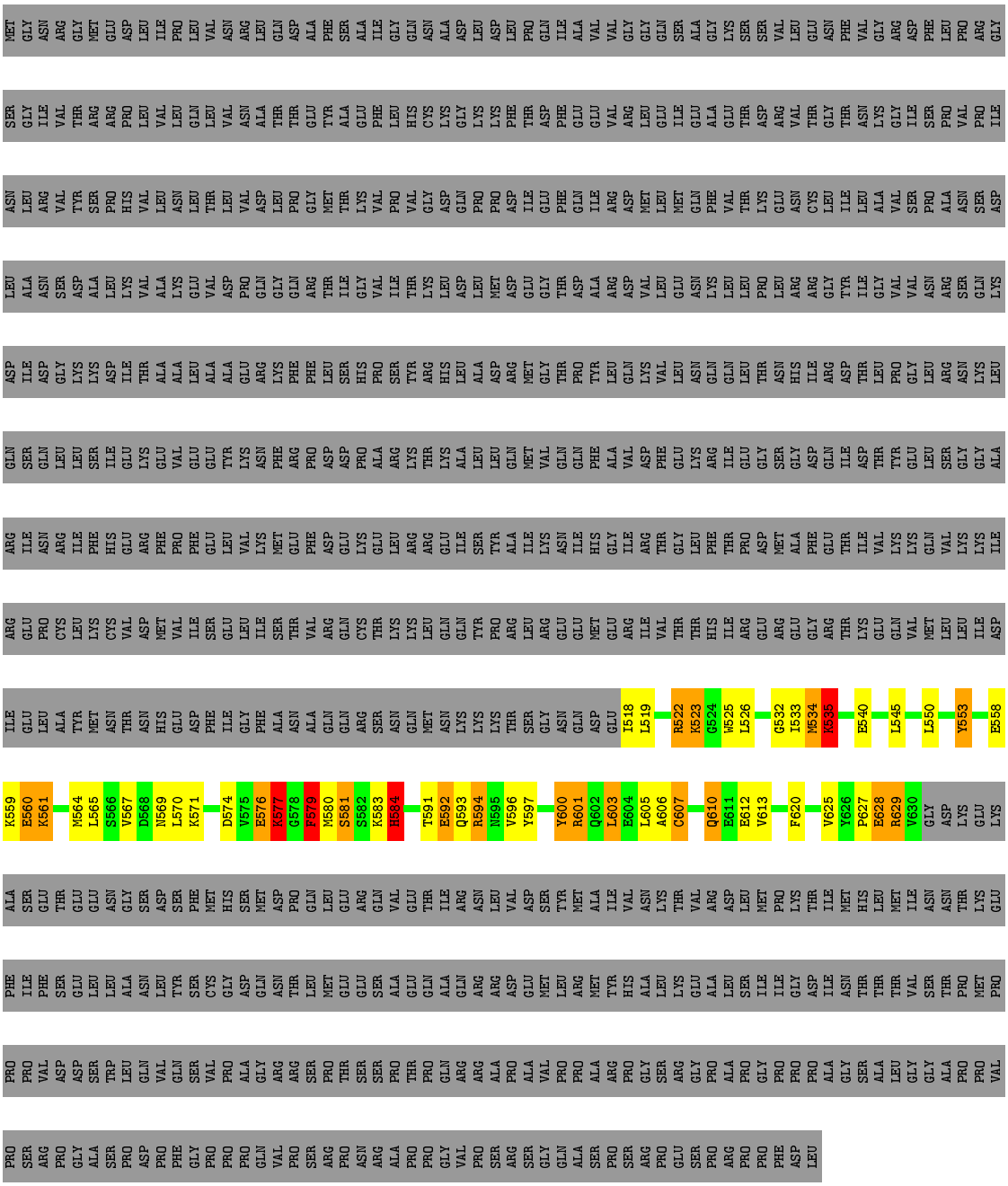
- Molecule 2: DYNAMIN-1

Chain B: 9% 9% 76%



- Molecule 2: DYNAMIN-1

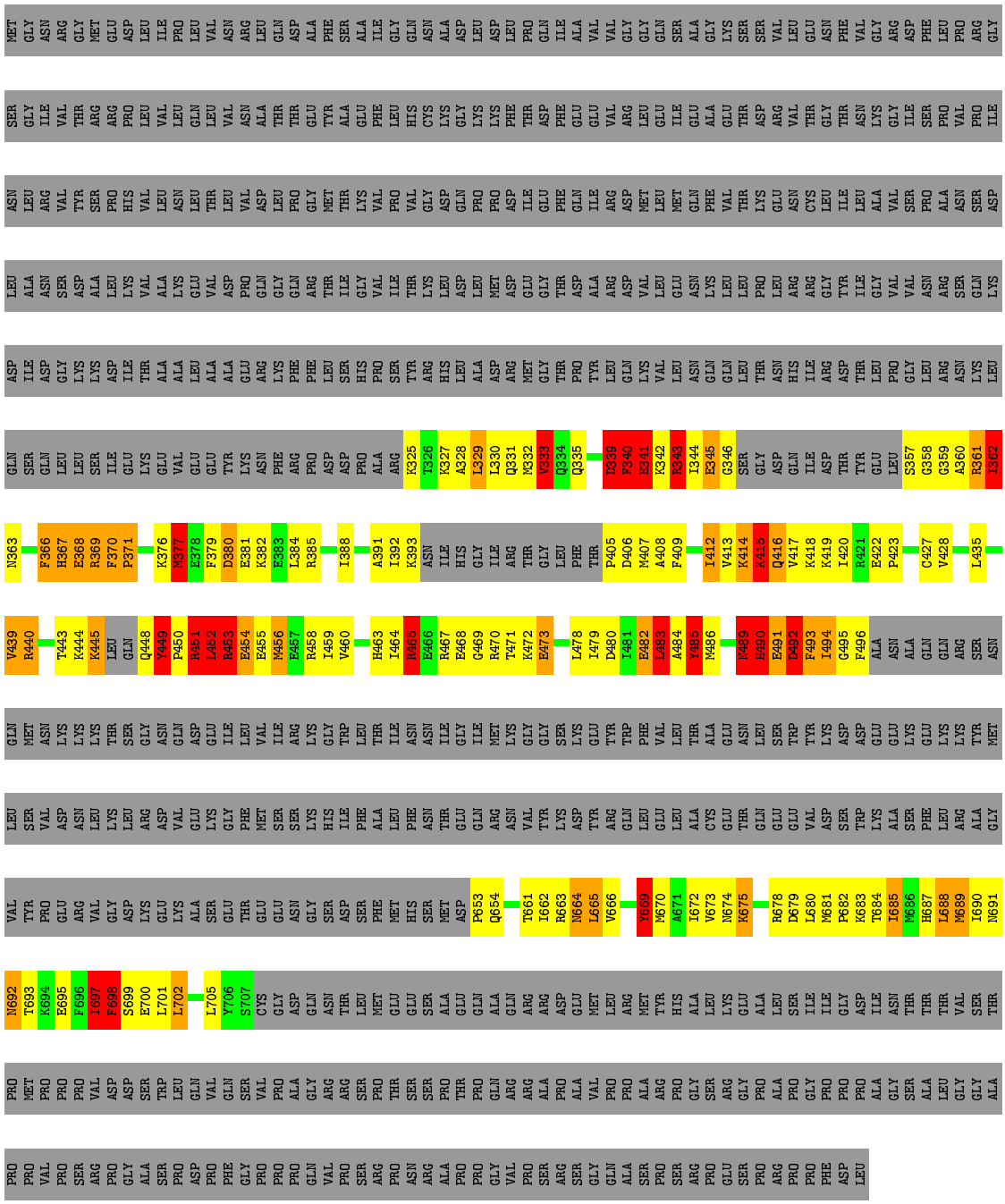
Chain C: 7% • • 87%



- Molecule 2: DYNAMIN-1

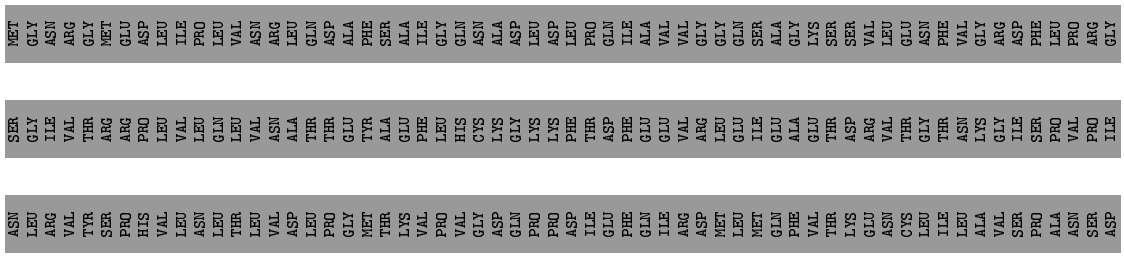
Chain E: 7% 10% • • 76%

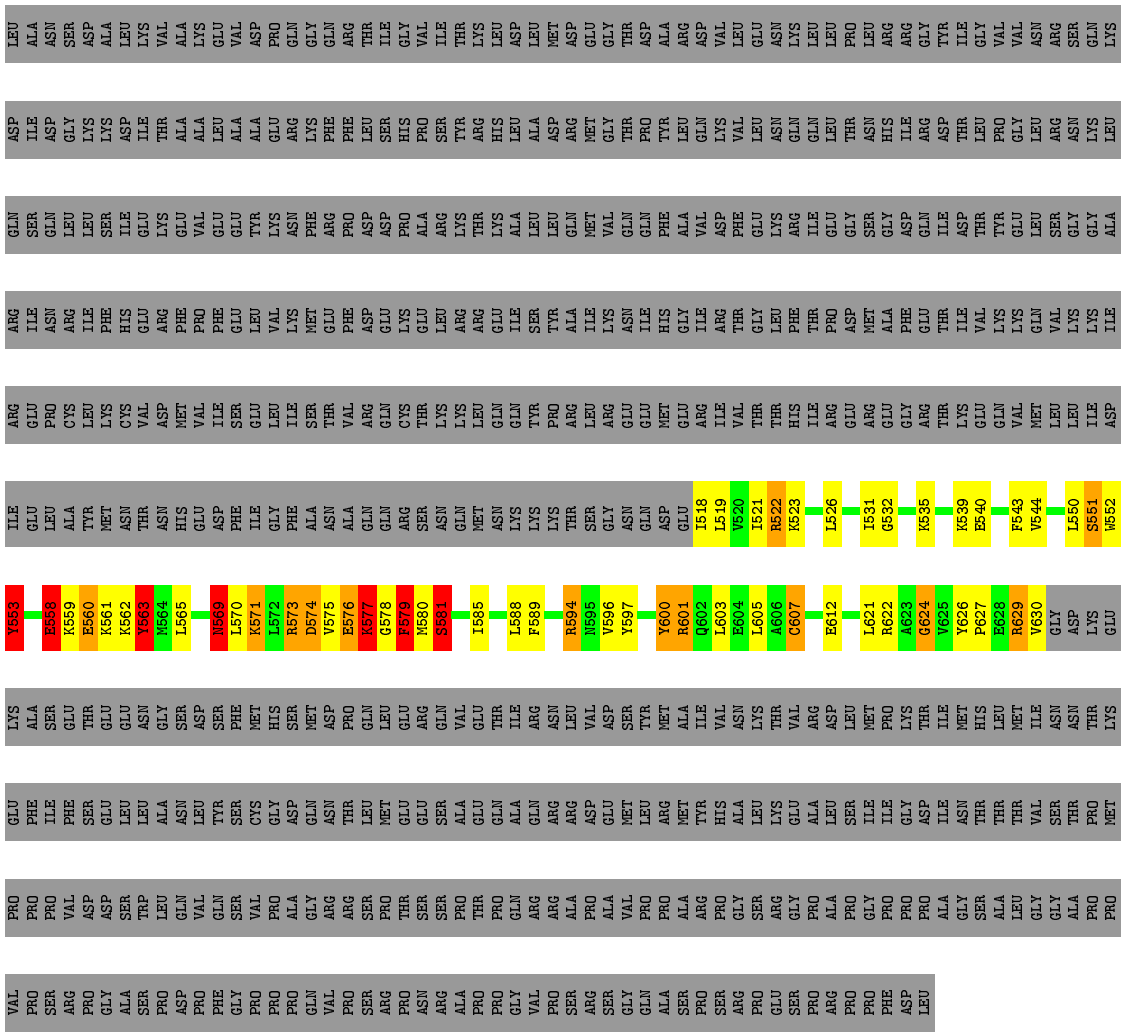
WORLDWIDE PDB PROTEIN DATA BANK
EMDataBank Unified Data Resource for 3DEM



- Molecule 2: DYNAMIN-1

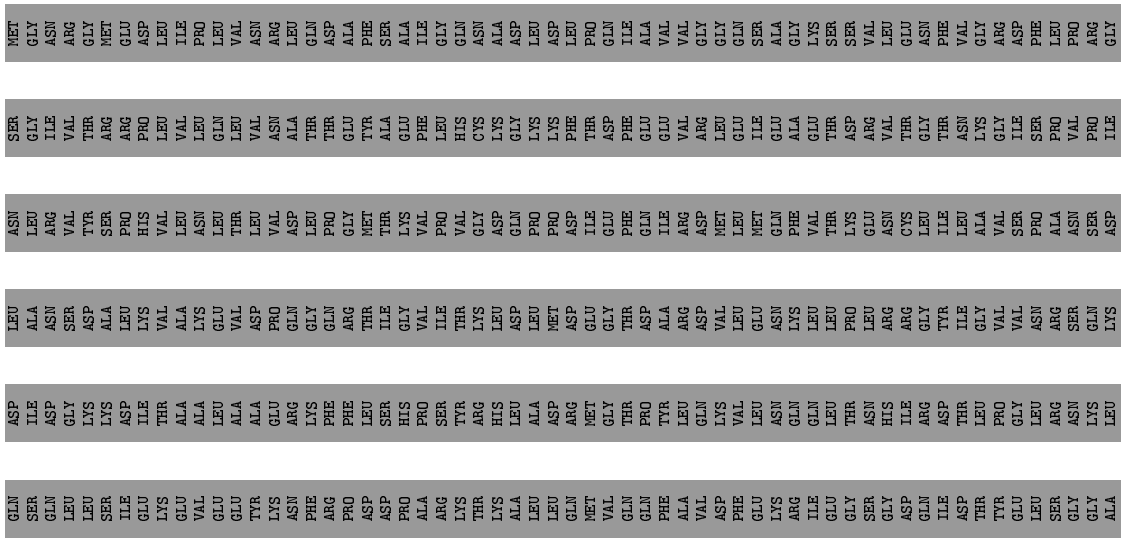
Chain F: 7% 87%





- Molecule 2: DYNAMIN-1

Chain H: 7% • • 87%



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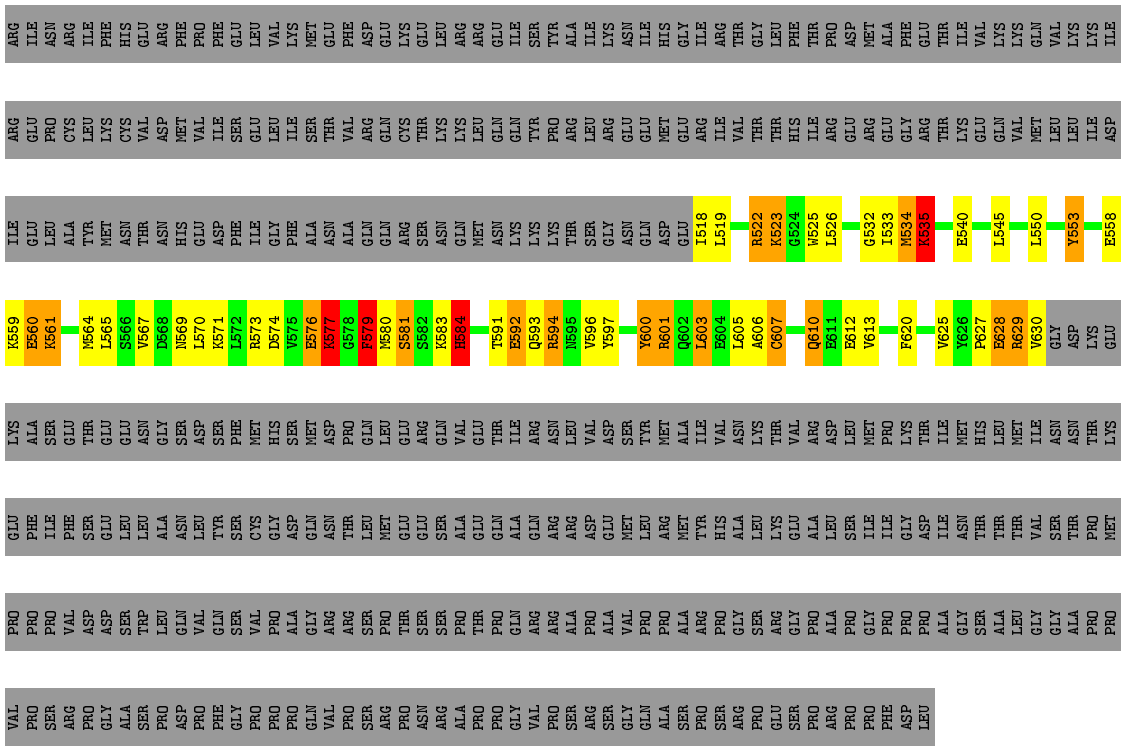
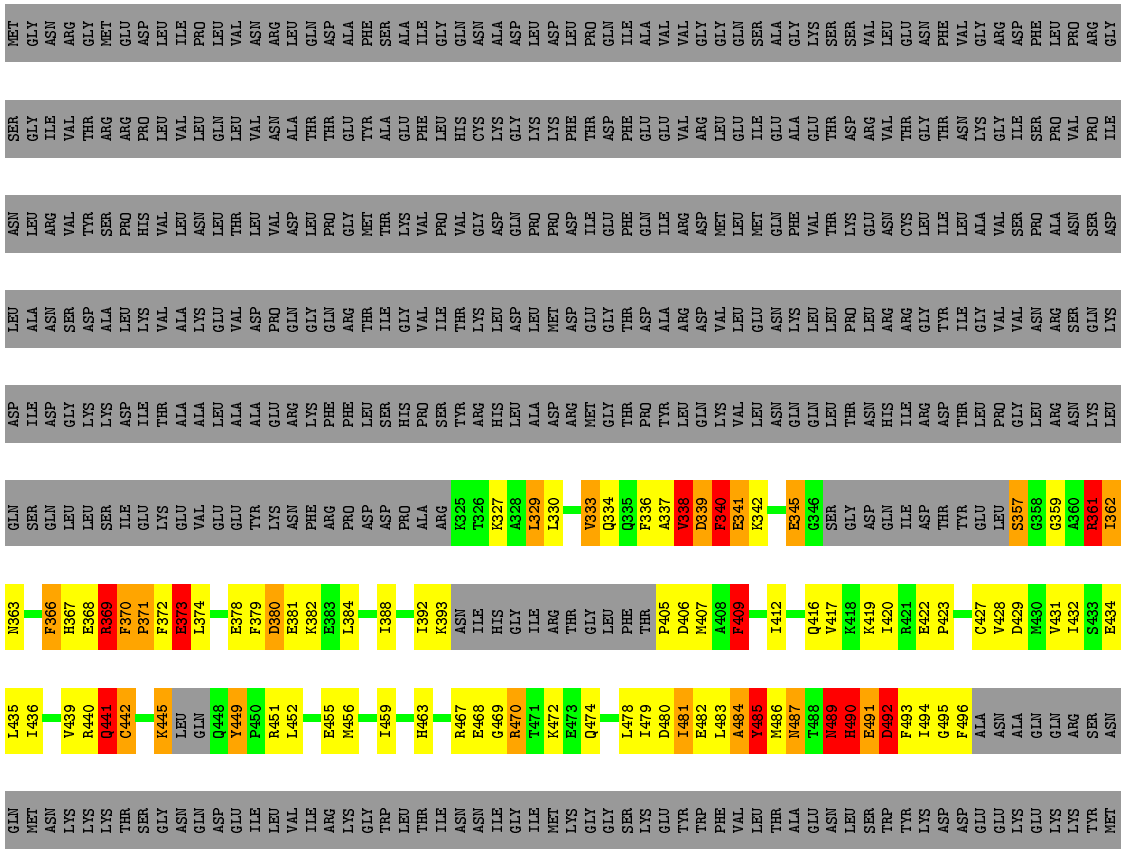


- Molecule 2: DYNAMIN-1

Chain I:



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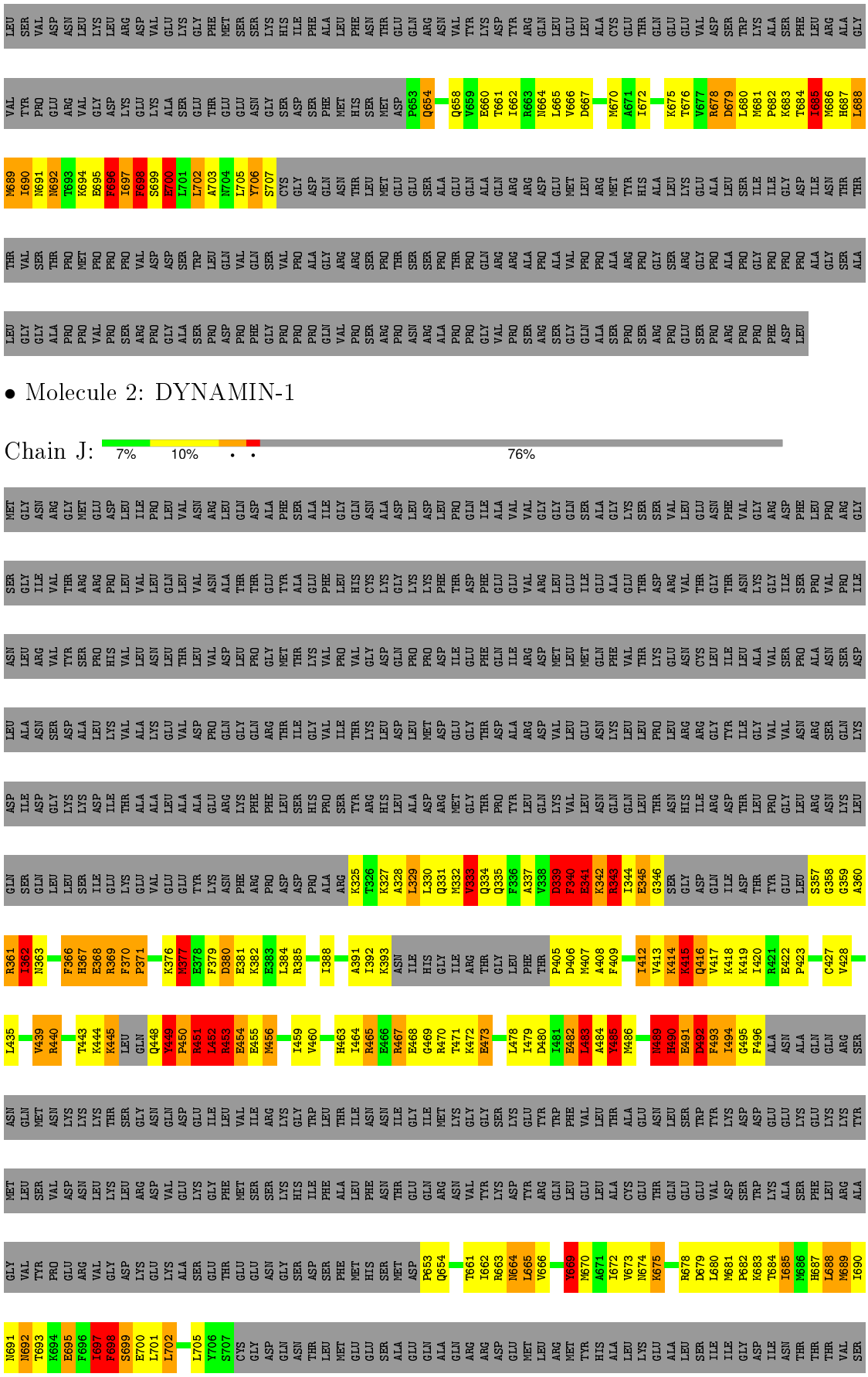

- Molecule 2: DYNAMIN-1

Chain J: 7% 10% • • 76%

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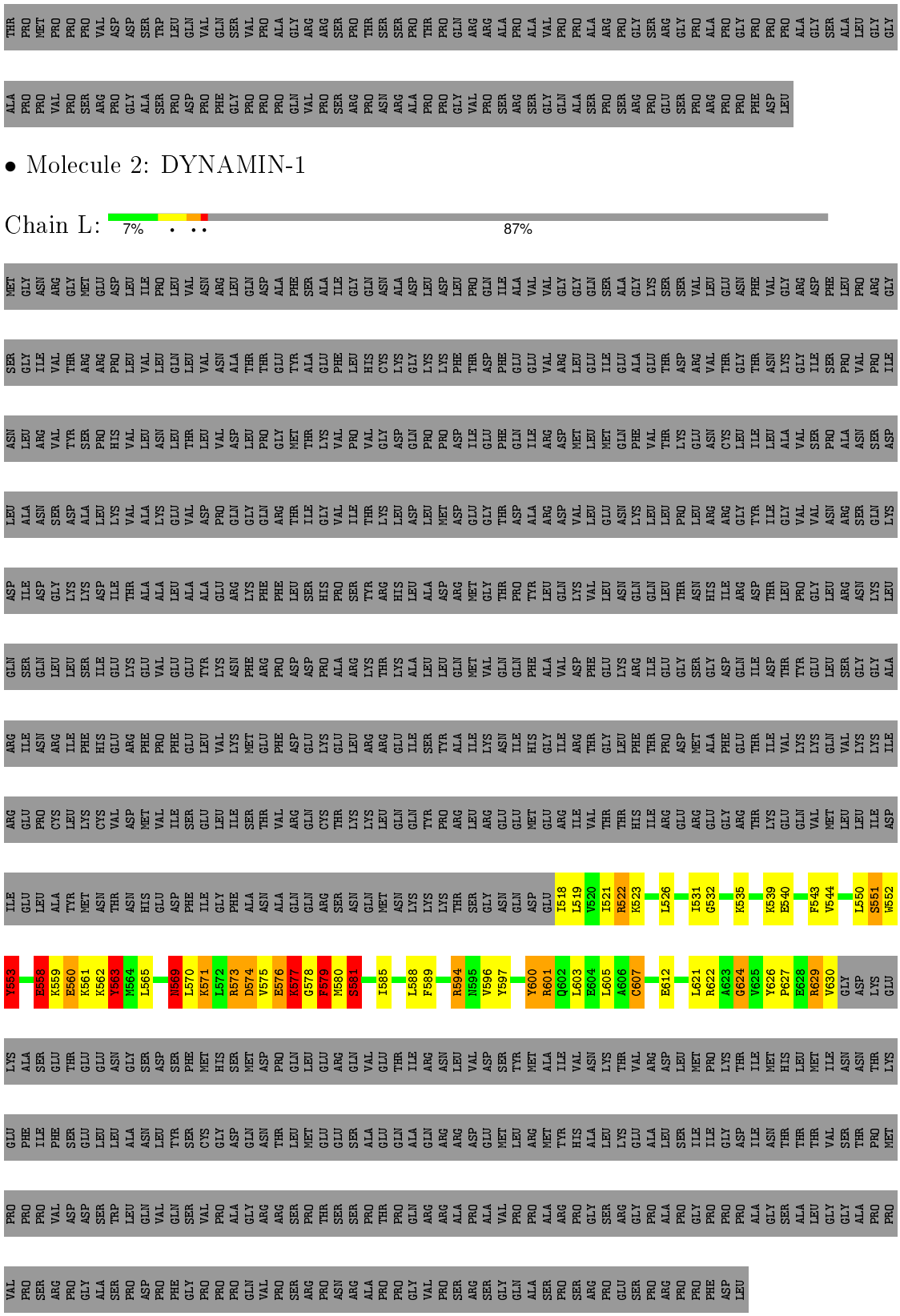

- Molecule 2: DYNAMIN-1

Chain L: 7% 87%

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 S0163 FLM	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.86	8/2683 (0.3%)	1.71	42/3630 (1.2%)
1	G	0.73	2/2604 (0.1%)	1.19	19/3524 (0.5%)
1	K	0.86	8/2683 (0.3%)	1.71	43/3630 (1.2%)
2	B	1.03	4/1718 (0.2%)	2.22	46/2293 (2.0%)
2	C	1.01	3/966 (0.3%)	1.74	34/1298 (2.6%)
2	E	1.18	6/1718 (0.3%)	2.25	67/2293 (2.9%)
2	F	1.01	4/966 (0.4%)	1.73	27/1298 (2.1%)
2	H	1.01	3/966 (0.3%)	1.74	34/1298 (2.6%)
2	I	1.03	4/1718 (0.2%)	2.22	46/2293 (2.0%)
2	J	1.18	6/1718 (0.3%)	2.25	67/2293 (2.9%)
2	L	1.02	3/966 (0.3%)	1.73	26/1298 (2.0%)
All	All	0.95	53/21310 (0.2%)	1.80	470/28672 (1.6%)

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	12
1	D	1	15
1	G	1	11
1	K	1	15
2	B	7	28
2	C	6	13
2	E	6	37
2	F	4	16
2	H	6	13
2	I	7	28
2	J	6	37
2	L	4	16
All	All	50	241

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	699	SER	CB-OG	-22.93	1.12	1.42
2	E	699	SER	CB-OG	-22.90	1.12	1.42
1	G	245	LYS	CA-CB	-9.85	1.32	1.53
1	A	245	LYS	CA-CB	-9.84	1.32	1.53
1	K	317	PHE	C-O	-9.47	1.05	1.23
1	D	317	PHE	C-O	-9.47	1.05	1.23
1	A	88	GLY	N-CA	-8.61	1.33	1.46
1	G	88	GLY	N-CA	-8.59	1.33	1.46
2	J	492	ASP	N-CA	-7.84	1.30	1.46
2	E	492	ASP	N-CA	-7.84	1.30	1.46
2	I	699	SER	CB-OG	-7.76	1.32	1.42
2	B	699	SER	CB-OG	-7.70	1.32	1.42
1	D	318	ARG	CA-C	-7.70	1.32	1.52
1	K	318	ARG	CA-C	-7.67	1.32	1.52
1	D	316	ASN	C-N	-7.36	1.17	1.34
1	K	316	ASN	C-N	-7.35	1.17	1.34
2	J	449	TYR	CD2-CE2	7.28	1.50	1.39
2	E	449	TYR	CD2-CE2	7.27	1.50	1.39
2	I	490	HIS	N-CA	-6.97	1.32	1.46
2	B	490	HIS	N-CA	-6.95	1.32	1.46
2	L	569	ASN	CA-CB	-6.91	1.35	1.53
2	F	569	ASN	CA-CB	-6.90	1.35	1.53
1	K	315	LYS	N-CA	-6.88	1.32	1.46
1	D	315	LYS	N-CA	-6.85	1.32	1.46
2	H	581	SER	N-CA	-6.75	1.32	1.46
2	C	581	SER	N-CA	-6.74	1.32	1.46
2	E	368	GLU	CD-OE1	-6.64	1.18	1.25
2	J	368	GLU	CD-OE1	-6.64	1.18	1.25
1	D	313	GLU	C-O	-6.54	1.10	1.23
1	K	313	GLU	C-O	-6.54	1.10	1.23
1	D	315	LYS	C-N	-6.44	1.19	1.34
1	K	315	LYS	C-N	-6.43	1.19	1.34
1	K	316	ASN	C-O	6.33	1.35	1.23
1	D	316	ASN	C-O	6.31	1.35	1.23
2	C	523	LYS	N-CA	-6.21	1.33	1.46
2	H	523	LYS	N-CA	-6.18	1.33	1.46
2	F	581	SER	N-CA	-6.11	1.34	1.46
2	L	581	SER	N-CA	-6.10	1.34	1.46
2	J	366	PHE	CA-CB	-5.66	1.41	1.53
2	E	366	PHE	CA-CB	-5.66	1.41	1.53
2	E	492	ASP	C-O	-5.47	1.12	1.23
2	J	492	ASP	C-O	-5.47	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	561	LYS	N-CA	-5.47	1.35	1.46
2	C	561	LYS	N-CA	-5.44	1.35	1.46
2	L	574	ASP	CA-CB	-5.30	1.42	1.53
2	F	574	ASP	CA-CB	-5.28	1.42	1.53
2	B	489	ASN	C-O	5.10	1.33	1.23
2	I	489	ASN	C-O	5.08	1.32	1.23
2	B	366	PHE	CA-CB	-5.04	1.42	1.53
1	D	245	LYS	CA-CB	-5.03	1.42	1.53
2	I	366	PHE	CA-CB	-5.02	1.43	1.53
2	F	561	LYS	N-CA	-5.01	1.36	1.46
1	K	245	LYS	CA-CB	-5.01	1.43	1.53

All (470) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	492	ASP	CB-CG-OD2	50.51	163.76	118.30
2	I	492	ASP	CB-CG-OD2	50.42	163.68	118.30
2	I	492	ASP	CB-CG-OD1	-45.51	77.34	118.30
2	B	492	ASP	CB-CG-OD1	-45.47	77.37	118.30
1	K	318	ARG	NE-CZ-NH2	39.72	140.16	120.30
1	D	318	ARG	NE-CZ-NH2	39.56	140.08	120.30
2	E	449	TYR	CB-CG-CD1	28.38	138.03	121.00
2	J	449	TYR	CB-CG-CD1	28.27	137.96	121.00
2	J	449	TYR	CZ-CE2-CD2	-27.66	94.91	119.80
2	E	449	TYR	CZ-CE2-CD2	-27.64	94.93	119.80
2	E	492	ASP	CB-CG-OD1	-24.62	96.14	118.30
2	J	492	ASP	CB-CG-OD1	-24.60	96.16	118.30
2	E	449	TYR	CB-CG-CD2	-24.55	106.27	121.00
2	J	449	TYR	CB-CG-CD2	-24.48	106.31	121.00
2	J	343	ARG	NE-CZ-NH1	-23.89	108.35	120.30
2	E	343	ARG	NE-CZ-NH1	-23.84	108.38	120.30
2	J	492	ASP	CB-CG-OD2	21.67	137.81	118.30
2	E	492	ASP	CB-CG-OD2	21.65	137.79	118.30
1	K	318	ARG	NH1-CZ-NH2	-18.77	98.76	119.40
1	D	318	ARG	NH1-CZ-NH2	-18.75	98.78	119.40
2	B	369	ARG	NE-CZ-NH1	-18.16	111.22	120.30
2	I	369	ARG	NE-CZ-NH1	-18.14	111.23	120.30
1	D	315	LYS	C-N-CA	18.06	166.84	121.70
1	K	315	LYS	C-N-CA	18.04	166.80	121.70
1	K	317	PHE	O-C-N	-17.44	94.80	122.70
1	D	317	PHE	O-C-N	-17.43	94.81	122.70
1	K	316	ASN	O-C-N	-17.34	94.96	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	316	ASN	O-C-N	-17.33	94.97	122.70
1	K	316	ASN	C-N-CA	16.52	162.99	121.70
1	D	316	ASN	C-N-CA	16.51	162.98	121.70
1	K	315	LYS	O-C-N	-16.32	96.58	122.70
1	D	315	LYS	O-C-N	-16.32	96.59	122.70
1	K	315	LYS	CA-C-N	14.74	149.63	117.20
1	D	315	LYS	CA-C-N	14.74	149.62	117.20
1	K	314	TYR	C-N-CA	14.04	156.81	121.70
1	D	314	TYR	C-N-CA	14.02	156.75	121.70
2	E	699	SER	N-CA-CB	-13.75	89.88	110.50
2	J	699	SER	N-CA-CB	-13.75	89.88	110.50
1	K	316	ASN	CA-C-N	13.39	146.67	117.20
1	D	316	ASN	CA-C-N	13.38	146.64	117.20
1	K	313	GLU	O-C-N	-13.28	101.45	122.70
1	D	313	GLU	O-C-N	-13.25	101.50	122.70
2	F	553	TYR	CB-CG-CD2	-13.01	113.19	121.00
2	L	553	TYR	CB-CG-CD2	-12.99	113.21	121.00
2	L	553	TYR	CB-CG-CD1	12.78	128.67	121.00
2	E	449	TYR	CE1-CZ-CE2	-12.78	99.36	119.80
2	F	553	TYR	CB-CG-CD1	12.78	128.67	121.00
1	K	314	TYR	O-C-N	-12.78	102.26	122.70
1	D	317	PHE	CA-C-N	12.77	145.30	117.20
1	K	317	PHE	CA-C-N	12.76	145.26	117.20
2	J	449	TYR	CE1-CZ-CE2	-12.75	99.40	119.80
1	D	314	TYR	O-C-N	-12.73	102.33	122.70
2	J	485	TYR	CB-CG-CD2	-12.73	113.36	121.00
2	E	485	TYR	CB-CG-CD2	-12.72	113.37	121.00
2	J	368	GLU	N-CA-CB	12.71	133.47	110.60
2	E	368	GLU	N-CA-CB	12.69	133.44	110.60
1	K	228	ARG	CB-CG-CD	12.14	143.16	111.60
1	D	228	ARG	CB-CG-CD	12.12	143.10	111.60
2	I	366	PHE	N-CA-CB	11.65	131.57	110.60
2	B	366	PHE	N-CA-CB	11.58	131.45	110.60
2	C	522	ARG	C-N-CA	11.39	150.18	121.70
2	H	522	ARG	C-N-CA	11.39	150.17	121.70
2	B	449	TYR	CB-CG-CD2	-11.31	114.21	121.00
1	K	87	LYS	CG-CD-CE	11.30	145.81	111.90
1	D	87	LYS	CG-CD-CE	11.29	145.76	111.90
2	I	449	TYR	CB-CG-CD2	-11.24	114.25	121.00
2	C	523	LYS	N-CA-CB	11.21	130.77	110.60
2	H	523	LYS	N-CA-CB	11.20	130.76	110.60
2	F	569	ASN	CA-CB-CG	11.15	137.93	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	569	ASN	CA-CB-CG	11.14	137.91	113.40
2	J	342	LYS	CB-CG-CD	10.62	139.20	111.60
2	E	342	LYS	CB-CG-CD	10.61	139.18	111.60
2	E	485	TYR	CG-CD2-CE2	-10.53	112.88	121.30
2	J	485	TYR	CG-CD2-CE2	-10.49	112.91	121.30
1	D	145	VAL	CG1-CB-CG2	-10.43	94.21	110.90
1	K	145	VAL	CG1-CB-CG2	-10.42	94.23	110.90
2	H	592	GLU	CG-CD-OE2	-10.36	97.59	118.30
2	C	592	GLU	CG-CD-OE2	-10.35	97.59	118.30
2	J	366	PHE	N-CA-CB	10.24	129.04	110.60
2	E	366	PHE	N-CA-CB	10.22	129.00	110.60
2	C	592	GLU	OE1-CD-OE2	10.00	135.30	123.30
2	H	592	GLU	OE1-CD-OE2	9.99	135.29	123.30
1	A	228	ARG	CB-CG-CD	9.86	137.22	111.60
1	G	228	ARG	CB-CG-CD	9.81	137.12	111.60
2	C	580	MET	C-N-CA	9.77	146.12	121.70
2	H	580	MET	C-N-CA	9.76	146.09	121.70
2	B	441	GLN	N-CA-CB	9.74	128.13	110.60
2	I	441	GLN	N-CA-CB	9.73	128.11	110.60
2	E	449	TYR	CG-CD2-CE2	-9.60	113.62	121.30
2	J	449	TYR	CG-CD2-CE2	-9.58	113.63	121.30
2	I	700	GLU	N-CA-CB	9.46	127.62	110.60
2	B	700	GLU	N-CA-CB	9.44	127.60	110.60
1	K	318	ARG	CA-C-O	-9.34	100.48	120.10
1	D	318	ARG	CA-C-O	-9.33	100.50	120.10
2	B	489	ASN	O-C-N	-9.32	107.79	122.70
2	I	489	ASN	O-C-N	-9.29	107.84	122.70
1	G	67	ARG	NE-CZ-NH1	-9.27	115.66	120.30
1	A	67	ARG	NE-CZ-NH1	-9.27	115.67	120.30
2	J	454	GLU	OE1-CD-OE2	9.26	134.41	123.30
2	E	454	GLU	OE1-CD-OE2	9.26	134.41	123.30
2	E	695	GLU	OE1-CD-OE2	-9.10	112.38	123.30
1	D	318	ARG	CG-CD-NE	9.09	130.89	111.80
1	G	67	ARG	NE-CZ-NH2	9.09	124.85	120.30
1	A	67	ARG	NE-CZ-NH2	9.09	124.84	120.30
1	K	318	ARG	CG-CD-NE	9.09	130.89	111.80
2	J	695	GLU	OE1-CD-OE2	-9.07	112.42	123.30
2	B	449	TYR	CB-CG-CD1	9.04	126.42	121.00
2	I	449	TYR	CB-CG-CD1	9.02	126.41	121.00
2	B	440	ARG	C-N-CA	8.89	143.92	121.70
2	I	440	ARG	C-N-CA	8.88	143.91	121.70
2	I	706	TYR	CB-CG-CD1	8.87	126.32	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	140	MET	CA-CB-CG	8.84	128.32	113.30
1	K	140	MET	CA-CB-CG	8.83	128.32	113.30
1	A	245	LYS	CA-CB-CG	8.83	132.82	113.40
1	G	245	LYS	CA-CB-CG	8.82	132.81	113.40
2	B	706	TYR	CB-CG-CD1	8.75	126.25	121.00
2	L	580	MET	C-N-CA	8.68	143.40	121.70
2	F	580	MET	C-N-CA	8.66	143.34	121.70
2	F	574	ASP	CB-CG-OD1	-8.57	110.58	118.30
1	A	123	ARG	NE-CZ-NH1	-8.57	116.01	120.30
1	G	123	ARG	NE-CZ-NH1	-8.53	116.03	120.30
2	L	574	ASP	CB-CG-OD1	-8.52	110.64	118.30
2	I	706	TYR	CB-CG-CD2	-8.50	115.90	121.00
2	J	453	ARG	CG-CD-NE	-8.48	93.98	111.80
1	K	314	TYR	CA-C-N	8.48	135.87	117.20
1	A	87	LYS	C-N-CA	8.48	140.11	122.30
2	E	453	ARG	CG-CD-NE	-8.48	94.00	111.80
1	D	314	TYR	CA-C-N	8.46	135.81	117.20
1	G	87	LYS	C-N-CA	8.45	140.04	122.30
2	B	706	TYR	CB-CG-CD2	-8.42	115.95	121.00
2	H	629	ARG	NE-CZ-NH1	-8.35	116.13	120.30
1	D	317	PHE	N-CA-C	8.32	133.47	111.00
1	K	317	PHE	N-CA-C	8.31	133.44	111.00
2	B	706	TYR	N-CA-CB	8.29	125.52	110.60
2	I	706	TYR	N-CA-CB	8.26	125.46	110.60
2	C	629	ARG	NE-CZ-NH1	-8.22	116.19	120.30
2	E	439	VAL	CG1-CB-CG2	-8.20	97.78	110.90
2	J	439	VAL	CG1-CB-CG2	-8.20	97.79	110.90
2	J	484	ALA	N-CA-CB	8.16	121.52	110.10
2	E	484	ALA	N-CA-CB	8.15	121.51	110.10
2	J	460	VAL	CA-CB-CG2	-8.15	98.68	110.90
2	C	591	THR	C-N-CA	8.12	142.00	121.70
2	E	460	VAL	CA-CB-CG2	-8.12	98.72	110.90
2	H	591	THR	C-N-CA	8.11	141.99	121.70
2	E	485	TYR	CB-CG-CD1	8.11	125.86	121.00
2	J	485	TYR	CB-CG-CD1	8.11	125.86	121.00
1	A	245	LYS	CB-CA-C	8.10	126.60	110.40
1	G	245	LYS	CB-CA-C	8.10	126.60	110.40
1	K	316	ASN	N-CA-C	8.07	132.80	111.00
1	D	316	ASN	N-CA-C	8.06	132.78	111.00
2	F	522	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	D	228	ARG	CG-CD-NE	8.04	128.68	111.80
2	L	522	ARG	NE-CZ-NH1	-8.03	116.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	228	ARG	CG-CD-NE	8.03	128.66	111.80
1	D	260	LEU	N-CA-CB	8.02	126.44	110.40
2	C	535	LYS	CA-CB-CG	7.99	130.98	113.40
2	H	535	LYS	CA-CB-CG	7.98	130.96	113.40
1	K	260	LEU	N-CA-CB	7.98	126.37	110.40
2	J	449	TYR	CE1-CZ-OH	7.97	141.61	120.10
2	E	449	TYR	CE1-CZ-OH	7.96	141.59	120.10
2	F	558	GLU	CA-CB-CG	7.88	130.73	113.40
2	L	558	GLU	CA-CB-CG	7.86	130.69	113.40
2	H	591	THR	O-C-N	-7.86	110.13	122.70
2	C	591	THR	O-C-N	-7.85	110.14	122.70
1	D	310	GLU	O-C-N	-7.81	110.20	122.70
1	K	310	GLU	O-C-N	-7.80	110.22	122.70
2	C	577	LYS	C-N-CA	7.79	138.65	122.30
2	H	577	LYS	C-N-CA	7.76	138.59	122.30
2	E	456	MET	CG-SD-CE	7.74	112.58	100.20
1	K	87	LYS	CB-CG-CD	-7.72	91.53	111.60
1	D	87	LYS	CB-CG-CD	-7.71	91.55	111.60
2	J	456	MET	CG-SD-CE	7.70	112.53	100.20
1	G	88	GLY	N-CA-C	7.68	132.31	113.10
2	F	574	ASP	N-CA-CB	7.67	124.40	110.60
1	A	88	GLY	N-CA-C	7.67	132.26	113.10
2	L	574	ASP	N-CA-CB	7.66	124.39	110.60
2	H	560	GLU	C-N-CA	7.65	140.83	121.70
2	C	560	GLU	C-N-CA	7.64	140.80	121.70
2	E	695	GLU	CG-CD-OE1	7.63	133.55	118.30
2	J	695	GLU	CG-CD-OE1	7.62	133.55	118.30
2	C	592	GLU	N-CA-CB	7.61	124.30	110.60
2	B	698	PHE	CB-CG-CD2	-7.61	115.47	120.80
2	H	592	GLU	N-CA-CB	7.61	124.30	110.60
2	H	580	MET	CA-CB-CG	7.60	126.22	113.30
2	C	580	MET	CA-CB-CG	7.59	126.21	113.30
2	I	698	PHE	CB-CG-CD2	-7.55	115.51	120.80
2	F	569	ASN	CB-CA-C	7.48	125.36	110.40
2	B	338	VAL	C-N-CA	7.47	140.38	121.70
2	L	560	GLU	C-N-CA	7.47	140.37	121.70
2	I	338	VAL	C-N-CA	7.45	140.33	121.70
2	L	569	ASN	CB-CA-C	7.45	125.31	110.40
2	B	492	ASP	OD1-CG-OD2	-7.42	109.20	123.30
2	F	560	GLU	C-N-CA	7.41	140.22	121.70
2	E	343	ARG	CG-CD-NE	7.39	127.31	111.80
2	J	343	ARG	CG-CD-NE	7.38	127.30	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	610	GLN	O-C-N	-7.38	110.89	122.70
2	E	340	PHE	CB-CG-CD1	-7.38	115.64	120.80
1	G	73	LEU	N-CA-CB	7.38	125.15	110.40
2	I	492	ASP	OD1-CG-OD2	-7.37	109.30	123.30
1	A	73	LEU	N-CA-CB	7.37	125.14	110.40
1	D	317	PHE	CB-CG-CD1	-7.37	115.64	120.80
2	C	610	GLN	O-C-N	-7.35	110.94	122.70
2	E	489	ASN	O-C-N	-7.33	110.97	122.70
2	J	489	ASN	O-C-N	-7.33	110.97	122.70
2	F	569	ASN	CB-CG-OD1	7.32	136.24	121.60
2	L	569	ASN	CB-CG-OD1	7.31	136.23	121.60
2	H	601	ARG	C-N-CA	7.31	139.98	121.70
2	J	340	PHE	CB-CG-CD1	-7.31	115.69	120.80
1	K	317	PHE	CB-CG-CD1	-7.30	115.69	120.80
2	E	377	MET	N-CA-CB	7.29	123.73	110.60
2	J	377	MET	N-CA-CB	7.29	123.72	110.60
2	C	601	ARG	C-N-CA	7.28	139.90	121.70
2	E	473	GLU	CA-CB-CG	7.25	129.35	113.40
1	A	87	LYS	CG-CD-CE	7.24	133.60	111.90
1	G	87	LYS	CG-CD-CE	7.23	133.60	111.90
2	J	473	GLU	CA-CB-CG	7.23	129.31	113.40
2	I	699	SER	C-N-CA	7.20	139.71	121.70
2	B	699	SER	C-N-CA	7.19	139.68	121.70
2	E	341	GLU	N-CA-CB	7.13	123.44	110.60
2	J	341	GLU	N-CA-CB	7.13	123.43	110.60
2	L	563	TYR	N-CA-CB	7.13	123.43	110.60
2	F	563	TYR	N-CA-CB	7.12	123.42	110.60
2	L	577	LYS	C-N-CA	7.12	137.25	122.30
2	I	485	TYR	CG-CD2-CE2	-7.11	115.61	121.30
2	E	452	LEU	N-CA-CB	7.11	124.62	110.40
2	F	577	LYS	C-N-CA	7.11	137.24	122.30
2	J	452	LEU	N-CA-CB	7.11	124.62	110.40
1	D	180	ASP	N-CA-CB	7.10	123.39	110.60
1	K	180	ASP	N-CA-CB	7.10	123.38	110.60
2	I	440	ARG	O-C-N	-7.09	111.35	122.70
2	B	485	TYR	CG-CD2-CE2	-7.08	115.63	121.30
2	B	440	ARG	O-C-N	-7.08	111.38	122.70
2	J	342	LYS	CA-CB-CG	7.03	128.86	113.40
2	E	342	LYS	CA-CB-CG	7.02	128.85	113.40
1	D	318	ARG	CA-C-N	7.00	136.71	117.10
1	K	318	ARG	CA-C-N	7.00	136.70	117.10
2	F	629	ARG	NE-CZ-NH2	-7.00	116.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	601	ARG	C-N-CA	6.97	139.12	121.70
2	L	629	ARG	NE-CZ-NH2	-6.94	116.83	120.30
2	F	601	ARG	C-N-CA	6.94	139.05	121.70
2	I	373	GLU	O-C-N	-6.90	111.66	122.70
2	B	373	GLU	O-C-N	-6.88	111.69	122.70
2	B	361	ARG	CG-CD-NE	6.86	126.21	111.80
2	I	361	ARG	CG-CD-NE	6.86	126.20	111.80
2	L	569	ASN	CB-CG-ND2	-6.84	100.29	116.70
2	F	569	ASN	CB-CG-ND2	-6.83	100.32	116.70
2	B	487	ASN	CB-CG-ND2	-6.82	100.34	116.70
2	I	487	ASN	CB-CG-ND2	-6.80	100.38	116.70
2	E	485	TYR	CE1-CZ-CE2	-6.77	108.97	119.80
2	J	485	TYR	CE1-CZ-CE2	-6.76	108.98	119.80
1	D	317	PHE	CZ-CE2-CD2	-6.74	112.01	120.10
2	F	581	SER	N-CA-CB	6.74	120.61	110.50
1	K	317	PHE	CZ-CE2-CD2	-6.71	112.04	120.10
2	L	581	SER	N-CA-CB	6.71	120.56	110.50
2	B	678	ARG	NE-CZ-NH2	6.69	123.64	120.30
2	J	341	GLU	CG-CD-OE2	-6.68	104.94	118.30
2	I	678	ARG	NE-CZ-NH2	6.67	123.64	120.30
2	E	341	GLU	CG-CD-OE2	-6.63	105.03	118.30
2	B	362	ILE	N-CA-C	-6.61	93.16	111.00
2	I	362	ILE	N-CA-C	-6.58	93.23	111.00
2	I	490	HIS	N-CA-CB	6.57	122.43	110.60
2	B	490	HIS	N-CA-CB	6.56	122.41	110.60
2	J	697	ILE	O-C-N	-6.54	112.23	122.70
2	I	492	ASP	N-CA-CB	-6.54	98.82	110.60
2	E	697	ILE	O-C-N	-6.53	112.25	122.70
2	B	492	ASP	N-CA-CB	-6.53	98.85	110.60
1	D	318	ARG	CB-CA-C	6.52	123.44	110.40
2	I	372	PHE	O-C-N	-6.52	112.27	122.70
2	C	581	SER	N-CA-CB	6.51	120.27	110.50
1	K	318	ARG	CB-CA-C	6.51	123.41	110.40
2	E	483	LEU	C-N-CA	6.50	137.94	121.70
2	H	581	SER	N-CA-CB	6.50	120.24	110.50
2	J	483	LEU	C-N-CA	6.48	137.90	121.70
2	J	451	ARG	C-N-CA	6.47	137.89	121.70
2	J	483	LEU	O-C-N	-6.47	112.34	122.70
2	B	372	PHE	O-C-N	-6.47	112.35	122.70
2	E	451	ARG	C-N-CA	6.47	137.87	121.70
2	E	483	LEU	O-C-N	-6.46	112.36	122.70
2	L	561	LYS	N-CA-CB	6.45	122.21	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	561	LYS	N-CA-CB	6.45	122.20	110.60
2	J	669	TYR	CB-CG-CD2	6.44	124.86	121.00
2	E	453	ARG	NE-CZ-NH1	-6.43	117.09	120.30
2	E	669	TYR	CB-CG-CD2	6.42	124.85	121.00
2	H	534	MET	N-CA-CB	6.41	122.14	110.60
2	H	561	LYS	N-CA-CB	6.41	122.14	110.60
2	C	561	LYS	N-CA-CB	6.40	122.12	110.60
2	C	534	MET	N-CA-CB	6.39	122.10	110.60
2	J	453	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	K	228	ARG	CD-NE-CZ	6.36	132.50	123.60
2	J	368	GLU	OE1-CD-OE2	-6.35	115.68	123.30
2	B	441	GLN	C-N-CA	6.35	137.57	121.70
2	E	368	GLU	OE1-CD-OE2	-6.34	115.69	123.30
2	E	362	ILE	N-CA-C	-6.34	93.89	111.00
2	I	441	GLN	C-N-CA	6.33	137.53	121.70
2	J	362	ILE	N-CA-C	-6.33	93.91	111.00
2	H	601	ARG	O-C-N	-6.32	112.59	122.70
2	J	415	LYS	CA-CB-CG	6.32	127.31	113.40
2	E	415	LYS	CA-CB-CG	6.32	127.30	113.40
1	D	228	ARG	CD-NE-CZ	6.32	132.44	123.60
2	C	601	ARG	O-C-N	-6.29	112.63	122.70
2	J	376	LYS	C-N-CA	6.25	137.34	121.70
2	E	376	LYS	C-N-CA	6.23	137.28	121.70
1	A	123	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	G	123	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	C	629	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	L	601	ARG	O-C-N	-6.07	112.99	122.70
2	F	601	ARG	O-C-N	-6.03	113.05	122.70
2	H	610	GLN	CA-C-O	6.03	132.75	120.10
2	J	492	ASP	CA-C-N	6.02	130.45	117.20
2	H	629	ARG	NE-CZ-NH2	-6.01	117.29	120.30
2	J	440	ARG	NE-CZ-NH2	-6.01	117.29	120.30
2	C	610	GLN	CA-C-O	6.01	132.72	120.10
1	G	741	ILE	CA-CB-CG1	-6.01	99.58	111.00
2	E	492	ASP	CA-C-N	6.00	130.41	117.20
1	K	245	LYS	CB-CG-CD	-6.00	96.00	111.60
2	C	559	LYS	C-N-CA	6.00	136.69	121.70
2	H	559	LYS	C-N-CA	6.00	136.69	121.70
1	A	741	ILE	CA-CB-CG1	-5.99	99.62	111.00
2	I	696	PHE	O-C-N	-5.99	113.12	122.70
2	C	600	TYR	N-CA-C	5.98	127.16	111.00
1	D	245	LYS	CB-CG-CD	-5.98	96.04	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	600	TYR	N-CA-C	5.97	127.13	111.00
2	B	696	PHE	O-C-N	-5.96	113.16	122.70
2	J	343	ARG	CD-NE-CZ	5.94	131.92	123.60
2	E	440	ARG	NE-CZ-NH2	-5.93	117.33	120.30
2	E	343	ARG	CD-NE-CZ	5.93	131.90	123.60
2	J	449	TYR	CA-CB-CG	5.92	124.64	113.40
2	E	449	TYR	CA-CB-CG	5.89	124.60	113.40
1	K	270	ASP	C-N-CA	5.88	136.41	121.70
1	D	270	ASP	C-N-CA	5.88	136.39	121.70
2	F	573	ARG	NE-CZ-NH2	5.86	123.23	120.30
2	I	696	PHE	N-CA-CB	5.86	121.14	110.60
2	B	696	PHE	N-CA-CB	5.84	121.11	110.60
2	L	573	ARG	NE-CZ-NH2	5.83	123.22	120.30
2	C	522	ARG	N-CA-CB	5.81	121.06	110.60
2	H	522	ARG	N-CA-CB	5.80	121.05	110.60
1	A	741	ILE	CB-CG1-CD1	-5.80	97.67	113.90
1	G	741	ILE	CB-CG1-CD1	-5.79	97.68	113.90
2	B	679	ASP	C-N-CA	5.73	136.01	121.70
2	I	679	ASP	C-N-CA	5.72	136.01	121.70
1	G	223	LYS	CB-CG-CD	5.71	126.44	111.60
2	J	333	VAL	CA-CB-CG2	5.71	119.46	110.90
1	A	223	LYS	CB-CG-CD	5.70	126.43	111.60
2	E	333	VAL	CA-CB-CG2	5.70	119.45	110.90
2	J	465	ARG	NE-CZ-NH1	-5.70	117.45	120.30
2	C	533	ILE	CB-CG1-CD1	-5.69	97.97	113.90
2	E	465	ARG	NE-CZ-NH1	-5.69	117.45	120.30
2	H	533	ILE	CB-CG1-CD1	-5.68	97.99	113.90
1	D	178	ASN	C-N-CA	5.68	135.89	121.70
1	K	178	ASN	C-N-CA	5.67	135.88	121.70
2	F	577	LYS	O-C-N	-5.67	113.56	123.20
2	L	577	LYS	O-C-N	-5.66	113.58	123.20
2	J	451	ARG	O-C-N	-5.64	113.67	122.70
2	E	451	ARG	O-C-N	-5.62	113.70	122.70
2	H	533	ILE	O-C-N	-5.62	113.70	122.70
2	C	533	ILE	O-C-N	-5.61	113.73	122.70
2	E	492	ASP	N-CA-C	5.60	126.13	111.00
2	B	441	GLN	O-C-N	-5.60	113.74	122.70
2	J	492	ASP	N-CA-C	5.59	126.09	111.00
1	D	297	ARG	CB-CG-CD	5.58	126.11	111.60
1	K	297	ARG	CB-CG-CD	5.58	126.11	111.60
1	G	270	ASP	C-N-CA	5.57	135.62	121.70
2	I	441	GLN	O-C-N	-5.55	113.82	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	600	TYR	N-CA-C	5.55	125.98	111.00
2	B	685	ILE	O-C-N	-5.55	113.83	122.70
2	F	600	TYR	N-CA-C	5.54	125.97	111.00
1	A	270	ASP	C-N-CA	5.54	135.55	121.70
1	K	160	LEU	CB-CG-CD1	-5.54	101.59	111.00
2	B	480	ASP	C-N-CA	5.53	135.53	121.70
1	D	160	LEU	CB-CG-CD1	-5.53	101.59	111.00
2	I	685	ILE	O-C-N	-5.53	113.85	122.70
2	E	465	ARG	NE-CZ-NH2	5.53	123.06	120.30
2	I	480	ASP	C-N-CA	5.51	135.49	121.70
2	C	577	LYS	O-C-N	-5.51	113.83	123.20
2	I	698	PHE	C-N-CA	5.51	135.47	121.70
2	H	577	LYS	O-C-N	-5.50	113.84	123.20
2	J	465	ARG	NE-CZ-NH2	5.49	123.05	120.30
2	B	698	PHE	C-N-CA	5.49	135.42	121.70
2	B	449	TYR	CA-CB-CG	5.48	123.81	113.40
2	E	452	LEU	CB-CG-CD2	-5.46	101.71	111.00
2	J	452	LEU	CB-CG-CD2	-5.46	101.72	111.00
1	G	73	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	A	73	LEU	CB-CG-CD1	-5.45	101.74	111.00
2	H	580	MET	N-CA-CB	5.44	120.39	110.60
2	L	559	LYS	C-N-CA	5.44	135.29	121.70
2	I	449	TYR	CA-CB-CG	5.43	123.72	113.40
2	F	559	LYS	C-N-CA	5.43	135.28	121.70
2	E	415	LYS	CB-CG-CD	5.43	125.72	111.60
2	J	415	LYS	CB-CG-CD	5.42	125.70	111.60
1	K	310	GLU	C-N-CA	5.42	135.26	121.70
1	D	315	LYS	N-CA-C	5.42	125.64	111.00
1	D	310	GLU	C-N-CA	5.42	135.25	121.70
2	C	580	MET	N-CA-CB	5.41	120.35	110.60
2	C	584	HIS	N-CA-CB	5.41	120.33	110.60
2	H	584	HIS	N-CA-CB	5.41	120.33	110.60
2	J	698	PHE	CZ-CE2-CD2	-5.40	113.62	120.10
1	K	315	LYS	N-CA-C	5.39	125.56	111.00
1	A	189	VAL	CA-CB-CG2	-5.39	102.82	110.90
2	F	574	ASP	CB-CG-OD2	5.38	123.14	118.30
2	J	452	LEU	CA-CB-CG	5.38	127.67	115.30
2	I	342	LYS	CB-CG-CD	5.38	125.59	111.60
2	L	574	ASP	CB-CG-OD2	5.38	123.14	118.30
2	B	342	LYS	CB-CG-CD	5.37	125.57	111.60
2	E	452	LEU	CA-CB-CG	5.37	127.66	115.30
1	K	312	GLU	O-C-N	-5.37	114.11	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	698	PHE	CZ-CE2-CD2	-5.36	113.67	120.10
1	G	189	VAL	CA-CB-CG2	-5.36	102.86	110.90
2	B	490	HIS	ND1-CG-CD2	-5.36	98.50	106.00
2	L	560	GLU	N-CA-CB	5.35	120.22	110.60
1	D	312	GLU	O-C-N	-5.34	114.15	122.70
2	I	490	HIS	ND1-CG-CD2	-5.33	98.53	106.00
2	E	697	ILE	CG1-CB-CG2	-5.31	99.71	111.40
2	F	560	GLU	N-CA-CB	5.31	120.16	110.60
2	E	485	TYR	CG-CD1-CE1	-5.30	117.06	121.30
2	J	697	ILE	CG1-CB-CG2	-5.30	99.73	111.40
1	K	160	LEU	CA-CB-CG	5.30	127.49	115.30
1	D	160	LEU	CA-CB-CG	5.30	127.48	115.30
2	J	333	VAL	N-CA-CB	5.27	123.10	111.50
2	E	333	VAL	N-CA-CB	5.27	123.09	111.50
2	E	450	PRO	N-CA-CB	-5.25	96.82	102.60
2	E	449	TYR	CD1-CG-CD2	-5.25	112.13	117.90
2	H	533	ILE	C-N-CA	5.24	134.81	121.70
2	J	450	PRO	N-CA-CB	-5.24	96.83	102.60
2	J	485	TYR	CG-CD1-CE1	-5.23	117.11	121.30
2	I	342	LYS	CA-CB-CG	5.22	124.89	113.40
2	C	533	ILE	C-N-CA	5.22	134.75	121.70
2	J	449	TYR	CD1-CG-CD2	-5.22	112.16	117.90
2	B	342	LYS	CA-CB-CG	5.21	124.86	113.40
1	G	244	GLY	O-C-N	-5.19	114.40	122.70
2	H	560	GLU	N-CA-C	5.18	125.00	111.00
2	J	494	ILE	CA-CB-CG1	5.18	120.85	111.00
2	C	560	GLU	N-CA-C	5.18	124.98	111.00
2	E	340	PHE	N-CA-C	5.18	124.98	111.00
2	B	489	ASN	N-CA-CB	5.18	119.92	110.60
2	I	340	PHE	N-CA-C	5.18	124.97	111.00
2	E	367	HIS	O-C-N	-5.17	114.42	122.70
2	J	367	HIS	O-C-N	-5.17	114.42	122.70
2	J	340	PHE	N-CA-C	5.17	124.95	111.00
2	C	580	MET	O-C-N	-5.16	114.44	122.70
2	B	340	PHE	N-CA-C	5.16	124.93	111.00
2	J	456	MET	CB-CG-SD	-5.15	96.95	112.40
2	E	494	ILE	CA-CB-CG1	5.15	120.78	111.00
2	E	456	MET	CB-CG-SD	-5.14	96.97	112.40
1	A	244	GLY	O-C-N	-5.13	114.48	122.70
2	H	580	MET	O-C-N	-5.13	114.50	122.70
2	I	372	PHE	CA-C-O	5.12	130.85	120.10
2	I	489	ASN	N-CA-CB	5.12	119.81	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	340	PHE	CB-CG-CD1	-5.11	117.23	120.80
2	B	372	PHE	CA-C-O	5.10	130.81	120.10
2	B	340	PHE	CB-CG-CD1	-5.10	117.23	120.80
2	I	409	PHE	C-N-CA	5.10	134.45	121.70
2	C	610	GLN	N-CA-CB	5.10	119.78	110.60
1	D	260	LEU	CB-CG-CD1	-5.10	102.33	111.00
2	B	409	PHE	C-N-CA	5.09	134.44	121.70
2	H	610	GLN	N-CA-CB	5.09	119.76	110.60
1	A	85	HIS	O-C-N	-5.09	114.56	122.70
2	E	339	ASP	N-CA-CB	5.09	119.75	110.60
2	L	560	GLU	CA-C-N	5.08	128.39	117.20
1	K	260	LEU	CB-CG-CD1	-5.08	102.36	111.00
2	C	581	SER	N-CA-C	5.08	124.72	111.00
2	H	581	SER	N-CA-C	5.08	124.72	111.00
2	B	456	MET	CG-SD-CE	5.06	108.30	100.20
2	I	456	MET	CG-SD-CE	5.06	108.30	100.20
1	G	85	HIS	O-C-N	-5.06	114.61	122.70
2	I	696	PHE	CA-C-O	5.04	130.68	120.10
2	B	696	PHE	CA-C-O	5.03	130.66	120.10
2	F	560	GLU	CA-C-N	5.03	128.27	117.20
2	J	339	ASP	N-CA-CB	5.03	119.65	110.60
1	K	313	GLU	CA-C-N	5.01	128.22	117.20
2	F	553	TYR	N-CA-CB	5.00	119.60	110.60

All (50) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	726	ASP	CA
2	B	366	PHE	CA
2	B	373	GLU	CA
2	B	441	GLN	CA
2	B	442	CYS	CA
2	B	445	LYS	CA
2	B	490	HIS	CA
2	B	700	GLU	CA
2	C	522	ARG	CA
2	C	534	MET	CA
2	C	560	GLU	CA
2	C	581	SER	CA
2	C	592	GLU	CA
2	C	610	GLN	CA
1	D	316	ASN	CA

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Mol	Chain	Res	Type	Atom
2	E	366	PHE	CA
2	E	368	GLU	CA
2	E	377	MET	CA
2	E	445	LYS	CA
2	E	484	ALA	CA
2	E	707	SER	CA
2	F	560	GLU	CA
2	F	563	TYR	CA
2	F	569	ASN	CA
2	F	581	SER	CA
1	G	726	ASP	CA
2	H	522	ARG	CA
2	H	534	MET	CA
2	H	560	GLU	CA
2	H	581	SER	CA
2	H	592	GLU	CA
2	H	610	GLN	CA
2	I	366	PHE	CA
2	I	373	GLU	CA
2	I	441	GLN	CA
2	I	442	CYS	CA
2	I	445	LYS	CA
2	I	490	HIS	CA
2	I	700	GLU	CA
2	J	366	PHE	CA
2	J	368	GLU	CA
2	J	377	MET	CA
2	J	445	LYS	CA
2	J	484	ALA	CA
2	J	707	SER	CA
1	K	316	ASN	CA
2	L	560	GLU	CA
2	L	563	TYR	CA
2	L	569	ASN	CA
2	L	581	SER	CA

All (241) 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

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Mol	Chain	Res	Type	Group
1	A	197	GLY	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	333	VAL	Mainchain
2	B	338	VAL	Mainchain
2	B	339	ASP	Mainchain
2	B	340	PHE	Sidechain,Mainchain
2	B	341	GLU	Mainchain
2	B	361	ARG	Mainchain
2	B	369	ARG	Sidechain
2	B	370	PHE	Sidechain
2	B	371	PRO	Mainchain
2	B	373	GLU	Mainchain
2	B	409	PHE	Sidechain
2	B	441	GLN	Mainchain
2	B	455	GLU	Sidechain
2	B	467	ARG	Mainchain
2	B	469	GLY	Mainchain
2	B	470	ARG	Sidechain
2	B	483	LEU	Mainchain
2	B	484	ALA	Mainchain
2	B	485	TYR	Sidechain
2	B	487	ASN	Sidechain
2	B	489	ASN	Mainchain,Peptide
2	B	490	HIS	Mainchain
2	B	654	GLN	Mainchain
2	B	686	MET	Mainchain
2	B	698	PHE	Sidechain
2	B	706	TYR	Sidechain
2	C	522	ARG	Sidechain,Mainchain
2	C	532	GLY	Mainchain
2	C	553	TYR	Mainchain
2	C	569	ASN	Mainchain
2	C	574	ASP	Mainchain
2	C	576	GLU	Mainchain
2	C	579	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	C	584	HIS	Sidechain
2	C	593	GLN	Sidechain
2	C	594	ARG	Sidechain
2	C	607	CYS	Mainchain
2	C	629	ARG	Sidechain
1	D	180	ASP	Sidechain
1	D	221	GLU	Mainchain
1	D	244	GLY	Mainchain
1	D	313	GLU	Mainchain
1	D	314	TYR	Sidechain
1	D	315	LYS	Mainchain
1	D	316	ASN	Mainchain,Peptide
1	D	317	PHE	Sidechain,Mainchain
1	D	318	ARG	Sidechain
1	D	32	PRO	Mainchain
1	D	43	GLY	Mainchain
1	D	60	GLY	Mainchain
1	D	62	GLY	Mainchain
2	E	333	VAL	Mainchain
2	E	339	ASP	Mainchain
2	E	340	PHE	Sidechain,Mainchain
2	E	341	GLU	Sidechain,Mainchain
2	E	343	ARG	Sidechain
2	E	358	GLY	Mainchain
2	E	361	ARG	Mainchain
2	E	362	ILE	Mainchain
2	E	370	PHE	Sidechain
2	E	371	PRO	Mainchain
2	E	414	LYS	Mainchain
2	E	415	LYS	Mainchain
2	E	440	ARG	Sidechain
2	E	449	TYR	Sidechain,Mainchain,Peptide
2	E	451	ARG	Mainchain
2	E	453	ARG	Sidechain
2	E	463	HIS	Sidechain
2	E	465	ARG	Sidechain
2	E	467	ARG	Mainchain
2	E	469	GLY	Mainchain
2	E	470	ARG	Sidechain
2	E	482	GLU	Mainchain
2	E	483	LEU	Mainchain
2	E	485	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	E	489	ASN	Mainchain
2	E	490	HIS	Sidechain
2	E	653	PRO	Mainchain
2	E	665	LEU	Mainchain
2	E	669	TYR	Sidechain
2	E	674	ASN	Sidechain
2	E	675	LYS	Mainchain
2	E	698	PHE	Sidechain
2	E	700	GLU	Mainchain
2	F	522	ARG	Sidechain
2	F	532	GLY	Mainchain
2	F	553	TYR	Sidechain,Mainchain
2	F	558	GLU	Sidechain
2	F	563	TYR	Sidechain,Mainchain
2	F	569	ASN	Sidechain,Mainchain
2	F	576	GLU	Mainchain
2	F	579	PHE	Sidechain
2	F	581	SER	Mainchain
2	F	594	ARG	Sidechain
2	F	607	CYS	Mainchain
2	F	624	GLY	Mainchain
2	F	629	ARG	Sidechain
1	G	105	THR	Mainchain
1	G	123	ARG	Sidechain
1	G	177	ALA	Mainchain
1	G	206	LYS	Mainchain
1	G	228	ARG	Sidechain
1	G	233	GLY	Mainchain
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	522	ARG	Sidechain,Mainchain
2	H	532	GLY	Mainchain
2	H	553	TYR	Mainchain
2	H	569	ASN	Mainchain
2	H	574	ASP	Mainchain
2	H	576	GLU	Mainchain
2	H	579	PHE	Sidechain
2	H	584	HIS	Sidechain
2	H	593	GLN	Sidechain

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Mol	Chain	Res	Type	Group
2	H	594	ARG	Sidechain
2	H	607	CYS	Mainchain
2	H	629	ARG	Sidechain
2	I	333	VAL	Mainchain
2	I	338	VAL	Mainchain
2	I	339	ASP	Mainchain
2	I	340	PHE	Sidechain,Mainchain
2	I	341	GLU	Mainchain
2	I	361	ARG	Mainchain
2	I	369	ARG	Sidechain
2	I	370	PHE	Sidechain
2	I	371	PRO	Mainchain
2	I	373	GLU	Mainchain
2	I	409	PHE	Sidechain
2	I	441	GLN	Mainchain
2	I	455	GLU	Sidechain
2	I	467	ARG	Mainchain
2	I	469	GLY	Mainchain
2	I	470	ARG	Sidechain
2	I	483	LEU	Mainchain
2	I	484	ALA	Mainchain
2	I	485	TYR	Sidechain
2	I	487	ASN	Sidechain
2	I	489	ASN	Mainchain,Peptide
2	I	490	HIS	Mainchain
2	I	654	GLN	Mainchain
2	I	686	MET	Mainchain
2	I	698	PHE	Sidechain
2	I	706	TYR	Sidechain
2	J	333	VAL	Mainchain
2	J	339	ASP	Mainchain
2	J	340	PHE	Sidechain,Mainchain
2	J	341	GLU	Sidechain,Mainchain
2	J	343	ARG	Sidechain
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	414	LYS	Mainchain
2	J	415	LYS	Mainchain
2	J	440	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	J	449	TYR	Sidechain,Mainchain,Peptide
2	J	451	ARG	Mainchain
2	J	453	ARG	Sidechain
2	J	463	HIS	Sidechain
2	J	465	ARG	Sidechain
2	J	467	ARG	Mainchain
2	J	469	GLY	Mainchain
2	J	470	ARG	Sidechain
2	J	482	GLU	Mainchain
2	J	483	LEU	Mainchain
2	J	485	TYR	Sidechain
2	J	489	ASN	Mainchain
2	J	490	HIS	Sidechain
2	J	653	PRO	Mainchain
2	J	665	LEU	Mainchain
2	J	669	TYR	Sidechain
2	J	674	ASN	Sidechain
2	J	675	LYS	Mainchain
2	J	698	PHE	Sidechain
2	J	700	GLU	Mainchain
1	K	180	ASP	Sidechain
1	K	221	GLU	Mainchain
1	K	244	GLY	Mainchain
1	K	313	GLU	Mainchain
1	K	314	TYR	Sidechain
1	K	315	LYS	Mainchain
1	K	316	ASN	Mainchain,Peptide
1	K	317	PHE	Sidechain,Mainchain
1	K	318	ARG	Sidechain
1	K	32	PRO	Mainchain
1	K	43	GLY	Mainchain
1	K	60	GLY	Mainchain
1	K	62	GLY	Mainchain
2	L	522	ARG	Sidechain
2	L	532	GLY	Mainchain
2	L	553	TYR	Sidechain,Mainchain
2	L	558	GLU	Sidechain
2	L	563	TYR	Sidechain,Mainchain
2	L	569	ASN	Sidechain,Mainchain
2	L	576	GLU	Mainchain
2	L	579	PHE	Sidechain
2	L	581	SER	Mainchain

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Mol	Chain	Res	Type	Group
2	L	594	ARG	Sidechain
2	L	607	CYS	Mainchain
2	L	624	GLY	Mainchain
2	L	629	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2567	0	2629	75	0
1	D	2643	0	2691	117	0
1	G	2567	0	2629	76	0
1	K	2643	0	2691	130	0
2	B	1697	0	1748	123	0
2	C	946	0	934	23	0
2	E	1697	0	1749	169	0
2	F	946	0	936	30	0
2	H	946	0	934	24	0
2	I	1697	0	1747	162	0
2	J	1697	0	1749	193	0
2	L	946	0	936	29	0
All	All	20992	0	21373	984	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 23.

All (984) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:454:GLU:OE1	1:K:271:ARG:NH1	1.72	1.21
1:D:317:PHE:CZ	2:E:332:MET:O	1.94	1.20
2:J:332:MET:O	1:K:317:PHE:CZ	1.94	1.18
2:J:453:ARG:N	1:K:318:ARG:HD2	1.55	1.17
1:D:318:ARG:HD2	2:E:453:ARG:N	1.55	1.14
2:I:341:GLU:CG	2:J:341:GLU:OE2	1.97	1.12
1:D:315:LYS:C	2:E:448:GLN:HE22	1.60	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:448:GLN:HE22	1:K:315:LYS:C	1.60	1.04
2:J:449:TYR:CB	1:K:318:ARG:HE	1.66	1.03
1:D:318:ARG:HE	2:E:449:TYR:CB	1.66	1.02
1:D:318:ARG:NE	2:E:449:TYR:CB	2.23	0.99
2:E:465:ARG:HH12	1:K:198:GLN:NE2	1.58	0.99
2:J:449:TYR:CB	1:K:318:ARG:NE	2.23	0.98
2:J:332:MET:O	1:K:317:PHE:HZ	1.38	0.97
1:D:317:PHE:CZ	2:E:332:MET:C	2.32	0.96
2:I:341:GLU:HG2	2:J:341:GLU:OE2	1.65	0.96
2:E:393:LYS:HE3	2:J:361:ARG:HD2	1.47	0.96
1:D:317:PHE:HZ	2:E:332:MET:O	1.38	0.96
2:I:341:GLU:CD	2:J:341:GLU:OE2	2.04	0.95
2:J:448:GLN:NE2	1:K:315:LYS:C	2.21	0.94
2:J:332:MET:C	1:K:317:PHE:CZ	2.32	0.94
1:D:315:LYS:C	2:E:448:GLN:NE2	2.21	0.93
2:B:702:LEU:H	2:B:702:LEU:HD23	1.34	0.93
2:J:453:ARG:H	1:K:318:ARG:HD2	1.25	0.92
2:I:700:GLU:HG2	2:J:698:PHE:HE1	1.31	0.92
1:G:207:LEU:HB2	1:G:235:VAL:HG22	1.52	0.91
2:I:702:LEU:HD23	2:I:702:LEU:H	1.34	0.91
1:D:316:ASN:N	2:E:448:GLN:NE2	2.19	0.91
1:A:12:LEU:HB3	1:A:745:ILE:HG12	1.52	0.91
1:D:318:ARG:HD2	2:E:453:ARG:H	1.25	0.90
1:G:12:LEU:HB3	1:G:745:ILE:HG12	1.52	0.90
2:J:332:MET:SD	1:K:317:PHE:HA	2.12	0.90
2:J:448:GLN:NE2	1:K:316:ASN:N	2.19	0.90
2:E:465:ARG:NH1	1:K:198:GLN:NE2	2.18	0.90
1:K:137:LEU:HB3	1:K:160:LEU:HD22	1.54	0.89
1:A:207:LEU:HB2	1:A:235:VAL:HG22	1.52	0.89
1:A:67:ARG:HD3	1:A:105:THR:HA	1.54	0.89
1:D:137:LEU:HB3	1:D:160:LEU:HD22	1.54	0.89
1:D:317:PHE:HA	2:E:332:MET:SD	2.12	0.89
2:J:449:TYR:HB2	1:K:318:ARG:NE	1.86	0.89
1:G:67:ARG:HD3	1:G:105:THR:HA	1.54	0.88
2:E:489:ASN:HA	2:I:676:THR:HG21	1.55	0.88
2:B:653:PRO:CD	2:I:345:GLU:O	2.21	0.88
1:D:318:ARG:NE	2:E:449:TYR:HB2	1.86	0.88
2:J:445:LYS:HG3	1:K:316:ASN:HB2	1.55	0.87
2:B:676:THR:HG21	2:J:489:ASN:HA	1.55	0.87
1:D:316:ASN:HD21	2:E:331:GLN:NE2	1.71	0.87
2:C:561:LYS:HD2	2:C:564:MET:HB2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:331:GLN:NE2	1:K:316:ASN:HD21	1.71	0.86
1:D:316:ASN:HB2	2:E:445:LYS:HG3	1.55	0.86
1:G:31:LEU:HG	1:G:285:LEU:HD22	1.58	0.86
2:J:459:ILE:HD12	2:J:705:LEU:HD22	1.58	0.86
2:E:459:ILE:HD12	2:E:705:LEU:HD22	1.58	0.85
1:A:31:LEU:HG	1:A:285:LEU:HD22	1.58	0.85
2:H:561:LYS:HD2	2:H:564:MET:HB2	1.57	0.85
2:L:523:LYS:HE2	2:L:544:VAL:HG13	1.58	0.85
2:I:392:ILE:HD13	2:I:662:ILE:HG13	1.57	0.85
2:F:523:LYS:HE2	2:F:544:VAL:HG13	1.58	0.85
2:B:392:ILE:HD13	2:B:662:ILE:HG13	1.57	0.84
2:J:345:GLU:OE1	2:J:345:GLU:HA	1.77	0.84
1:K:16:LEU:HD23	1:K:29:LEU:HD11	1.58	0.84
2:E:345:GLU:OE1	2:E:345:GLU:HA	1.77	0.84
2:J:331:GLN:CD	1:K:316:ASN:HD21	1.80	0.83
1:D:16:LEU:HD23	1:D:29:LEU:HD11	1.58	0.83
1:D:316:ASN:HD21	2:E:331:GLN:CD	1.80	0.83
1:K:36:VAL:HG13	1:K:48:LEU:HD13	1.59	0.82
1:D:36:VAL:HG13	1:D:48:LEU:HD13	1.60	0.82
1:K:83:PHE:HB2	1:K:86:CYS:HB2	1.61	0.82
2:B:345:GLU:HA	2:B:345:GLU:OE1	1.79	0.81
2:E:393:LYS:HE3	2:J:361:ARG:CD	2.05	0.81
2:E:702:LEU:N	2:E:702:LEU:HD23	1.95	0.81
2:J:702:LEU:HD23	2:J:702:LEU:N	1.95	0.81
2:I:345:GLU:HA	2:I:345:GLU:OE1	1.78	0.81
1:D:83:PHE:HB2	1:D:86:CYS:HB2	1.61	0.81
2:C:620:PHE:HB3	2:C:625:VAL:HB	1.63	0.81
2:E:465:ARG:HH12	1:K:198:GLN:HE22	1.23	0.80
2:H:620:PHE:HB3	2:H:625:VAL:HB	1.63	0.80
1:K:40:GLN:HB2	1:K:141:THR:HG22	1.62	0.80
2:J:444:LYS:HB3	1:K:318:ARG:O	1.82	0.79
1:D:318:ARG:O	2:E:444:LYS:HB3	1.82	0.79
1:D:36:VAL:HG22	1:D:48:LEU:HD22	1.64	0.79
1:D:12:LEU:HD23	1:D:745:ILE:HG12	1.64	0.79
1:K:36:VAL:HG22	1:K:48:LEU:HD22	1.64	0.79
2:B:661:THR:HG23	2:J:675:LYS:HE2	1.63	0.79
2:E:675:LYS:HE2	2:I:661:THR:HG23	1.63	0.79
1:K:12:LEU:HD23	1:K:745:ILE:HG12	1.64	0.78
1:D:40:GLN:HB2	1:D:141:THR:HG22	1.62	0.78
2:J:384:LEU:HB3	2:J:666:VAL:HG13	1.65	0.78
2:E:465:ARG:HH22	1:K:198:GLN:NE2	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:329:LEU:HG	2:E:702:LEU:HD22	1.66	0.78
1:D:318:ARG:HE	2:E:449:TYR:HB3	1.47	0.78
2:J:329:LEU:HG	2:J:702:LEU:HD22	1.66	0.78
1:D:10:ILE:HG23	1:D:130:LEU:HD11	1.64	0.78
1:D:318:ARG:HE	2:E:449:TYR:HB2	1.43	0.78
2:I:702:LEU:N	2:I:702:LEU:HD23	2.00	0.78
2:E:384:LEU:HB3	2:E:666:VAL:HG13	1.65	0.78
2:E:471:THR:HG21	2:E:689:MET:HG2	1.66	0.77
1:D:314:TYR:O	2:E:448:GLN:NE2	2.17	0.77
2:J:335:GLN:HG2	2:J:445:LYS:HE2	1.66	0.77
2:J:448:GLN:NE2	1:K:314:TYR:O	2.17	0.77
2:E:335:GLN:HG2	2:E:445:LYS:HE2	1.66	0.77
2:J:449:TYR:HB3	1:K:318:ARG:HE	1.47	0.77
1:A:206:LYS:HE2	1:A:238:SER:HA	1.66	0.77
2:I:422:GLU:HB3	2:I:423:PRO:HD3	1.66	0.77
1:G:206:LYS:HE2	1:G:238:SER:HA	1.66	0.77
2:B:422:GLU:HB3	2:B:423:PRO:HD3	1.66	0.77
2:J:471:THR:HG21	2:J:689:MET:HG2	1.65	0.77
2:B:702:LEU:N	2:B:702:LEU:HD23	2.00	0.76
1:K:10:ILE:HG23	1:K:130:LEU:HD11	1.64	0.76
2:E:380:ASP:HA	2:E:670:MET:HB3	1.66	0.76
2:I:463:HIS:CE1	2:J:334:GLN:NE2	2.54	0.76
1:A:59:ARG:HB3	1:A:242:ILE:HG23	1.67	0.76
2:J:380:ASP:HA	2:J:670:MET:HB3	1.66	0.76
1:G:59:ARG:HB3	1:G:242:ILE:HG23	1.67	0.75
1:K:181:LEU:HD23	1:K:219:VAL:HG21	1.67	0.75
1:G:27:ALA:HB1	1:G:296:LEU:HD12	1.68	0.75
1:A:191:LYS:HA	1:A:195:PRO:HA	1.69	0.75
2:E:661:THR:HG22	2:E:665:LEU:HD21	1.69	0.75
2:J:661:THR:HG22	2:J:665:LEU:HD21	1.69	0.75
1:G:191:LYS:HA	1:G:195:PRO:HA	1.69	0.75
1:D:181:LEU:HD23	1:D:219:VAL:HG21	1.67	0.75
1:K:142:LYS:HE3	1:K:184:SER:HA	1.68	0.74
2:J:422:GLU:HB3	2:J:423:PRO:HD3	1.69	0.74
1:D:142:LYS:HE3	1:D:184:SER:HA	1.67	0.74
2:I:700:GLU:HG2	2:J:698:PHE:CE1	2.20	0.74
2:J:449:TYR:HB2	1:K:318:ARG:HE	1.43	0.74
2:E:465:ARG:NH2	1:K:198:GLN:NE2	2.35	0.74
2:L:531:ILE:HD12	2:L:535:LYS:HD3	1.68	0.74
2:I:459:ILE:HD12	2:I:705:LEU:HD13	1.70	0.73
2:E:422:GLU:HB3	2:E:423:PRO:HD3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:531:ILE:HD12	2:F:535:LYS:HD3	1.68	0.73
1:A:27:ALA:HB1	1:A:296:LEU:HD12	1.68	0.73
2:I:696:PHE:HA	2:I:700:GLU:HG3	1.70	0.73
2:B:459:ILE:HD12	2:B:705:LEU:HD13	1.70	0.72
2:B:696:PHE:HA	2:B:700:GLU:HG3	1.70	0.72
2:B:688:LEU:HD23	2:B:688:LEU:N	2.03	0.72
2:E:490:HIS:CG	2:E:491:GLU:H	2.07	0.72
2:J:453:ARG:H	1:K:318:ARG:CD	1.98	0.72
2:I:463:HIS:HE1	2:J:334:GLN:NE2	1.87	0.72
1:A:48:LEU:HG	1:A:134:LEU:HD23	1.72	0.72
2:I:694:LYS:NZ	2:J:341:GLU:OE2	2.23	0.72
2:B:489:ASN:HB3	2:B:665:LEU:HD22	1.72	0.72
2:I:489:ASN:HB3	2:I:665:LEU:HD22	1.72	0.72
2:J:490:HIS:CG	2:J:491:GLU:H	2.07	0.72
2:I:694:LYS:CE	2:J:341:GLU:HG3	2.20	0.71
2:I:707:SER:HA	2:J:702:LEU:HB2	1.72	0.71
2:B:380:ASP:HA	2:B:670:MET:HB3	1.72	0.71
2:I:688:LEU:N	2:I:688:LEU:HD23	2.03	0.71
1:G:48:LEU:HG	1:G:134:LEU:HD23	1.72	0.71
2:I:380:ASP:HA	2:I:670:MET:HB3	1.72	0.71
1:A:83:PHE:HZ	1:A:97:VAL:HG13	1.55	0.71
1:D:318:ARG:CD	2:E:453:ARG:H	1.98	0.71
2:I:463:HIS:CE1	2:J:334:GLN:HE22	2.08	0.71
2:J:702:LEU:H	2:J:702:LEU:HD23	1.56	0.70
1:A:57:LEU:HD22	1:A:136:ASP:HB2	1.74	0.70
1:D:206:LYS:HG2	1:D:209:LEU:HD12	1.73	0.70
1:G:83:PHE:HZ	1:G:97:VAL:HG13	1.55	0.70
1:D:318:ARG:CD	2:E:449:TYR:HB2	2.21	0.70
2:C:518:ILE:HG13	2:C:519:LEU:H	1.56	0.70
2:B:442:CYS:HB3	2:B:445:LYS:HZ2	1.57	0.70
1:G:57:LEU:HD22	1:G:136:ASP:HB2	1.73	0.70
2:I:687:HIS:CD2	2:I:688:LEU:HD21	2.27	0.70
1:A:29:LEU:HD23	1:A:289:ILE:HG12	1.74	0.70
2:B:439:VAL:HG12	2:B:697:ILE:HB	1.74	0.70
1:K:206:LYS:HG2	1:K:209:LEU:HD12	1.73	0.70
2:I:442:CYS:HB3	2:I:445:LYS:HZ2	1.57	0.70
2:B:687:HIS:CD2	2:B:688:LEU:CD2	2.75	0.69
2:I:687:HIS:CD2	2:I:688:LEU:CD2	2.75	0.69
2:J:449:TYR:HB2	1:K:318:ARG:CD	2.21	0.69
2:I:341:GLU:CD	2:J:341:GLU:CD	2.50	0.69
2:B:687:HIS:CD2	2:B:688:LEU:HD21	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:ASN:HB3	2:E:332:MET:HG2	1.73	0.69
2:E:454:GLU:CD	1:K:271:ARG:NH1	2.45	0.69
2:I:439:VAL:HG12	2:I:697:ILE:HB	1.74	0.69
2:I:695:GLU:HG3	2:J:337:ALA:C	2.13	0.69
2:E:687:HIS:CD2	2:E:688:LEU:HD21	2.28	0.69
2:E:384:LEU:HD11	2:E:412:ILE:HG23	1.74	0.69
2:J:332:MET:HG2	1:K:316:ASN:HB3	1.73	0.69
1:G:12:LEU:HD13	1:G:745:ILE:HA	1.75	0.69
2:J:687:HIS:CD2	2:J:688:LEU:CD2	2.75	0.69
2:E:687:HIS:CD2	2:E:688:LEU:CD2	2.75	0.68
1:A:12:LEU:HD13	1:A:745:ILE:HA	1.75	0.68
2:E:702:LEU:H	2:E:702:LEU:HD23	1.56	0.68
2:H:518:ILE:HG13	2:H:519:LEU:H	1.56	0.68
2:J:687:HIS:CD2	2:J:688:LEU:HD21	2.28	0.68
1:D:316:ASN:ND2	2:E:331:GLN:CD	2.47	0.68
2:J:331:GLN:CD	1:K:316:ASN:ND2	2.47	0.68
2:J:384:LEU:HD11	2:J:412:ILE:HG23	1.74	0.68
1:G:29:LEU:HD23	1:G:289:ILE:HG12	1.74	0.68
2:J:448:GLN:HE22	1:K:315:LYS:CA	2.07	0.68
2:J:392:ILE:HA	2:J:408:ALA:HB2	1.75	0.68
2:I:388:ILE:HG21	2:I:666:VAL:HG21	1.76	0.68
2:I:334:GLN:OE1	2:J:695:GLU:HG3	1.94	0.68
2:E:417:VAL:HB	2:E:479:ILE:HG23	1.74	0.68
2:B:388:ILE:HG21	2:B:666:VAL:HG21	1.76	0.68
2:E:688:LEU:N	2:E:688:LEU:HD23	2.08	0.68
2:B:653:PRO:HD3	2:I:345:GLU:O	1.92	0.67
2:J:417:VAL:HB	2:J:479:ILE:HG23	1.75	0.67
2:I:694:LYS:HE2	2:J:341:GLU:HG3	1.76	0.67
2:E:392:ILE:HA	2:E:408:ALA:HB2	1.75	0.67
1:K:13:VAL:HG11	1:K:31:LEU:HD21	1.75	0.67
1:D:207:LEU:HD22	1:D:220:LEU:HD11	1.77	0.67
1:K:207:LEU:HD22	1:K:220:LEU:HD11	1.77	0.67
2:B:333:VAL:O	2:B:333:VAL:HG12	1.93	0.67
2:E:465:ARG:CZ	1:K:198:GLN:NE2	2.58	0.67
2:B:388:ILE:HG12	2:B:666:VAL:HG11	1.77	0.67
2:F:552:TRP:HH2	2:F:565:LEU:HD13	1.59	0.67
2:F:518:ILE:HG13	2:F:519:LEU:H	1.60	0.67
1:D:318:ARG:H	2:E:453:ARG:HB3	1.59	0.67
1:K:40:GLN:HG3	1:K:63:ILE:HB	1.76	0.67
2:I:388:ILE:HG12	2:I:666:VAL:HG11	1.77	0.67
2:J:453:ARG:HB3	1:K:318:ARG:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:GLN:HG3	1:D:63:ILE:HB	1.76	0.67
2:J:688:LEU:HD23	2:J:688:LEU:N	2.08	0.67
2:L:518:ILE:HG13	2:L:519:LEU:H	1.60	0.67
1:D:315:LYS:CA	2:E:448:GLN:HE22	2.07	0.67
2:I:703:ALA:HA	2:J:699:SER:HA	1.75	0.67
2:I:333:VAL:HG12	2:I:333:VAL:O	1.93	0.67
1:D:13:VAL:HG11	1:D:31:LEU:HD21	1.75	0.66
2:J:420:ILE:HG13	2:J:673:VAL:HG21	1.78	0.66
2:E:420:ILE:HG13	2:E:673:VAL:HG21	1.78	0.66
2:I:490:HIS:CG	2:I:491:GLU:H	2.14	0.66
2:E:494:ILE:HD13	2:I:678:ARG:HD2	1.76	0.66
2:B:678:ARG:HD2	2:J:494:ILE:HD13	1.76	0.66
2:I:384:LEU:HD12	2:I:412:ILE:HG13	1.77	0.66
2:J:414:LYS:HG2	2:J:483:LEU:HB3	1.78	0.66
1:D:67:ARG:HH21	1:D:120:ILE:HG12	1.61	0.66
1:K:67:ARG:HH21	1:K:120:ILE:HG12	1.61	0.66
2:L:552:TRP:HH2	2:L:565:LEU:HD13	1.60	0.66
2:B:490:HIS:CG	2:B:491:GLU:H	2.14	0.66
2:B:384:LEU:HD12	2:B:412:ILE:HG13	1.77	0.66
2:B:653:PRO:HD2	2:I:345:GLU:O	1.95	0.65
2:E:414:LYS:HG2	2:E:483:LEU:HB3	1.77	0.65
2:E:675:LYS:HD3	2:I:665:LEU:HD21	1.79	0.65
2:J:681:MET:HB2	2:J:682:PRO:HD3	1.78	0.65
2:E:681:MET:HB2	2:E:682:PRO:HD3	1.77	0.65
2:B:665:LEU:HD21	2:J:675:LYS:HD3	1.79	0.65
2:J:444:LYS:O	1:K:318:ARG:N	2.15	0.65
1:K:13:VAL:HG13	1:K:29:LEU:HD13	1.79	0.65
2:B:388:ILE:HG12	2:B:666:VAL:HG21	1.78	0.65
2:E:465:ARG:NH1	1:K:198:GLN:HE22	1.89	0.64
2:I:388:ILE:HG12	2:I:666:VAL:HG21	1.79	0.64
1:D:13:VAL:HG13	1:D:29:LEU:HD13	1.79	0.64
2:J:690:ILE:HG22	2:J:691:ASN:N	2.12	0.64
2:B:384:LEU:HD22	2:B:670:MET:HG2	1.79	0.64
1:A:217:ARG:HG3	1:A:265:TYR:HE1	1.62	0.64
1:G:56:PHE:HB3	1:G:94:PHE:HB3	1.78	0.64
2:I:384:LEU:HD22	2:I:670:MET:HG2	1.79	0.64
1:G:217:ARG:HG3	1:G:265:TYR:HE1	1.62	0.64
1:D:171:ILE:HD12	1:D:193:VAL:HG21	1.80	0.64
1:K:40:GLN:HE22	1:K:145:VAL:HG11	1.63	0.64
1:A:56:PHE:HB3	1:A:94:PHE:HB3	1.78	0.64
2:I:687:HIS:HE1	2:J:342:LYS:HD3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:695:GLU:HG3	2:J:337:ALA:O	1.96	0.64
2:B:329:LEU:HG	2:B:702:LEU:HA	1.79	0.63
1:K:171:ILE:HD12	1:K:193:VAL:HG21	1.80	0.63
2:I:329:LEU:HG	2:I:702:LEU:HA	1.79	0.63
1:D:40:GLN:HE22	1:D:145:VAL:HG11	1.63	0.63
2:J:692:ASN:C	2:J:692:ASN:HD22	2.00	0.63
2:C:607:CYS:HB3	2:C:612:GLU:HB3	1.81	0.63
2:B:692:ASN:C	2:B:692:ASN:HD22	2.02	0.63
2:F:573:ARG:HB2	2:F:630:VAL:HA	1.80	0.62
1:D:13:VAL:HG13	1:D:29:LEU:HB3	1.80	0.62
1:K:13:VAL:HG13	1:K:29:LEU:HB3	1.80	0.62
1:K:181:LEU:HD21	1:K:219:VAL:HG11	1.81	0.62
2:E:690:ILE:HG22	2:E:691:ASN:N	2.12	0.62
2:B:452:LEU:C	2:B:452:LEU:HD13	2.19	0.62
2:I:692:ASN:HD22	2:I:692:ASN:C	2.02	0.62
2:E:692:ASN:HD22	2:E:692:ASN:C	2.00	0.62
2:I:452:LEU:C	2:I:452:LEU:HD13	2.19	0.62
2:H:607:CYS:HB3	2:H:612:GLU:HB3	1.81	0.62
1:A:161:MET:HA	1:A:164:VAL:HG22	1.82	0.62
1:A:176:PRO:HB3	1:A:206:LYS:HD2	1.81	0.61
1:G:161:MET:HA	1:G:164:VAL:HG22	1.82	0.61
1:K:208:ASP:HB3	1:K:258:PHE:HB2	1.83	0.61
1:D:208:ASP:HB3	1:D:258:PHE:HB2	1.82	0.61
1:G:176:PRO:HB3	1:G:206:LYS:HD2	1.81	0.61
2:I:490:HIS:CD2	2:I:491:GLU:H	2.18	0.61
2:L:573:ARG:HB2	2:L:630:VAL:HA	1.80	0.61
2:L:570:LEU:HD13	2:L:588:LEU:HD13	1.82	0.61
2:B:490:HIS:CD2	2:B:491:GLU:H	2.18	0.61
1:D:181:LEU:HD21	1:D:219:VAL:HG11	1.81	0.61
1:D:318:ARG:N	2:E:453:ARG:HB3	2.15	0.61
2:E:385:ARG:HH12	2:E:663:ARG:HA	1.66	0.61
2:J:385:ARG:HH12	2:J:663:ARG:HA	1.66	0.61
1:G:23:ILE:HG22	1:G:25:GLN:HG2	1.83	0.61
1:A:23:ILE:HG22	1:A:25:GLN:HG2	1.83	0.61
1:A:87:LYS:HE2	1:A:88:GLY:HA3	1.83	0.61
1:D:318:ARG:N	2:E:444:LYS:O	2.15	0.61
1:D:135:VAL:HG12	1:D:137:LEU:HG	1.83	0.61
1:A:209:LEU:HD11	1:A:238:SER:HB3	1.83	0.61
1:G:87:LYS:HE2	1:G:88:GLY:HA3	1.83	0.61
1:G:232:ILE:HG21	1:G:277:LEU:HA	1.82	0.60
2:J:453:ARG:HB3	1:K:318:ARG:N	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:702:LEU:CD2	2:I:702:LEU:H	2.09	0.60
2:E:494:ILE:HG13	2:I:675:LYS:HE2	1.84	0.60
1:G:209:LEU:HD11	1:G:238:SER:HB3	1.83	0.60
2:H:518:ILE:HG13	2:H:519:LEU:N	2.16	0.60
2:F:570:LEU:HD13	2:F:588:LEU:HD13	1.82	0.60
2:E:465:ARG:NH1	1:K:198:GLN:HE21	1.98	0.60
2:B:675:LYS:HE2	2:J:494:ILE:HG13	1.84	0.60
2:L:518:ILE:HG13	2:L:519:LEU:N	2.16	0.60
2:I:698:PHE:CZ	2:J:691:ASN:ND2	2.70	0.60
1:A:232:ILE:HG21	1:A:277:LEU:HA	1.82	0.60
2:E:491:GLU:OE2	2:E:492:ASP:HA	2.02	0.59
2:B:489:ASN:OD1	2:B:489:ASN:N	2.35	0.59
2:C:518:ILE:HG13	2:C:519:LEU:N	2.16	0.59
1:K:229:ARG:HG3	1:K:280:VAL:HG11	1.85	0.59
1:K:135:VAL:HG12	1:K:137:LEU:HG	1.83	0.59
2:I:694:LYS:HE2	2:J:341:GLU:CG	2.32	0.59
1:D:201:ILE:HD12	1:D:277:LEU:HD12	1.83	0.59
1:A:94:PHE:HZ	1:A:124:VAL:HG11	1.68	0.59
2:J:491:GLU:OE2	2:J:492:ASP:HA	2.02	0.59
2:I:374:LEU:HD13	2:I:423:PRO:HB2	1.84	0.59
2:B:374:LEU:HD13	2:B:423:PRO:HB2	1.84	0.59
1:G:94:PHE:HZ	1:G:124:VAL:HG11	1.68	0.59
2:E:379:PHE:HE1	2:E:419:LYS:HB2	1.68	0.59
2:I:392:ILE:HG13	2:I:393:LYS:HG2	1.85	0.59
2:J:471:THR:HG22	2:J:688:LEU:HB2	1.85	0.59
1:K:201:ILE:HD12	1:K:277:LEU:HD12	1.83	0.59
2:L:579:PHE:HD1	2:L:579:PHE:N	2.01	0.59
1:K:10:ILE:HB	1:K:11:PRO:HD3	1.85	0.59
1:G:70:VAL:HG23	1:G:119:PRO:HB3	1.85	0.59
2:F:579:PHE:N	2:F:579:PHE:HD1	2.01	0.59
2:J:379:PHE:HE1	2:J:419:LYS:HB2	1.68	0.59
2:F:518:ILE:HG13	2:F:519:LEU:N	2.16	0.59
1:K:42:ALA:HB1	1:K:174:VAL:HG12	1.84	0.59
1:A:70:VAL:HG23	1:A:119:PRO:HB3	1.85	0.59
1:D:87:LYS:HB2	1:D:87:LYS:HZ3	1.67	0.58
1:D:319:PRO:O	2:E:444:LYS:NZ	2.30	0.58
2:B:690:ILE:HG22	2:B:691:ASN:N	2.17	0.58
2:B:392:ILE:HG13	2:B:393:LYS:HG2	1.85	0.58
2:I:489:ASN:OD1	2:I:489:ASN:N	2.35	0.58
2:E:471:THR:HG22	2:E:688:LEU:HB2	1.85	0.58
2:H:565:LEU:HD11	2:H:570:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:465:ARG:HH22	1:K:198:GLN:HE22	1.51	0.58
1:D:10:ILE:HB	1:D:11:PRO:HD3	1.85	0.58
2:I:681:MET:HB2	2:I:682:PRO:HD3	1.86	0.58
1:D:42:ALA:HB1	1:D:174:VAL:HG12	1.84	0.58
2:C:579:PHE:N	2:C:579:PHE:CD1	2.70	0.58
2:J:702:LEU:N	2:J:702:LEU:CD2	2.67	0.58
2:I:690:ILE:HG22	2:I:691:ASN:N	2.17	0.58
1:D:229:ARG:HG3	1:D:280:VAL:HG11	1.85	0.58
2:I:338:VAL:HG11	2:J:687:HIS:ND1	2.18	0.58
2:F:579:PHE:N	2:F:579:PHE:CD1	2.72	0.58
2:H:579:PHE:CD1	2:H:579:PHE:N	2.70	0.58
2:F:531:ILE:HG23	2:F:535:LYS:HD3	1.86	0.58
1:A:140:MET:HE2	1:A:160:LEU:HD21	1.86	0.58
2:I:707:SER:CA	2:J:702:LEU:HB2	2.30	0.57
1:D:317:PHE:CA	2:E:332:MET:SD	2.88	0.57
1:D:317:PHE:CD1	2:E:332:MET:SD	2.97	0.57
2:L:579:PHE:CD1	2:L:579:PHE:N	2.71	0.57
2:J:332:MET:SD	1:K:317:PHE:CD1	2.97	0.57
2:I:341:GLU:OE2	2:J:341:GLU:OE2	2.22	0.57
2:J:489:ASN:OD1	2:J:489:ASN:N	2.35	0.57
2:L:531:ILE:HG23	2:L:535:LYS:HD3	1.86	0.57
1:G:13:VAL:HG11	1:G:289:ILE:HD13	1.87	0.57
2:C:579:PHE:N	2:C:579:PHE:HD1	2.03	0.57
2:H:579:PHE:HD1	2:H:579:PHE:N	2.03	0.57
2:E:428:VAL:HG11	2:E:472:LYS:HG3	1.86	0.57
1:A:13:VAL:HG11	1:A:289:ILE:HD13	1.87	0.57
1:G:69:LEU:HD13	1:G:101:ILE:HG12	1.86	0.57
2:I:481:ILE:HG22	2:I:482:GLU:OE1	2.05	0.57
2:J:444:LYS:NZ	1:K:319:PRO:O	2.30	0.57
2:I:687:HIS:CE1	2:J:342:LYS:HD3	2.40	0.57
2:B:702:LEU:CD2	2:B:702:LEU:N	2.65	0.56
2:E:490:HIS:CD2	2:E:491:GLU:H	2.22	0.56
2:J:392:ILE:HG13	2:J:393:LYS:HG2	1.87	0.56
2:L:577:LYS:HE3	2:L:577:LYS:H	1.70	0.56
2:C:565:LEU:HD11	2:C:570:LEU:HD21	1.85	0.56
2:B:681:MET:HB2	2:B:682:PRO:HD3	1.86	0.56
2:J:428:VAL:HG11	2:J:472:LYS:HG3	1.86	0.56
2:E:489:ASN:N	2:E:489:ASN:OD1	2.35	0.56
2:J:490:HIS:CD2	2:J:491:GLU:H	2.22	0.56
1:K:83:PHE:HZ	1:K:97:VAL:HG13	1.70	0.56
2:J:391:ALA:HB1	2:J:408:ALA:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:481:ILE:HG22	2:B:482:GLU:OE1	2.05	0.56
1:A:69:LEU:HD13	1:A:101:ILE:HG12	1.86	0.56
2:E:465:ARG:NH2	1:K:228:ARG:HH21	2.04	0.56
1:D:83:PHE:HZ	1:D:97:VAL:HG13	1.70	0.56
2:E:687:HIS:CG	2:E:688:LEU:HD23	2.41	0.56
2:B:687:HIS:CG	2:B:688:LEU:HD23	2.41	0.56
2:E:344:ILE:HD13	2:E:690:ILE:HG13	1.88	0.56
2:F:577:LYS:HE3	2:F:577:LYS:H	1.71	0.56
2:F:521:ILE:HD13	2:F:622:ARG:HB3	1.87	0.56
2:I:379:PHE:HE2	2:I:419:LYS:HD3	1.71	0.56
2:L:521:ILE:HD13	2:L:622:ARG:HB3	1.87	0.56
2:J:478:LEU:HD12	2:J:680:LEU:HD23	1.88	0.56
2:E:391:ALA:HB1	2:E:408:ALA:HA	1.87	0.56
2:E:478:LEU:HD12	2:E:680:LEU:HD23	1.88	0.56
2:E:346:GLY:HA3	2:E:360:ALA:HB1	1.87	0.56
2:J:346:GLY:HA3	2:J:360:ALA:HB1	1.88	0.56
1:A:235:VAL:HB	1:A:255:GLU:HB2	1.87	0.56
2:E:392:ILE:HG13	2:E:393:LYS:HG2	1.87	0.56
2:I:702:LEU:CD2	2:I:702:LEU:N	2.65	0.56
2:B:495:GLY:O	2:B:496:PHE:HB2	2.05	0.56
2:H:535:LYS:O	2:H:535:LYS:HG3	2.06	0.55
2:E:702:LEU:CD2	2:E:702:LEU:N	2.67	0.55
2:I:495:GLY:O	2:I:496:PHE:HB2	2.05	0.55
2:B:379:PHE:HE2	2:B:419:LYS:HD3	1.71	0.55
1:G:66:ARG:HB2	1:G:105:THR:HG21	1.88	0.55
2:I:687:HIS:CG	2:I:688:LEU:HD23	2.41	0.55
2:E:458:ARG:HG3	1:K:229:ARG:HH22	1.71	0.55
1:D:170:LEU:HD21	1:D:281:LEU:HD22	1.89	0.55
1:G:235:VAL:HB	1:G:255:GLU:HB2	1.87	0.55
2:J:687:HIS:CG	2:J:688:LEU:HD23	2.41	0.55
1:K:170:LEU:HD21	1:K:281:LEU:HD22	1.89	0.55
2:I:698:PHE:HZ	2:J:691:ASN:ND2	2.03	0.55
2:J:452:LEU:HD13	2:J:452:LEU:C	2.27	0.55
1:D:317:PHE:O	2:E:449:TYR:HD1	1.89	0.55
2:J:344:ILE:HD13	2:J:690:ILE:HG13	1.88	0.55
2:E:452:LEU:C	2:E:452:LEU:HD13	2.27	0.54
2:B:329:LEU:HD21	2:B:705:LEU:HG	1.89	0.54
2:I:329:LEU:HD21	2:I:705:LEU:HG	1.90	0.54
2:E:662:ILE:HD13	2:E:665:LEU:HD12	1.90	0.54
2:C:535:LYS:O	2:C:535:LYS:HG3	2.06	0.54
2:J:662:ILE:HD13	2:J:665:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:698:PHE:CE1	2:J:691:ASN:CG	2.81	0.54
2:J:495:GLY:O	2:J:496:PHE:HB2	2.08	0.54
2:J:445:LYS:HG3	1:K:316:ASN:CB	2.34	0.54
1:A:66:ARG:HB2	1:A:105:THR:HG21	1.88	0.54
2:C:596:VAL:HG11	2:C:603:LEU:HB2	1.89	0.54
2:J:449:TYR:HD1	1:K:317:PHE:O	1.89	0.54
1:D:316:ASN:N	2:E:448:GLN:HE21	2.02	0.54
1:D:17:GLN:HG3	1:D:29:LEU:HD12	1.90	0.54
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.71	0.54
1:K:17:GLN:HG3	1:K:29:LEU:HD12	1.90	0.54
2:E:495:GLY:O	2:E:496:PHE:HB2	2.08	0.54
2:B:494:ILE:HG23	2:J:675:LYS:HD2	1.90	0.54
2:E:675:LYS:HD2	2:I:494:ILE:HG23	1.90	0.54
1:G:33:GLN:HB2	1:G:133:THR:HB	1.90	0.54
1:G:15:ARG:HG3	1:G:15:ARG:HH11	1.71	0.54
2:J:362:ILE:CG2	2:J:363:ASN:N	2.71	0.53
2:B:379:PHE:CZ	2:B:416:GLN:HG2	2.44	0.53
1:A:33:GLN:HB2	1:A:133:THR:HB	1.89	0.53
2:J:416:GLN:HG2	2:J:670:MET:HE2	1.89	0.53
2:I:362:ILE:CG2	2:I:363:ASN:N	2.72	0.53
2:I:459:ILE:HG21	2:I:705:LEU:HD22	1.90	0.53
2:B:388:ILE:HG13	2:B:409:PHE:HA	1.90	0.53
1:G:274:THR:HB	1:G:275:PRO:HD3	1.90	0.53
2:B:362:ILE:CG2	2:B:363:ASN:N	2.72	0.53
2:J:345:GLU:OE1	2:J:345:GLU:CA	2.55	0.53
2:H:596:VAL:HG11	2:H:603:LEU:HB2	1.89	0.53
2:I:703:ALA:CA	2:J:699:SER:HA	2.39	0.53
1:A:274:THR:HB	1:A:275:PRO:HD3	1.90	0.53
2:B:459:ILE:HG21	2:B:705:LEU:HD22	1.90	0.53
2:E:362:ILE:CG2	2:E:363:ASN:N	2.71	0.53
2:I:345:GLU:CA	2:I:345:GLU:OE1	2.55	0.53
2:I:698:PHE:HE1	2:J:691:ASN:CG	2.12	0.52
1:D:316:ASN:ND2	2:E:331:GLN:NE2	2.51	0.52
2:I:379:PHE:CZ	2:I:416:GLN:HG2	2.44	0.52
1:G:140:MET:HE2	1:G:160:LEU:HD21	1.91	0.52
2:I:388:ILE:HG13	2:I:409:PHE:HA	1.90	0.52
2:F:578:GLY:HA3	2:F:585:ILE:HD12	1.90	0.52
2:H:553:TYR:CG	2:H:558:GLU:HG2	2.45	0.52
1:D:58:PRO:HG3	1:D:101:ILE:HG22	1.91	0.52
2:J:448:GLN:HE21	1:K:316:ASN:N	2.02	0.52
2:B:370:PHE:N	2:B:371:PRO:HD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:340:PHE:CD2	2:B:694:LYS:HG3	2.45	0.52
2:B:345:GLU:CA	2:B:345:GLU:OE1	2.55	0.52
2:J:332:MET:SD	1:K:317:PHE:CA	2.88	0.51
2:I:370:PHE:N	2:I:371:PRO:HD2	2.25	0.51
2:I:340:PHE:CD2	2:I:694:LYS:HG3	2.45	0.51
2:E:333:VAL:HG23	2:E:333:VAL:O	2.10	0.51
1:D:316:ASN:CB	2:E:445:LYS:HG3	2.34	0.51
2:C:553:TYR:CG	2:C:558:GLU:HG2	2.45	0.51
1:G:300:LEU:HB3	1:G:735:LEU:HD22	1.93	0.51
2:L:578:GLY:HA3	2:L:585:ILE:HD12	1.90	0.51
1:A:300:LEU:HB3	1:A:735:LEU:HD22	1.93	0.51
2:C:577:LYS:HE3	2:C:577:LYS:H	1.76	0.51
1:D:62:GLY:HA3	1:D:113:LYS:HE2	1.93	0.51
1:K:58:PRO:HG3	1:K:101:ILE:HG22	1.91	0.51
1:K:62:GLY:HA3	1:K:113:LYS:HE2	1.93	0.51
2:J:333:VAL:O	2:J:333:VAL:HG23	2.10	0.51
2:F:607:CYS:HB3	2:F:612:GLU:HB3	1.91	0.51
2:L:607:CYS:HB3	2:L:612:GLU:HB3	1.91	0.51
1:A:31:LEU:HD21	1:A:130:LEU:HD12	1.92	0.51
2:E:490:HIS:CG	2:E:491:GLU:N	2.75	0.51
2:I:694:LYS:HE2	2:J:341:GLU:CD	2.31	0.51
2:B:688:LEU:O	2:B:689:MET:C	2.48	0.51
2:J:370:PHE:N	2:J:371:PRO:HD2	2.26	0.51
1:G:31:LEU:HD21	1:G:130:LEU:HD12	1.92	0.51
2:I:334:GLN:CD	2:J:695:GLU:HG3	2.31	0.51
2:B:672:ILE:HD13	2:J:491:GLU:HA	1.93	0.50
2:I:367:HIS:CG	2:I:682:PRO:HB3	2.47	0.50
2:B:496:PHE:CE2	2:B:660:GLU:HG2	2.46	0.50
2:I:698:PHE:HZ	2:J:691:ASN:HD21	1.59	0.50
2:E:688:LEU:O	2:E:689:MET:C	2.46	0.50
1:G:83:PHE:HB2	1:G:86:CYS:HB2	1.94	0.50
1:D:310:GLU:HA	1:D:313:GLU:HG2	1.94	0.50
2:I:496:PHE:CE2	2:I:660:GLU:HG2	2.46	0.50
2:B:374:LEU:HG	2:B:678:ARG:HB3	1.94	0.50
2:E:491:GLU:HA	2:I:672:ILE:HD13	1.93	0.50
1:A:83:PHE:HB2	1:A:86:CYS:HB2	1.94	0.50
2:J:688:LEU:O	2:J:689:MET:C	2.46	0.50
2:B:687:HIS:HD2	2:B:688:LEU:HD21	1.77	0.50
1:G:217:ARG:HD2	1:G:264:SER:HB3	1.94	0.50
1:K:87:LYS:HZ3	1:K:87:LYS:HB2	1.75	0.50
2:E:345:GLU:OE1	2:E:345:GLU:CA	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:703:ALA:CB	2:J:699:SER:HA	2.41	0.50
2:B:359:GLY:HA2	2:B:362:ILE:HG22	1.93	0.50
2:E:343:ARG:HH21	2:E:359:GLY:H	1.59	0.50
2:L:526:LEU:HD13	2:L:605:LEU:HD22	1.94	0.50
2:J:343:ARG:HH21	2:J:359:GLY:H	1.59	0.49
2:J:392:ILE:HG22	2:J:408:ALA:HB1	1.93	0.49
2:E:362:ILE:HG23	2:E:363:ASN:N	2.27	0.49
2:H:577:LYS:HE3	2:H:577:LYS:H	1.76	0.49
1:D:319:PRO:C	2:E:444:LYS:HE3	2.33	0.49
2:I:374:LEU:HG	2:I:678:ARG:HB3	1.94	0.49
2:E:370:PHE:N	2:E:371:PRO:HD2	2.26	0.49
2:J:444:LYS:HE3	1:K:319:PRO:C	2.33	0.49
2:J:449:TYR:HB2	2:J:453:ARG:H	1.77	0.49
2:J:340:PHE:CZ	2:J:439:VAL:HG12	2.47	0.49
2:E:392:ILE:HG22	2:E:408:ALA:HB1	1.93	0.49
2:B:367:HIS:CG	2:B:682:PRO:HB3	2.46	0.49
2:F:526:LEU:HD13	2:F:605:LEU:HD22	1.94	0.49
2:J:453:ARG:HG3	2:J:454:GLU:N	2.27	0.49
1:D:140:MET:HE3	1:D:160:LEU:HD12	1.93	0.49
2:I:359:GLY:HA2	2:I:362:ILE:HG22	1.93	0.49
1:D:307:ILE:HB	1:D:728:MET:HG3	1.95	0.49
2:L:562:LYS:O	2:L:563:TYR:HB3	2.12	0.49
2:E:449:TYR:HB2	2:E:453:ARG:H	1.78	0.49
1:A:217:ARG:HD2	1:A:264:SER:HB3	1.94	0.49
1:K:307:ILE:HB	1:K:728:MET:HG3	1.95	0.49
1:K:43:GLY:HA3	1:K:236:ASN:HD22	1.78	0.49
2:E:453:ARG:HG3	2:E:454:GLU:N	2.27	0.49
2:B:494:ILE:HG23	2:J:675:LYS:CD	2.43	0.49
2:B:336:PHE:CD2	2:B:697:ILE:HD11	2.48	0.49
1:A:33:GLN:CB	1:A:133:THR:HB	2.43	0.49
2:F:562:LYS:O	2:F:563:TYR:HB3	2.13	0.49
1:G:37:VAL:HG22	1:G:171:ILE:HG23	1.94	0.49
1:D:173:ALA:HB2	1:D:190:ALA:HB2	1.94	0.49
2:I:336:PHE:CD2	2:I:697:ILE:HD11	2.48	0.49
1:K:161:MET:HA	1:K:164:VAL:HG22	1.95	0.49
2:E:340:PHE:HZ	2:E:439:VAL:HG12	1.78	0.49
2:I:362:ILE:HG23	2:I:363:ASN:N	2.28	0.48
2:B:362:ILE:HG23	2:B:363:ASN:N	2.28	0.48
2:B:340:PHE:O	2:B:341:GLU:C	2.50	0.48
2:J:362:ILE:HG23	2:J:363:ASN:N	2.27	0.48
1:K:140:MET:HE3	1:K:160:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:490:HIS:NE2	2:I:672:ILE:HG21	2.28	0.48
2:I:688:LEU:O	2:I:689:MET:C	2.47	0.48
1:A:40:GLN:O	1:A:41:SER:HB3	2.13	0.48
1:K:310:GLU:HA	1:K:313:GLU:HG2	1.94	0.48
2:B:490:HIS:NE2	2:B:672:ILE:HG21	2.28	0.48
2:J:417:VAL:HB	2:J:479:ILE:CG2	2.43	0.48
2:J:413:VAL:HG21	2:J:486:MET:H	1.79	0.48
1:D:43:GLY:HA3	1:D:236:ASN:HD22	1.78	0.48
2:J:687:HIS:HD2	2:J:688:LEU:HD21	1.78	0.48
1:K:43:GLY:HA3	1:K:236:ASN:ND2	2.29	0.48
2:E:340:PHE:CZ	2:E:439:VAL:HG12	2.47	0.48
1:D:43:GLY:HA3	1:D:236:ASN:ND2	2.29	0.48
1:A:37:VAL:HG22	1:A:171:ILE:HG23	1.94	0.48
1:D:161:MET:HA	1:D:164:VAL:HG22	1.95	0.48
1:G:33:GLN:CB	1:G:133:THR:HB	2.43	0.48
2:H:525:TRP:HB3	2:H:540:GLU:HG2	1.96	0.48
2:C:525:TRP:HB3	2:C:540:GLU:HG2	1.96	0.48
1:D:170:LEU:HD11	1:D:281:LEU:HD22	1.96	0.48
2:J:413:VAL:HA	2:J:669:TYR:CE2	2.49	0.48
1:K:173:ALA:HB2	1:K:190:ALA:HB2	1.94	0.48
2:E:413:VAL:HA	2:E:669:TYR:CE2	2.49	0.48
1:G:40:GLN:O	1:G:41:SER:HB3	2.13	0.48
2:E:675:LYS:CD	2:I:494:ILE:HG23	2.43	0.48
1:G:83:PHE:CZ	1:G:97:VAL:HG13	2.43	0.48
2:L:526:LEU:HD13	2:L:605:LEU:HB3	1.95	0.48
2:F:526:LEU:HD13	2:F:605:LEU:HB3	1.95	0.48
2:B:378:GLU:HG2	2:B:420:ILE:HD13	1.95	0.48
1:G:9:LEU:HG	1:G:286:THR:HG23	1.96	0.48
1:A:9:LEU:HG	1:A:286:THR:HG23	1.95	0.48
2:I:378:GLU:HG2	2:I:420:ILE:HD13	1.95	0.48
1:K:83:PHE:CE2	1:K:122:LEU:HD22	2.49	0.48
2:J:435:LEU:HD12	2:J:690:ILE:HD12	1.96	0.48
2:B:336:PHE:CE2	2:B:697:ILE:HD11	2.49	0.48
2:I:336:PHE:CE2	2:I:697:ILE:HD11	2.49	0.48
1:K:170:LEU:HD11	1:K:281:LEU:HD22	1.96	0.48
2:J:340:PHE:HZ	2:J:439:VAL:HG12	1.78	0.47
2:B:370:PHE:CE1	2:B:427:CYS:HB2	2.49	0.47
2:B:361:ARG:O	2:B:362:ILE:C	2.52	0.47
2:E:485:TYR:CD1	2:I:484:ALA:HB3	2.49	0.47
1:D:83:PHE:CE2	1:D:122:LEU:HD22	2.49	0.47
2:E:687:HIS:HD2	2:E:688:LEU:HD21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:416:GLN:HG2	2:E:670:MET:HE2	1.96	0.47
1:K:235:VAL:HG11	1:K:254:ALA:HB3	1.97	0.47
2:J:490:HIS:CG	2:J:491:GLU:N	2.75	0.47
2:J:409:PHE:CE2	2:J:490:HIS:HB3	2.50	0.47
1:K:87:LYS:HZ2	1:K:87:LYS:H	1.63	0.47
1:K:59:ARG:HA	1:K:64:VAL:HG13	1.96	0.47
2:J:697:ILE:O	2:J:697:ILE:HD13	2.14	0.47
1:K:83:PHE:CZ	1:K:97:VAL:HG13	2.50	0.47
2:J:379:PHE:CE1	2:J:419:LYS:HB2	2.49	0.47
2:E:413:VAL:HG21	2:E:486:MET:H	1.79	0.47
1:D:55:ASP:HB3	1:D:98:ARG:HD3	1.96	0.47
2:I:478:LEU:HD11	2:I:680:LEU:HD23	1.96	0.47
2:J:662:ILE:HD13	2:J:665:LEU:CD1	2.45	0.47
2:E:435:LEU:HD12	2:E:690:ILE:HD12	1.96	0.47
1:D:59:ARG:HA	1:D:64:VAL:HG13	1.96	0.47
1:D:235:VAL:HG11	1:D:254:ALA:HB3	1.97	0.47
1:K:149:PRO:HD2	1:K:152:ILE:HD13	1.96	0.47
2:B:432:ILE:CD1	2:B:472:LYS:HE3	2.45	0.47
2:J:331:GLN:NE2	1:K:316:ASN:ND2	2.51	0.47
2:B:439:VAL:HA	2:B:697:ILE:HG13	1.97	0.47
2:I:439:VAL:HA	2:I:697:ILE:HG13	1.97	0.47
2:E:697:ILE:HD13	2:E:697:ILE:O	2.14	0.47
1:K:55:ASP:HB3	1:K:98:ARG:HD3	1.96	0.47
2:I:340:PHE:O	2:I:341:GLU:C	2.50	0.47
2:B:678:ARG:HD2	2:J:494:ILE:CD1	2.45	0.47
2:E:409:PHE:CE2	2:E:490:HIS:HB3	2.50	0.47
2:H:579:PHE:HD1	2:H:579:PHE:H	1.62	0.47
1:A:173:ALA:HB1	1:A:187:LEU:HD23	1.97	0.47
1:D:191:LYS:HZ1	1:D:225:LEU:HG	1.80	0.47
2:E:465:ARG:CZ	1:K:198:GLN:HE21	2.28	0.47
2:B:478:LEU:HD11	2:B:680:LEU:HD23	1.96	0.47
2:I:370:PHE:CE1	2:I:427:CYS:HB2	2.50	0.47
2:I:688:LEU:N	2:I:688:LEU:CD2	2.74	0.47
2:I:452:LEU:HD13	2:I:452:LEU:O	2.15	0.47
1:G:173:ALA:HB1	1:G:187:LEU:HD23	1.97	0.47
2:E:449:TYR:CD2	2:E:452:LEU:HB3	2.50	0.47
2:E:682:PRO:HB3	2:I:654:GLN:NE2	2.30	0.47
1:D:149:PRO:HD2	1:D:152:ILE:HD13	1.96	0.47
2:F:571:LYS:HB3	2:F:589:PHE:CZ	2.49	0.47
2:J:361:ARG:O	2:J:362:ILE:C	2.51	0.46
2:L:571:LYS:HB3	2:L:589:PHE:CZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:431:VAL:HG21	2:I:685:ILE:HG21	1.96	0.46
1:A:83:PHE:CZ	1:A:97:VAL:HG13	2.43	0.46
2:B:484:ALA:HB3	2:J:485:TYR:CD1	2.49	0.46
1:G:205:THR:HG22	1:G:236:ASN:HD22	1.81	0.46
2:I:432:ILE:CD1	2:I:472:LYS:HE3	2.45	0.46
1:A:205:THR:HG22	1:A:236:ASN:HD22	1.81	0.46
2:E:444:LYS:HD2	2:E:453:ARG:CD	2.45	0.46
2:I:694:LYS:CE	2:J:341:GLU:OE2	2.63	0.46
1:K:289:ILE:HG21	1:K:745:ILE:HD13	1.96	0.46
2:E:494:ILE:CD1	2:I:678:ARG:HD2	2.44	0.46
2:E:662:ILE:HD13	2:E:665:LEU:CD1	2.45	0.46
2:B:654:GLN:NE2	2:J:682:PRO:HB3	2.30	0.46
2:B:431:VAL:HG21	2:B:685:ILE:HG21	1.96	0.46
2:J:444:LYS:HD2	2:J:453:ARG:CD	2.45	0.46
2:E:325:LYS:HA	2:E:328:ALA:HB3	1.98	0.46
1:G:29:LEU:N	1:G:29:LEU:HD12	2.31	0.46
1:K:201:ILE:HG21	1:K:232:ILE:HD12	1.98	0.46
2:L:579:PHE:HD1	2:L:579:PHE:H	1.62	0.46
2:B:484:ALA:HB3	2:J:485:TYR:HD1	1.80	0.46
2:J:325:LYS:HA	2:J:328:ALA:HB3	1.98	0.46
1:K:140:MET:HE1	1:K:157:ARG:HG3	1.98	0.46
1:D:289:ILE:HG21	1:D:745:ILE:HD13	1.96	0.46
2:B:369:ARG:C	2:B:369:ARG:CD	2.84	0.46
1:G:259:PHE:HB3	1:G:272:MET:HB3	1.98	0.46
1:G:51:PHE:CD1	1:G:281:LEU:HD12	2.51	0.46
1:G:170:LEU:HD22	1:G:201:ILE:CG1	2.46	0.46
1:K:61:SER:HA	1:K:242:ILE:CD1	2.46	0.46
2:J:449:TYR:CD2	2:J:452:LEU:HB3	2.50	0.46
2:I:337:ALA:HB1	2:I:698:PHE:CD1	2.51	0.46
2:B:452:LEU:O	2:B:452:LEU:HD13	2.15	0.46
1:D:140:MET:CE	1:D:157:ARG:HA	2.46	0.45
2:I:687:HIS:HD2	2:I:688:LEU:HD21	1.77	0.45
1:A:29:LEU:HD12	1:A:29:LEU:N	2.31	0.45
1:K:229:ARG:HD2	1:K:280:VAL:HG21	1.99	0.45
2:F:579:PHE:HD1	2:F:579:PHE:H	1.62	0.45
1:A:9:LEU:HD23	1:A:290:ARG:CZ	2.46	0.45
2:E:485:TYR:HD1	2:I:484:ALA:HB3	1.80	0.45
1:K:23:ILE:HG22	1:K:25:GLN:HE21	1.82	0.45
2:E:388:ILE:HD11	2:E:412:ILE:HD11	1.98	0.45
2:E:662:ILE:HA	2:E:665:LEU:CD1	2.46	0.45
1:D:229:ARG:HD2	1:D:280:VAL:HG21	1.99	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:A:170:LEU:HD22	1:A:201:ILE:CG1	2.46	0.45
2:J:384:LEU:HD21	2:J:412:ILE:HG23	1.98	0.45
2:B:688:LEU:CD2	2:B:688:LEU:N	2.74	0.45
2:I:490:HIS:CD2	2:I:491:GLU:N	2.83	0.45
1:D:201:ILE:HG21	1:D:232:ILE:HD12	1.98	0.45
1:G:9:LEU:HD23	1:G:290:ARG:CZ	2.47	0.45
1:D:61:SER:HA	1:D:242:ILE:CD1	2.46	0.45
1:A:176:PRO:CB	1:A:206:LYS:HD2	2.46	0.45
2:B:409:PHE:CD1	2:B:666:VAL:HG13	2.51	0.45
1:A:98:ARG:HA	1:A:101:ILE:HD12	1.99	0.45
2:I:369:ARG:CD	2:I:369:ARG:C	2.84	0.45
2:B:490:HIS:CD2	2:B:491:GLU:N	2.83	0.45
2:J:329:LEU:HD23	2:J:702:LEU:HB3	1.99	0.45
2:E:675:LYS:CD	2:I:665:LEU:HD21	2.45	0.45
2:J:388:ILE:HD11	2:J:412:ILE:HD11	1.98	0.45
2:E:384:LEU:HD21	2:E:412:ILE:HG23	1.98	0.45
2:I:687:HIS:CD2	2:I:688:LEU:HD23	2.52	0.45
2:E:417:VAL:HB	2:E:479:ILE:CG2	2.43	0.45
1:D:61:SER:HA	1:D:242:ILE:HD13	1.99	0.45
1:D:74:VAL:HG21	1:D:123:ARG:NH2	2.31	0.45
2:E:683:LYS:HE2	2:I:658:GLN:HE21	1.82	0.45
2:I:676:THR:HG22	2:I:680:LEU:HD22	1.99	0.45
2:B:676:THR:HG22	2:B:680:LEU:HD22	1.99	0.45
2:B:370:PHE:CZ	2:B:374:LEU:HD21	2.52	0.45
2:B:374:LEU:HD13	2:B:423:PRO:CB	2.47	0.45
1:D:42:ALA:HB1	1:D:174:VAL:CG1	2.46	0.45
1:G:98:ARG:HA	1:G:101:ILE:HD12	1.99	0.45
2:B:367:HIS:CD2	2:B:682:PRO:HB3	2.52	0.45
2:H:545:LEU:HB2	2:H:550:LEU:HD13	1.98	0.45
2:B:470:ARG:HH11	2:B:470:ARG:HG3	1.82	0.45
2:I:374:LEU:HD13	2:I:423:PRO:CB	2.47	0.45
2:J:380:ASP:OD1	2:J:380:ASP:N	2.49	0.45
2:B:428:VAL:HG13	2:B:689:MET:CE	2.47	0.45
1:K:42:ALA:HB1	1:K:174:VAL:CG1	2.46	0.45
1:K:61:SER:HA	1:K:242:ILE:HD13	1.99	0.45
2:E:329:LEU:HD23	2:E:702:LEU:HB3	1.99	0.45
1:D:83:PHE:CZ	1:D:97:VAL:HG13	2.50	0.45
2:E:361:ARG:O	2:E:362:ILE:C	2.51	0.45
2:B:337:ALA:HB1	2:B:698:PHE:CD1	2.51	0.45
2:B:658:GLN:HE21	2:J:683:LYS:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:CD1	1:A:281:LEU:HD12	2.51	0.45
2:C:545:LEU:HB2	2:C:550:LEU:HD13	1.98	0.45
2:B:405:PRO:HA	2:B:662:ILE:CD1	2.47	0.45
2:I:370:PHE:CZ	2:I:374:LEU:HD21	2.52	0.45
2:E:380:ASP:N	2:E:380:ASP:OD1	2.49	0.45
2:E:493:PHE:CZ	2:E:665:LEU:HD23	2.52	0.45
2:I:474:GLN:HG2	2:I:688:LEU:CD1	2.47	0.45
1:K:74:VAL:HG21	1:K:123:ARG:NH2	2.31	0.45
1:G:309:LYS:HB3	1:G:309:LYS:NZ	2.31	0.45
1:K:140:MET:CE	1:K:157:ARG:HA	2.46	0.45
2:I:409:PHE:CD1	2:I:666:VAL:HG13	2.51	0.45
1:A:234:VAL:CG1	1:A:277:LEU:HD22	2.47	0.45
2:E:379:PHE:CE1	2:E:419:LYS:HB2	2.49	0.45
2:J:680:LEU:HA	2:J:680:LEU:HD12	1.88	0.45
1:K:113:LYS:HD2	1:K:113:LYS:N	2.32	0.45
2:B:429:ASP:HA	2:B:432:ILE:HD12	1.99	0.45
2:B:485:TYR:HB3	2:J:485:TYR:CE2	2.51	0.45
1:A:80:TYR:HB2	1:A:90:LYS:HB3	1.98	0.45
1:D:23:ILE:HG22	1:D:25:GLN:HE21	1.82	0.45
2:J:406:ASP:OD1	2:J:407:MET:N	2.50	0.44
2:B:474:GLN:HG2	2:B:688:LEU:CD1	2.47	0.44
2:I:703:ALA:HA	2:J:699:SER:CA	2.45	0.44
1:G:234:VAL:CG1	1:G:277:LEU:HD22	2.47	0.44
1:K:235:VAL:HG23	1:K:255:GLU:HA	1.99	0.44
2:I:429:ASP:HA	2:I:432:ILE:HD12	1.99	0.44
1:A:309:LYS:HB3	1:A:309:LYS:NZ	2.31	0.44
2:I:470:ARG:HG3	2:I:470:ARG:HH11	1.82	0.44
1:G:80:TYR:HB2	1:G:90:LYS:HB3	1.98	0.44
2:J:662:ILE:HA	2:J:665:LEU:CD1	2.46	0.44
2:I:490:HIS:CG	2:I:491:GLU:N	2.81	0.44
2:B:409:PHE:HD1	2:B:666:VAL:HG13	1.81	0.44
2:I:428:VAL:HG13	2:I:689:MET:CE	2.47	0.44
2:I:367:HIS:CD2	2:I:682:PRO:HB3	2.52	0.44
2:E:406:ASP:OD1	2:E:407:MET:N	2.50	0.44
2:I:405:PRO:HA	2:I:662:ILE:CD1	2.47	0.44
2:I:491:GLU:OE2	2:I:492:ASP:N	2.49	0.44
2:E:692:ASN:C	2:E:692:ASN:ND2	2.70	0.44
1:D:113:LYS:N	1:D:113:LYS:HD2	2.32	0.44
2:E:485:TYR:CE2	2:I:485:TYR:HB3	2.51	0.44
2:E:464:ILE:HG13	2:E:693:THR:HG23	1.98	0.44
2:J:464:ILE:HG13	2:J:693:THR:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:PHE:CE2	2:E:332:MET:HA	2.52	0.44
2:B:665:LEU:HD21	2:J:675:LYS:CD	2.46	0.44
2:I:409:PHE:HD1	2:I:666:VAL:HG13	1.81	0.44
1:K:58:PRO:HG3	1:K:101:ILE:CG2	2.47	0.44
2:H:600:TYR:O	2:H:601:ARG:HB2	2.18	0.44
2:B:490:HIS:CG	2:B:491:GLU:N	2.81	0.44
2:B:491:GLU:OE2	2:B:492:ASP:N	2.49	0.44
1:D:58:PRO:HG3	1:D:101:ILE:CG2	2.47	0.44
2:J:370:PHE:CE1	2:J:427:CYS:HB2	2.53	0.44
1:D:235:VAL:HG23	1:D:255:GLU:HA	1.99	0.44
1:D:235:VAL:CG2	1:D:255:GLU:HA	2.48	0.44
1:K:84:LEU:HD13	1:K:121:ASN:HD22	1.82	0.44
2:I:341:GLU:HG3	2:J:341:GLU:OE2	2.09	0.44
1:D:140:MET:HE1	1:D:157:ARG:HG3	2.00	0.44
1:D:84:LEU:HD13	1:D:121:ASN:HD22	1.82	0.44
2:I:417:VAL:HB	2:I:479:ILE:HG23	2.00	0.44
2:J:332:MET:HA	1:K:317:PHE:CE2	2.52	0.44
2:J:493:PHE:CZ	2:J:665:LEU:HD23	2.52	0.44
2:L:543:PHE:HD2	2:L:550:LEU:HD21	1.83	0.44
1:G:46:SER:HA	1:G:237:ARG:HH21	1.82	0.44
2:B:380:ASP:N	2:B:380:ASP:OD1	2.49	0.43
1:K:235:VAL:CG2	1:K:255:GLU:HA	2.48	0.43
2:I:474:GLN:HG2	2:I:688:LEU:HD12	2.00	0.43
2:I:380:ASP:OD1	2:I:380:ASP:N	2.49	0.43
1:A:83:PHE:CZ	1:A:122:LEU:HD22	2.53	0.43
2:C:596:VAL:HG13	2:C:597:TYR:HD1	1.83	0.43
2:E:370:PHE:CE1	2:E:427:CYS:HB2	2.53	0.43
2:I:357:SER:N	2:I:434:GLU:HG3	2.33	0.43
1:A:46:SER:HA	1:A:237:ARG:HH21	1.82	0.43
1:G:83:PHE:CZ	1:G:122:LEU:HD22	2.53	0.43
2:H:526:LEU:HD13	2:H:605:LEU:HB3	2.00	0.43
2:J:449:TYR:HA	2:J:450:PRO:HD2	1.94	0.43
2:E:491:GLU:HG2	2:E:491:GLU:O	2.18	0.43
2:J:344:ILE:HG21	2:J:690:ILE:HD11	2.01	0.43
1:G:232:ILE:CG1	1:G:280:VAL:HG21	2.49	0.43
1:A:232:ILE:CG1	1:A:280:VAL:HG21	2.49	0.43
2:I:361:ARG:O	2:I:362:ILE:C	2.52	0.43
2:J:369:ARG:CD	2:J:369:ARG:C	2.87	0.43
2:L:600:TYR:O	2:L:601:ARG:HB2	2.18	0.43
1:A:31:LEU:CD2	1:A:130:LEU:HD12	2.48	0.43
2:E:344:ILE:HG21	2:E:690:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:680:LEU:HD12	2:E:680:LEU:HA	1.87	0.43
2:F:624:GLY:HA2	2:F:626:TYR:CZ	2.54	0.43
2:C:526:LEU:HD13	2:C:605:LEU:HB3	2.00	0.43
1:G:16:LEU:HD21	1:G:742:ILE:HG12	2.00	0.43
2:I:459:ILE:HD13	2:I:705:LEU:HA	2.00	0.43
1:G:176:PRO:CB	1:G:206:LYS:HD2	2.46	0.43
2:B:474:GLN:HG2	2:B:688:LEU:HD12	2.00	0.43
2:L:621:LEU:HD23	2:L:627:PRO:HD3	2.01	0.43
2:L:573:ARG:CD	2:L:575:VAL:HG22	2.48	0.43
2:F:621:LEU:HD23	2:F:627:PRO:HD3	2.01	0.43
2:C:600:TYR:O	2:C:601:ARG:HB2	2.18	0.43
2:I:381:GLU:HG2	2:I:382:LYS:HG3	2.00	0.43
2:E:452:LEU:C	2:E:452:LEU:CD1	2.87	0.43
1:A:67:ARG:HH22	1:A:107:ARG:HH21	1.67	0.43
1:G:67:ARG:HH22	1:G:107:ARG:HH21	1.67	0.43
1:G:209:LEU:HD11	1:G:238:SER:CB	2.47	0.43
2:E:664:ASN:HA	2:E:664:ASN:HD22	1.62	0.43
2:H:596:VAL:HG13	2:H:597:TYR:HD1	1.83	0.43
1:A:9:LEU:CD1	1:A:286:THR:HG23	2.49	0.43
1:D:191:LYS:NZ	1:D:225:LEU:HG	2.33	0.43
1:G:63:ILE:HG21	1:G:148:GLN:HE22	1.84	0.43
1:G:66:ARG:HB2	1:G:105:THR:CG2	2.48	0.43
2:L:624:GLY:HA2	2:L:626:TYR:CZ	2.54	0.43
2:B:417:VAL:HB	2:B:479:ILE:HG23	2.00	0.43
2:B:683:LYS:HD3	2:J:405:PRO:CB	2.49	0.43
2:J:452:LEU:CD1	2:J:452:LEU:C	2.87	0.43
2:J:448:GLN:CD	1:K:314:TYR:O	2.57	0.43
2:I:694:LYS:HE2	2:J:341:GLU:OE2	2.19	0.43
2:E:329:LEU:CG	2:E:702:LEU:HD22	2.45	0.43
1:A:209:LEU:HD11	1:A:238:SER:CB	2.47	0.43
2:E:381:GLU:HG2	2:E:382:LYS:HG3	2.00	0.43
1:K:48:LEU:HB3	1:K:57:LEU:CD1	2.49	0.42
1:G:56:PHE:CB	1:G:94:PHE:HB3	2.48	0.42
2:F:573:ARG:CD	2:F:575:VAL:HG22	2.48	0.42
1:K:170:LEU:HD11	1:K:281:LEU:CD2	2.50	0.42
2:E:340:PHE:O	2:E:341:GLU:C	2.53	0.42
1:G:167:GLU:O	1:G:168:ASN:HB2	2.19	0.42
1:A:16:LEU:HD21	1:A:742:ILE:HG12	2.00	0.42
1:A:63:ILE:HG21	1:A:148:GLN:HE22	1.84	0.42
1:A:66:ARG:HB2	1:A:105:THR:CG2	2.48	0.42
1:D:48:LEU:HB3	1:D:57:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:567:VAL:HG13	2:C:625:VAL:CG2	2.50	0.42
2:H:567:VAL:HG13	2:H:625:VAL:CG2	2.50	0.42
1:K:289:ILE:HG21	1:K:745:ILE:HG21	2.02	0.42
2:B:374:LEU:HD22	2:B:374:LEU:H	1.84	0.42
2:I:463:HIS:HE1	2:J:334:GLN:CD	2.20	0.42
2:E:684:THR:HG22	2:E:685:ILE:N	2.34	0.42
2:J:467:ARG:HA	2:J:467:ARG:HD3	1.86	0.42
2:B:329:LEU:HA	2:B:329:LEU:HD12	1.87	0.42
2:B:459:ILE:HD13	2:B:705:LEU:HA	2.00	0.42
1:G:31:LEU:CD2	1:G:130:LEU:HD12	2.48	0.42
2:B:357:SER:N	2:B:434:GLU:HG3	2.33	0.42
2:E:405:PRO:CB	2:I:683:LYS:HD3	2.49	0.42
2:C:627:PRO:O	2:C:628:GLU:HB2	2.20	0.42
2:B:381:GLU:HG2	2:B:382:LYS:HG3	2.01	0.42
2:E:369:ARG:CD	2:E:369:ARG:C	2.87	0.42
1:K:13:VAL:HG13	1:K:29:LEU:CD1	2.49	0.42
2:I:374:LEU:HD22	2:I:374:LEU:H	1.84	0.42
2:B:371:PRO:HA	2:B:374:LEU:HD23	2.02	0.42
2:J:664:ASN:HA	2:J:664:ASN:HD22	1.62	0.42
2:B:406:ASP:OD1	2:B:407:MET:N	2.52	0.42
2:F:543:PHE:HD2	2:F:550:LEU:HD21	1.83	0.42
2:J:491:GLU:HG2	2:J:491:GLU:O	2.18	0.42
2:I:371:PRO:HA	2:I:374:LEU:HD23	2.02	0.42
1:K:191:LYS:NZ	1:K:225:LEU:HG	2.33	0.42
2:E:456:MET:HB2	2:E:456:MET:HE2	1.95	0.42
2:J:381:GLU:HG2	2:J:382:LYS:HG3	2.00	0.42
2:J:687:HIS:C	2:J:688:LEU:HD23	2.40	0.42
2:J:420:ILE:HD11	2:J:673:VAL:HG11	2.02	0.42
2:B:452:LEU:C	2:B:452:LEU:CD1	2.88	0.42
1:D:55:ASP:HB3	1:D:98:ARG:CD	2.50	0.42
1:A:167:GLU:O	1:A:168:ASN:HB2	2.19	0.42
1:D:237:ARG:HG3	1:D:251:ALA:HB2	2.02	0.42
1:D:140:MET:HE2	1:D:157:ARG:HA	2.00	0.42
2:B:388:ILE:CG1	2:B:409:PHE:HA	2.50	0.42
2:I:388:ILE:CG1	2:I:409:PHE:HA	2.50	0.42
2:I:452:LEU:C	2:I:452:LEU:CD1	2.88	0.42
1:G:140:MET:CE	1:G:160:LEU:HD21	2.49	0.42
2:I:406:ASP:OD1	2:I:407:MET:N	2.52	0.42
1:K:237:ARG:HG3	1:K:251:ALA:HB2	2.02	0.42
2:L:551:SER:HB2	2:L:553:TYR:HE1	1.85	0.42
2:H:627:PRO:O	2:H:628:GLU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:456:MET:SD	2:J:701:LEU:HD21	2.60	0.42
2:J:654:GLN:O	2:J:654:GLN:HG2	2.20	0.42
2:E:654:GLN:HG2	2:E:654:GLN:O	2.20	0.42
2:E:420:ILE:HD11	2:E:673:VAL:HG11	2.02	0.42
1:G:9:LEU:CD1	1:G:286:THR:HG23	2.49	0.42
1:K:234:VAL:HA	1:K:255:GLU:HG3	2.01	0.42
1:D:314:TYR:O	2:E:448:GLN:CD	2.57	0.42
1:D:316:ASN:HB3	2:E:332:MET:CG	2.47	0.42
1:G:23:ILE:HG12	1:G:734:ALA:HB1	2.02	0.42
1:D:170:LEU:HD11	1:D:281:LEU:CD2	2.50	0.42
2:J:684:THR:HG22	2:J:685:ILE:N	2.34	0.42
2:B:467:ARG:HA	2:B:467:ARG:HD3	1.87	0.42
2:F:600:TYR:O	2:F:601:ARG:HB2	2.18	0.42
2:I:707:SER:HA	2:J:702:LEU:CB	2.47	0.41
2:F:535:LYS:O	2:F:535:LYS:HG2	2.20	0.41
2:C:579:PHE:HD1	2:C:579:PHE:H	1.62	0.41
2:I:692:ASN:ND2	2:I:692:ASN:C	2.72	0.41
1:A:135:VAL:HG12	1:A:137:LEU:HG	2.02	0.41
1:K:34:ILE:HG22	1:K:48:LEU:HD11	2.01	0.41
2:E:329:LEU:HA	2:E:329:LEU:HD12	1.86	0.41
1:D:289:ILE:HG21	1:D:745:ILE:HG21	2.01	0.41
2:L:535:LYS:O	2:L:535:LYS:HG2	2.20	0.41
2:C:607:CYS:HB2	2:C:613:VAL:HG23	2.03	0.41
1:D:234:VAL:HA	1:D:255:GLU:HG3	2.02	0.41
1:K:55:ASP:HB3	1:K:98:ARG:CD	2.50	0.41
1:G:135:VAL:HG12	1:G:137:LEU:HG	2.02	0.41
2:E:687:HIS:C	2:E:688:LEU:HD23	2.40	0.41
2:E:493:PHE:CZ	2:E:664:ASN:HB3	2.55	0.41
1:D:66:ARG:O	1:D:67:ARG:HG3	2.20	0.41
1:A:23:ILE:HG12	1:A:734:ALA:HB1	2.02	0.41
2:E:478:LEU:CD1	2:E:680:LEU:HD23	2.50	0.41
2:H:553:TYR:CD1	2:H:558:GLU:HG2	2.56	0.41
2:L:539:LYS:HG2	2:L:540:GLU:H	1.85	0.41
2:J:455:GLU:HG2	2:J:705:LEU:CD1	2.50	0.41
2:J:493:PHE:CZ	2:J:664:ASN:HB3	2.55	0.41
1:G:134:LEU:N	1:G:134:LEU:HD12	2.36	0.41
2:J:478:LEU:CD1	2:J:680:LEU:HD23	2.50	0.41
1:K:191:LYS:HZ3	1:K:227:LEU:HG	1.85	0.41
1:D:78:THR:HB	1:D:80:TYR:CE1	2.56	0.41
2:L:596:VAL:HG13	2:L:597:TYR:HD1	1.85	0.41
2:J:340:PHE:O	2:J:341:GLU:C	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ILE:HG22	1:D:48:LEU:HD11	2.01	0.41
2:F:543:PHE:CD2	2:F:550:LEU:HD21	2.56	0.41
2:F:596:VAL:HG13	2:F:597:TYR:HD1	1.85	0.41
2:I:687:HIS:C	2:I:688:LEU:HD23	2.41	0.41
1:K:66:ARG:O	1:K:67:ARG:HG3	2.20	0.41
2:E:456:MET:SD	2:E:701:LEU:HD21	2.60	0.41
1:K:135:VAL:HG21	1:K:163:PHE:CD1	2.56	0.41
1:D:13:VAL:HG13	1:D:29:LEU:CD1	2.49	0.41
2:I:439:VAL:HA	2:I:697:ILE:HB	2.03	0.41
1:D:204:ILE:HB	1:D:207:LEU:HD11	2.03	0.41
2:B:654:GLN:O	2:B:654:GLN:HG2	2.20	0.41
1:G:63:ILE:HG21	1:G:148:GLN:NE2	2.36	0.41
2:F:551:SER:HB2	2:F:553:TYR:HE1	1.85	0.41
2:I:435:LEU:HD23	2:I:436:ILE:N	2.36	0.41
1:K:78:THR:HB	1:K:80:TYR:CE1	2.56	0.41
1:G:301:GLN:HA	1:G:301:GLN:HE21	1.85	0.41
2:H:583:LYS:HD2	2:H:606:ALA:HB1	2.03	0.41
2:E:406:ASP:HB3	2:I:680:LEU:HD11	2.02	0.41
2:B:680:LEU:HD11	2:J:406:ASP:HB3	2.02	0.41
2:J:687:HIS:CD2	2:J:688:LEU:HD23	2.53	0.41
2:I:490:HIS:CE1	2:I:672:ILE:HG21	2.56	0.41
1:A:134:LEU:HD12	1:A:134:LEU:N	2.35	0.41
2:I:384:LEU:HG	2:I:666:VAL:HG12	2.03	0.41
1:K:204:ILE:HB	1:K:207:LEU:HD11	2.03	0.41
2:B:333:VAL:O	2:B:333:VAL:CG1	2.66	0.41
2:I:654:GLN:O	2:I:654:GLN:HG2	2.20	0.41
2:J:692:ASN:ND2	2:J:692:ASN:C	2.70	0.41
2:B:684:THR:HG22	2:B:685:ILE:N	2.35	0.41
2:I:340:PHE:HD2	2:I:694:LYS:HG3	1.85	0.41
2:I:329:LEU:HD12	2:I:329:LEU:HA	1.88	0.41
2:B:439:VAL:HA	2:B:697:ILE:HB	2.03	0.41
2:H:607:CYS:HB2	2:H:613:VAL:HG23	2.03	0.41
2:B:340:PHE:HD2	2:B:694:LYS:HG3	1.85	0.41
2:I:684:THR:HG22	2:I:685:ILE:N	2.35	0.41
2:L:543:PHE:CD2	2:L:550:LEU:HD21	2.56	0.41
1:A:307:ILE:HG21	1:A:728:MET:HB3	2.03	0.41
1:G:138:PRO:HG2	1:G:159:MET:SD	2.61	0.41
1:K:274:THR:HB	1:K:275:PRO:HD3	2.03	0.41
1:D:315:LYS:HA	2:E:448:GLN:HE22	1.86	0.40
1:A:140:MET:CE	1:A:160:LEU:HD21	2.49	0.40
1:D:170:LEU:HD12	1:D:170:LEU:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:583:LYS:HD2	2:C:606:ALA:HB1	2.03	0.40
1:G:262:HIS:HA	1:G:263:PRO:HD2	1.90	0.40
2:B:435:LEU:HD23	2:B:436:ILE:N	2.35	0.40
1:D:274:THR:HB	1:D:275:PRO:HD3	2.03	0.40
2:B:490:HIS:CE1	2:B:672:ILE:HG21	2.56	0.40
2:E:455:GLU:HG2	2:E:705:LEU:CD1	2.50	0.40
2:F:573:ARG:HD2	2:F:575:VAL:HG22	2.04	0.40
1:A:164:VAL:HG21	1:A:193:VAL:HG11	2.03	0.40
1:A:87:LYS:O	1:A:87:LYS:HG3	2.20	0.40
1:K:201:ILE:HD12	1:K:277:LEU:CD1	2.51	0.40
1:A:63:ILE:HG21	1:A:148:GLN:NE2	2.36	0.40
2:F:539:LYS:HG2	2:F:540:GLU:H	1.85	0.40
2:E:391:ALA:CB	2:E:408:ALA:HA	2.50	0.40
1:K:140:MET:HE2	1:K:157:ARG:HA	2.03	0.40
2:J:489:ASN:C	2:J:490:HIS:O	2.59	0.40
2:J:384:LEU:HD21	2:J:412:ILE:CG2	2.52	0.40
2:C:553:TYR:CD1	2:C:558:GLU:HG2	2.56	0.40
2:I:369:ARG:HD3	2:I:369:ARG:C	2.42	0.40
2:J:456:MET:HE2	2:J:456:MET:HB2	1.95	0.40
2:B:330:LEU:HD22	2:B:330:LEU:HA	1.89	0.40
1:G:307:ILE:HG21	1:G:728:MET:HB3	2.03	0.40
1:D:135:VAL:HG21	1:D:163:PHE:CD1	2.56	0.40
2:B:384:LEU:HG	2:B:666:VAL:HG12	2.03	0.40
1:G:87:LYS:HG3	1:G:87:LYS:O	2.20	0.40
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.91	0.40
2:B:369:ARG:C	2:B:369:ARG:HD3	2.42	0.40
1:A:170:LEU:HD22	1:A:201:ILE:HG12	2.02	0.40
1:A:301:GLN:HA	1:A:301:GLN:HE21	1.85	0.40
1:A:138:PRO:HG2	1:A:159:MET:SD	2.62	0.40
1:G:66:ARG:HB3	1:G:115:ILE:HG22	2.04	0.40
2:B:384:LEU:HD22	2:B:670:MET:CG	2.50	0.40
2:I:384:LEU:HD22	2:I:670:MET:CG	2.50	0.40
1:G:164:VAL:HG21	1:G:193:VAL:HG11	2.04	0.40
2:H:573:ARG:HB2	2:H:630:VAL:HA	2.04	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%)	319 (96%)	13 (4%)	1 (0%)	46	83
1	G	325/864 (38%)	313 (96%)	10 (3%)	2 (1%)	30	74
1	K	333/864 (38%)	319 (96%)	13 (4%)	1 (0%)	46	83
2	B	194/864 (22%)	158 (81%)	28 (14%)	8 (4%)	3	35
2	C	111/864 (13%)	94 (85%)	12 (11%)	5 (4%)	3	33
2	E	194/864 (22%)	166 (86%)	23 (12%)	5 (3%)	7	45
2	F	111/864 (13%)	93 (84%)	16 (14%)	2 (2%)	11	53
2	H	111/864 (13%)	94 (85%)	12 (11%)	5 (4%)	3	33
2	I	194/864 (22%)	158 (81%)	29 (15%)	7 (4%)	4	38
2	J	194/864 (22%)	166 (86%)	23 (12%)	5 (3%)	7	45
2	L	111/864 (13%)	93 (84%)	16 (14%)	2 (2%)	11	53
All	All	2536/10368 (24%)	2286 (90%)	205 (8%)	45 (2%)	15	53

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	GLY
2	B	442	CYS
2	B	490	HIS
2	B	690	ILE
2	C	523	LYS
2	C	576	GLU
2	E	490	HIS
2	F	576	GLU
1	G	88	GLY
2	H	523	LYS
2	H	576	GLU
2	I	442	CYS

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Mol	Chain	Res	Type
2	I	490	HIS
2	I	690	ILE
2	J	490	HIS
2	L	576	GLU
2	B	492	ASP
2	C	534	MET
2	H	534	MET
2	I	492	ASP
2	B	689	MET
2	B	696	PHE
2	C	577	LYS
2	C	628	GLU
1	D	79	GLU
2	E	492	ASP
2	F	577	LYS
2	H	577	LYS
2	H	628	GLU
2	I	689	MET
2	I	696	PHE
2	J	492	ASP
1	K	79	GLU
2	L	577	LYS
2	E	377	MET
2	E	412	ILE
2	E	689	MET
2	J	377	MET
2	J	412	ILE
2	J	689	MET
1	A	87	LYS
1	G	87	LYS
2	B	481	ILE
2	I	481	ILE
2	B	365	ILE

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
1	K	295/761 (39%)	281 (95%)	14 (5%)	32	68
2	B	191/761 (25%)	158 (83%)	33 (17%)	2	17
2	C	102/761 (13%)	91 (89%)	11 (11%)	8	35
2	E	191/761 (25%)	151 (79%)	40 (21%)	1	10
2	F	102/761 (13%)	89 (87%)	13 (13%)	5	29
2	H	102/761 (13%)	91 (89%)	11 (11%)	8	35
2	I	191/761 (25%)	158 (83%)	33 (17%)	2	17
2	J	191/761 (25%)	151 (79%)	40 (21%)	1	10
2	L	102/761 (13%)	89 (87%)	13 (13%)	5	29
All	All	2336/9132 (26%)	2090 (90%)	246 (10%)	13	36

All (246) 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	366	PHE
2	B	368	GLU
2	B	369	ARG

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Mol	Chain	Res	Type
2	B	373	GLU
2	B	380	ASP
2	B	441	GLN
2	B	445	LYS
2	B	449	TYR
2	B	451	ARG
2	B	468	GLU
2	B	486	MET
2	B	489	ASN
2	B	490	HIS
2	B	491	GLU
2	B	492	ASP
2	B	493	PHE
2	B	664	ASN
2	B	667	ASP
2	B	679	ASP
2	B	685	ILE
2	B	688	LEU
2	B	692	ASN
2	B	697	ILE
2	B	698	PHE
2	B	700	GLU
2	B	702	LEU
2	C	535	LYS
2	C	560	GLU
2	C	571	LYS
2	C	577	LYS
2	C	579	PHE
2	C	581	SER
2	C	584	HIS
2	C	592	GLU
2	C	594	ARG
2	C	603	LEU
2	C	610	GLN
1	D	34	ILE
1	D	78	THR
1	D	87	LYS
1	D	99	LEU
1	D	113	LYS
1	D	140	MET
1	D	225	LEU
1	D	228	ARG

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Mol	Chain	Res	Type
1	D	248	ILE
1	D	260	LEU
1	D	297	ARG
1	D	304	LEU
1	D	316	ASN
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	366	PHE
2	E	367	HIS
2	E	368	GLU
2	E	369	ARG
2	E	377	MET
2	E	380	ASP
2	E	415	LYS
2	E	416	GLN
2	E	418	LYS
2	E	443	THR
2	E	445	LYS
2	E	449	TYR
2	E	451	ARG
2	E	452	LEU
2	E	453	ARG
2	E	468	GLU
2	E	473	GLU
2	E	480	ASP
2	E	482	GLU
2	E	483	LEU
2	E	489	ASN
2	E	491	GLU
2	E	493	PHE
2	E	664	ASN
2	E	672	ILE
2	E	678	ARG
2	E	679	ASP
2	E	685	ILE
2	E	688	LEU

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Mol	Chain	Res	Type
2	E	692	ASN
2	E	697	ILE
2	E	698	PHE
2	E	702	LEU
2	F	551	SER
2	F	553	TYR
2	F	558	GLU
2	F	560	GLU
2	F	563	TYR
2	F	569	ASN
2	F	571	LYS
2	F	574	ASP
2	F	577	LYS
2	F	579	PHE
2	F	581	SER
2	F	594	ARG
2	F	603	LEU
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	535	LYS
2	H	560	GLU
2	H	571	LYS
2	H	577	LYS
2	H	579	PHE
2	H	581	SER
2	H	584	HIS
2	H	592	GLU
2	H	594	ARG
2	H	603	LEU
2	H	610	GLN
2	I	327	LYS
2	I	329	LEU

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Mol	Chain	Res	Type
2	I	330	LEU
2	I	339	ASP
2	I	340	PHE
2	I	345	GLU
2	I	357	SER
2	I	366	PHE
2	I	368	GLU
2	I	369	ARG
2	I	373	GLU
2	I	380	ASP
2	I	441	GLN
2	I	445	LYS
2	I	449	TYR
2	I	451	ARG
2	I	468	GLU
2	I	486	MET
2	I	489	ASN
2	I	490	HIS
2	I	491	GLU
2	I	492	ASP
2	I	493	PHE
2	I	664	ASN
2	I	667	ASP
2	I	679	ASP
2	I	685	ILE
2	I	688	LEU
2	I	692	ASN
2	I	697	ILE
2	I	698	PHE
2	I	700	GLU
2	I	702	LEU
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
2	J	366	PHE
2	J	367	HIS
2	J	368	GLU
2	J	369	ARG

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Mol	Chain	Res	Type
2	J	377	MET
2	J	380	ASP
2	J	415	LYS
2	J	416	GLN
2	J	418	LYS
2	J	443	THR
2	J	445	LYS
2	J	449	TYR
2	J	451	ARG
2	J	452	LEU
2	J	453	ARG
2	J	468	GLU
2	J	473	GLU
2	J	480	ASP
2	J	482	GLU
2	J	483	LEU
2	J	489	ASN
2	J	491	GLU
2	J	493	PHE
2	J	664	ASN
2	J	672	ILE
2	J	678	ARG
2	J	679	ASP
2	J	685	ILE
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	140	MET
1	K	225	LEU
1	K	228	ARG
1	K	248	ILE
1	K	260	LEU
1	K	297	ARG
1	K	304	LEU
1	K	316	ASN

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Mol	Chain	Res	Type
1	K	318	ARG
2	L	551	SER
2	L	553	TYR
2	L	558	GLU
2	L	560	GLU
2	L	563	TYR
2	L	569	ASN
2	L	571	LYS
2	L	574	ASP
2	L	577	LYS
2	L	579	PHE
2	L	581	SER
2	L	594	ARG
2	L	603	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) 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	335	GLN
2	B	367	HIS
2	B	487	ASN
2	B	654	GLN
2	B	658	GLN
2	B	664	ASN
2	B	687	HIS
2	B	692	ASN
2	C	529	ASN
1	D	40	GLN
1	D	121	ASN
1	D	148	GLN
1	D	155	GLN
1	D	236	ASN
1	D	282	ASN
1	D	303	GLN
1	D	316	ASN
2	E	331	GLN
2	E	335	GLN

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Mol	Chain	Res	Type
2	E	448	GLN
2	E	490	HIS
2	E	658	GLN
2	E	664	ASN
2	E	687	HIS
2	E	692	ASN
2	F	610	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	I	335	GLN
2	I	367	HIS
2	I	463	HIS
2	I	487	ASN
2	I	654	GLN
2	I	658	GLN
2	I	664	ASN
2	I	687	HIS
2	I	692	ASN
2	J	331	GLN
2	J	335	GLN
2	J	448	GLN
2	J	490	HIS
2	J	658	GLN
2	J	664	ASN
2	J	687	HIS
2	J	691	ASN
2	J	692	ASN
1	K	40	GLN
1	K	121	ASN
1	K	148	GLN
1	K	155	GLN
1	K	198	GLN
1	K	236	ASN
1	K	282	ASN
1	K	303	GLN
1	K	316	ASN
2	L	610	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.