Full wwPDB EM Validation Report (i)

Mar 5, 2026 – 07:47 PM UTC

PDB ID	:	4UUD / pdb_00004uud
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 initial models	:	3ZYC, 1DYN, 3SNH

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

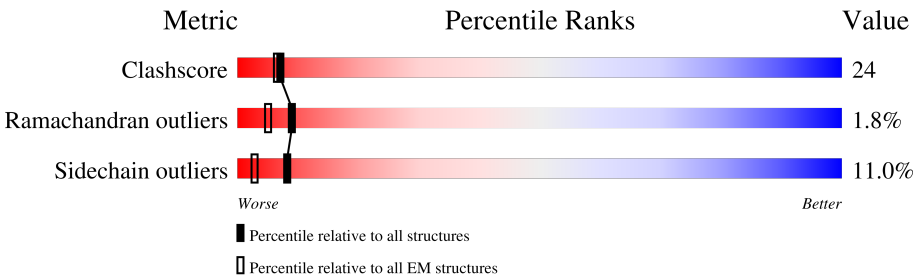
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

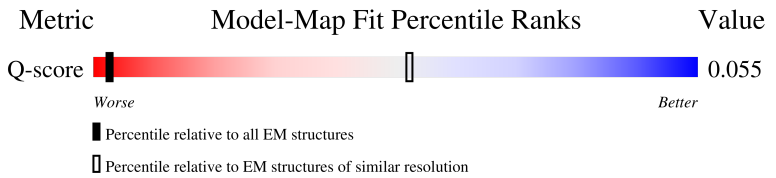
1 Overall quality at a glance (i)

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	96 (12.00 - 13.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	864	21% 14% • 62%
1	D	864	22% 13% • • 61%
1	G	864	21% 14% • 62%
1	K	864	22% 13% • • 61%

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Mol	Chain	Length	Quality of chain
2	B	864	7% 8% 6% • 76%
2	C	864	6% • •• 87%
2	E	864	6% 9% 6% • 76%
2	F	864	6% 5% •• 87%
2	H	864	6% • •• 87%
2	I	864	7% 9% 5% • 76%
2	J	864	6% 9% 6% • 76%
2	L	864	6% 5% •• 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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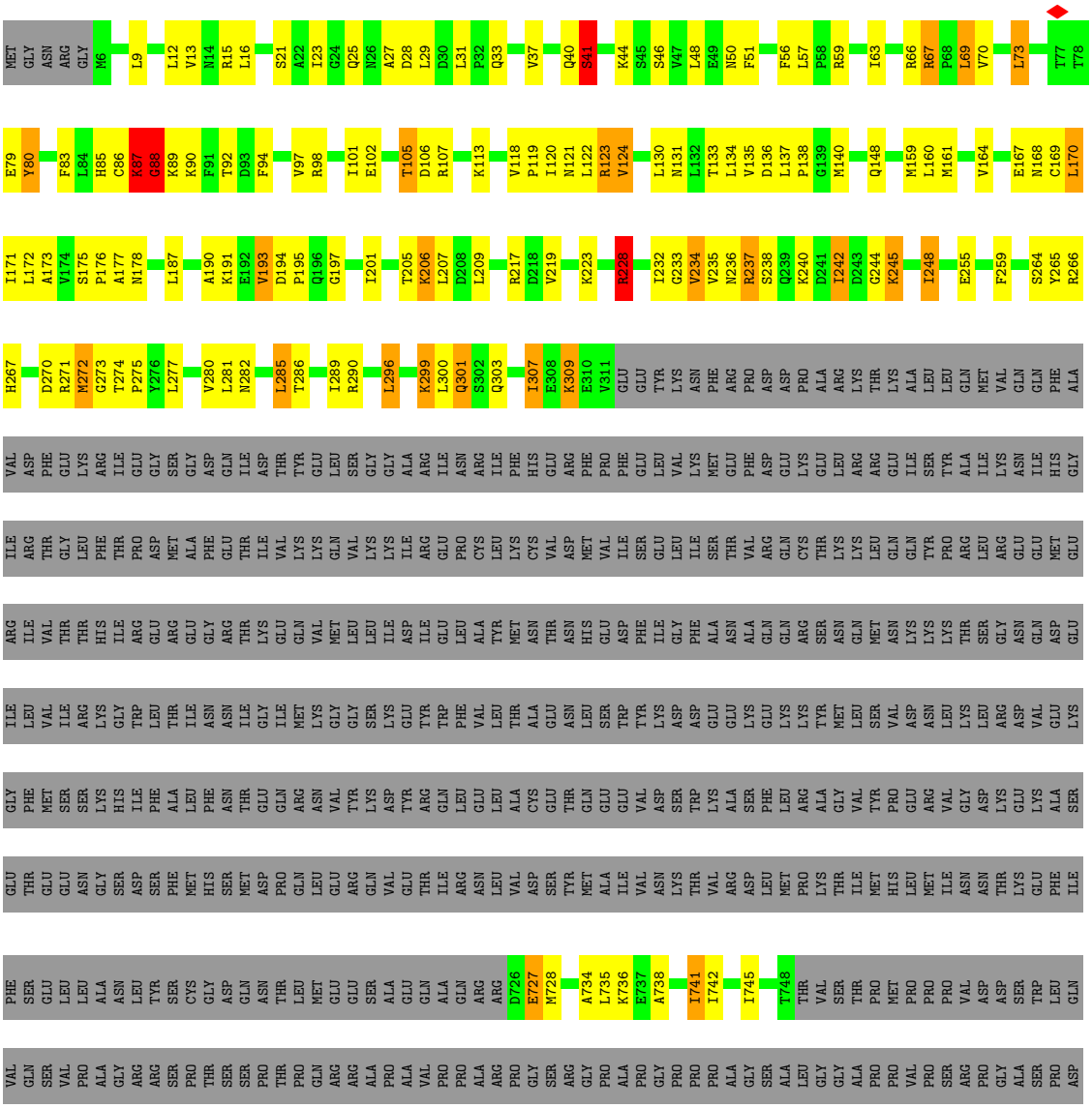
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L	113	946	609	158	175	4	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

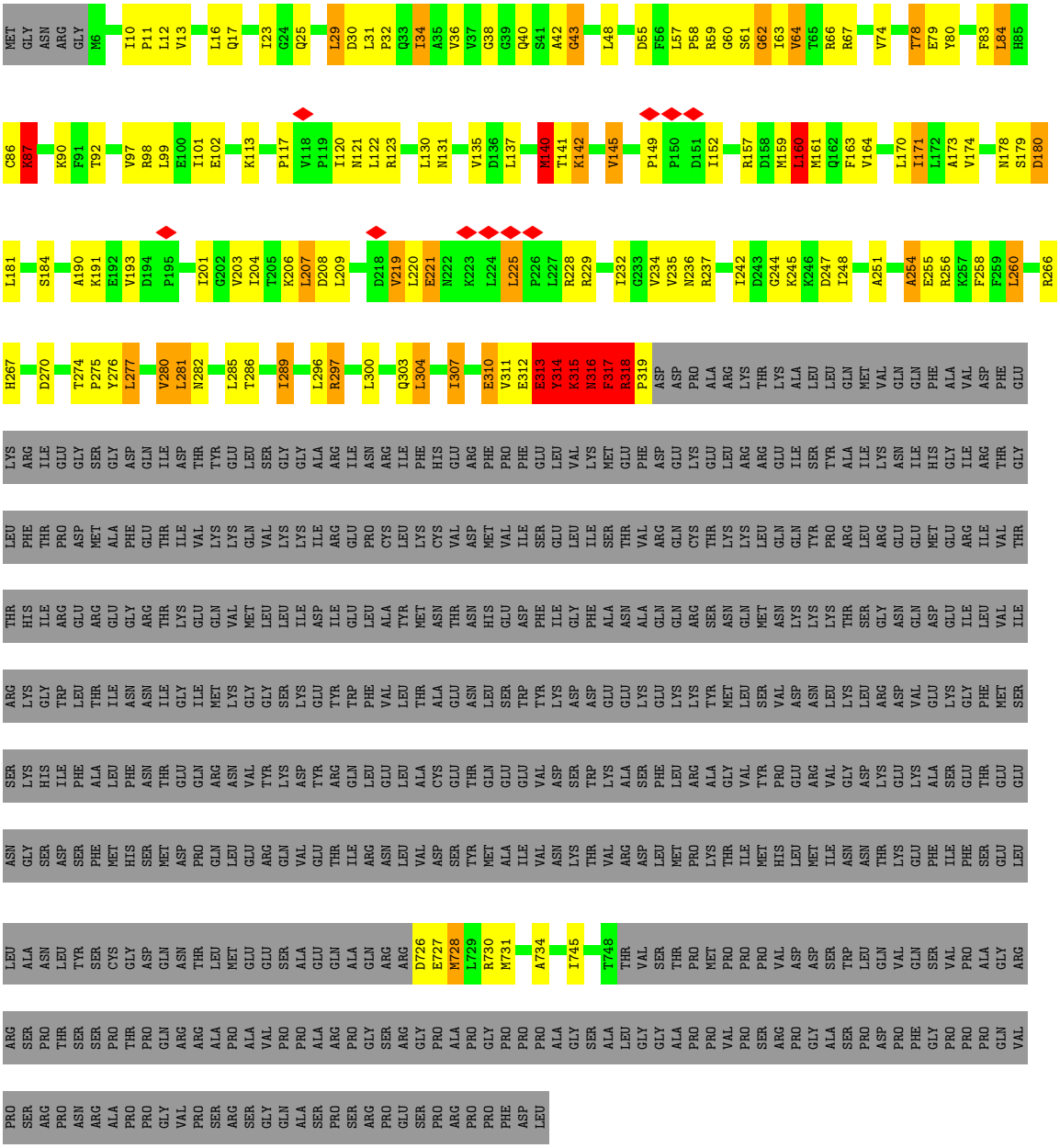
- Molecule 1: DYNAMIN-1

Chain A: 21% 14% • 62%



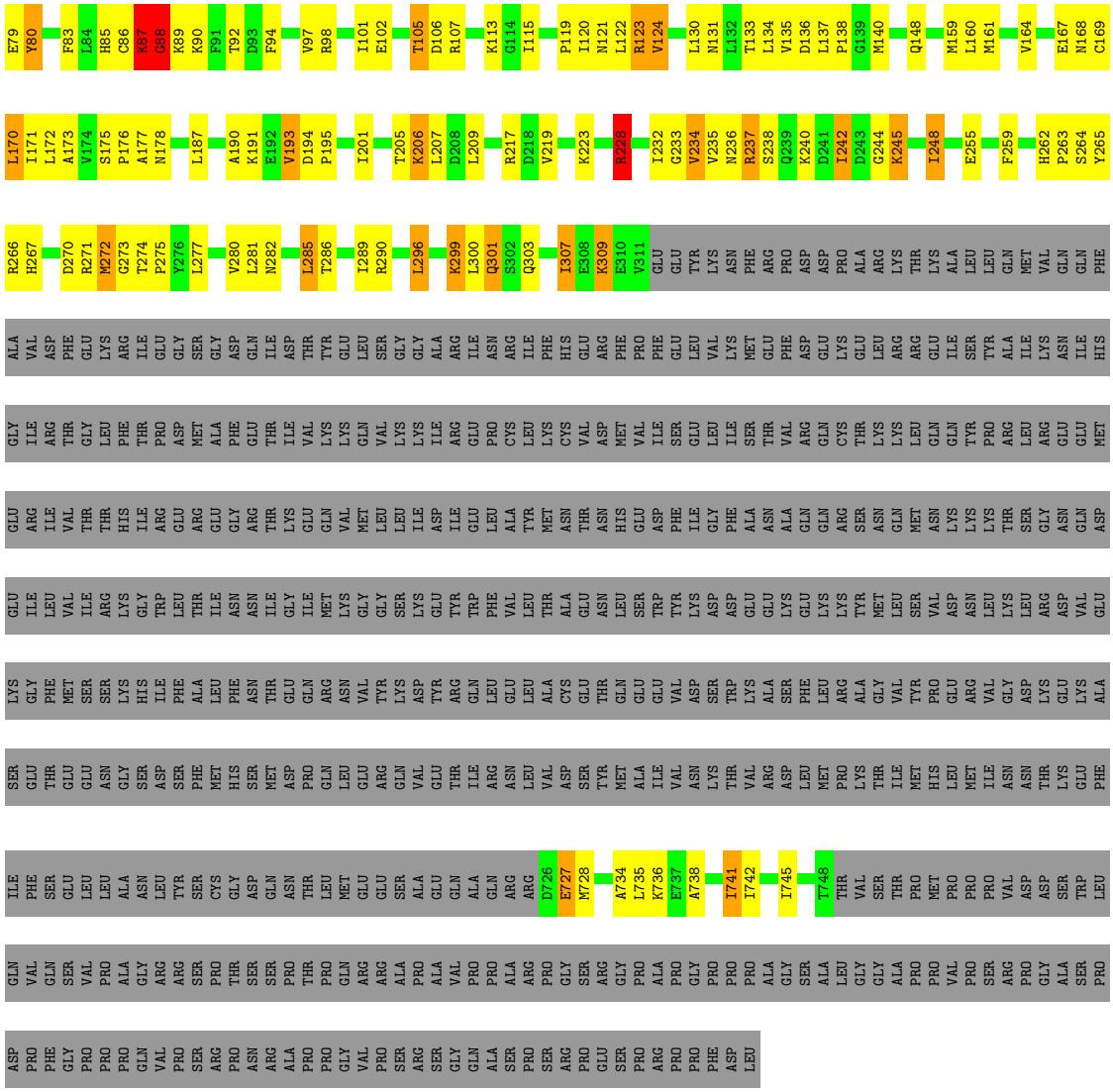
• Molecule 1: DYNAMIN-1

Chain D:



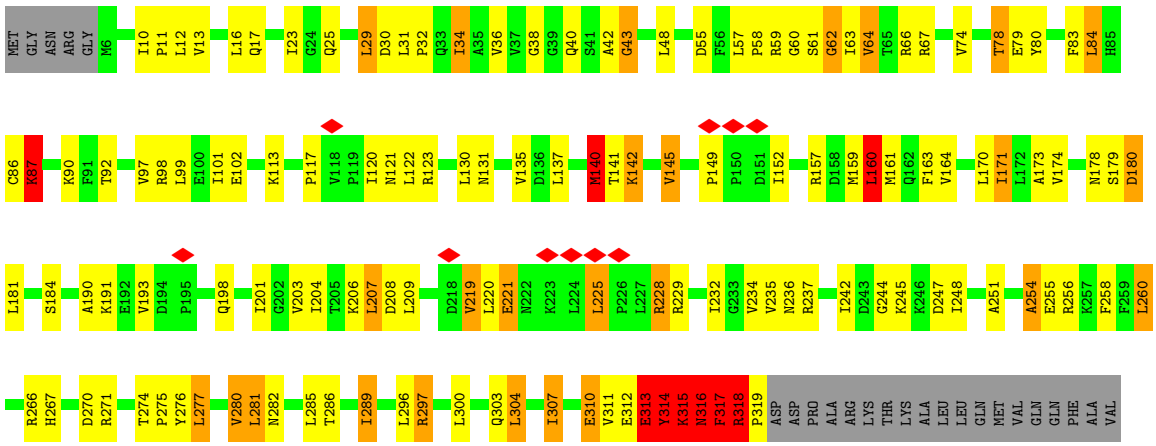
• Molecule 1: DYNAMIN-1

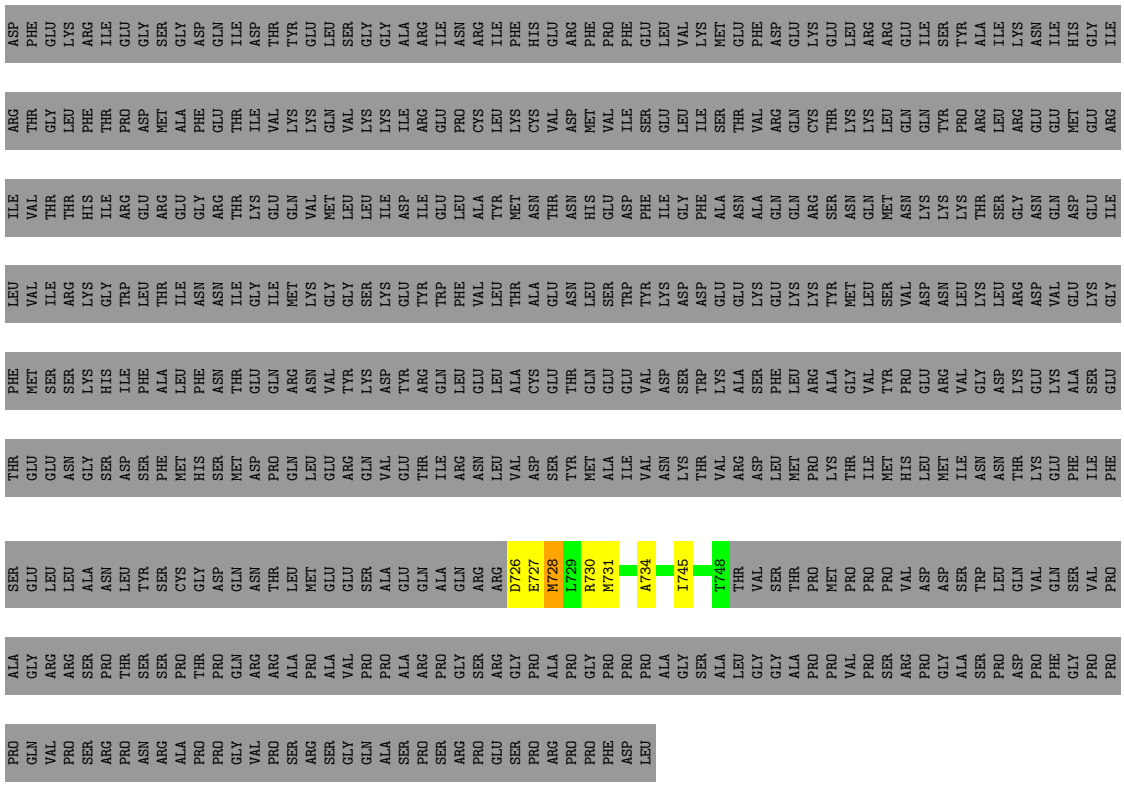
Chain G:



- Molecule 1: DYNAMIN-1

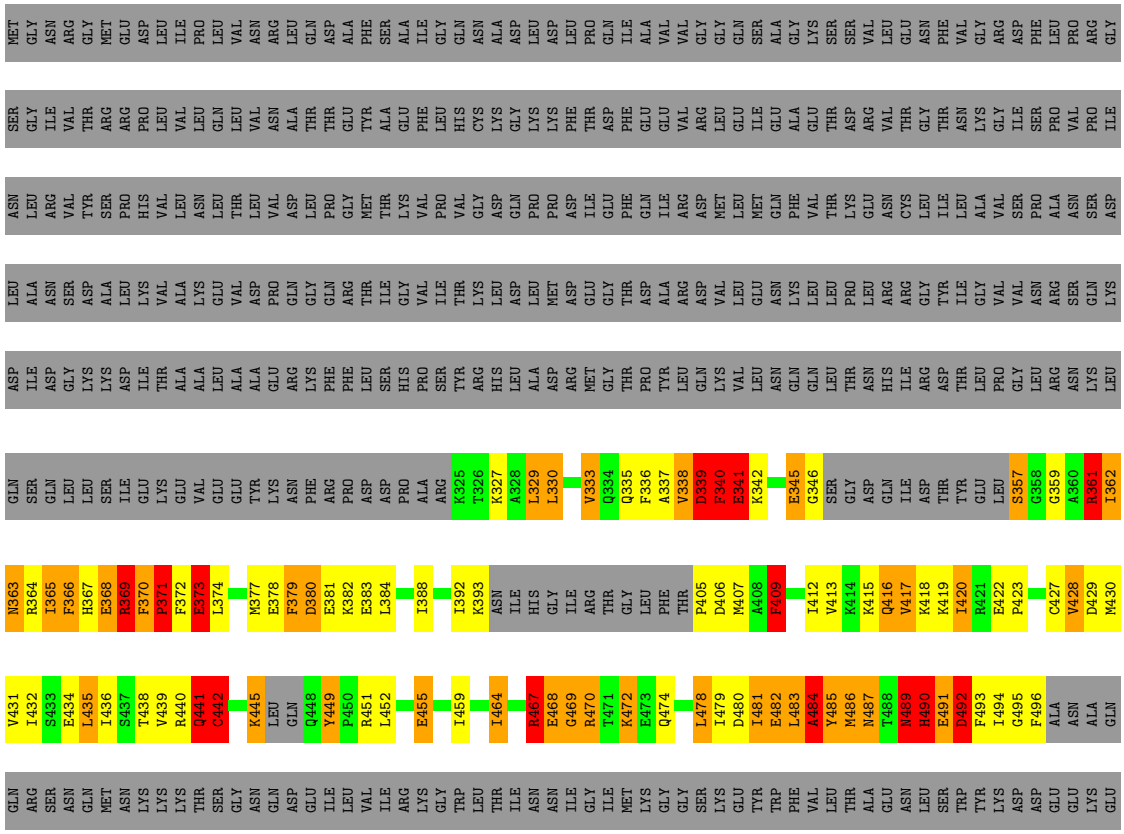
Chain K:

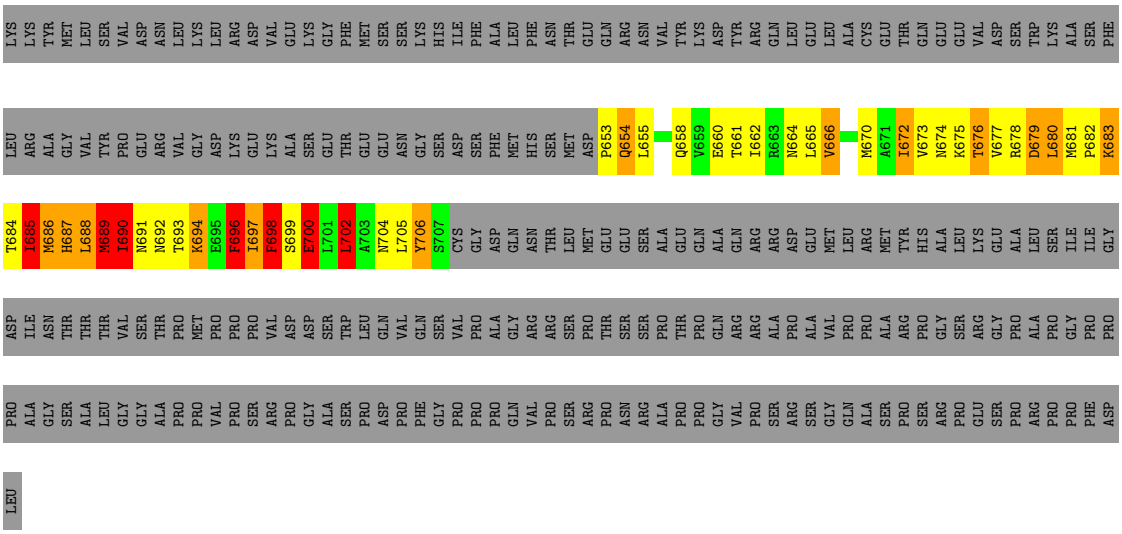




- Molecule 2: DYNAMIN-1

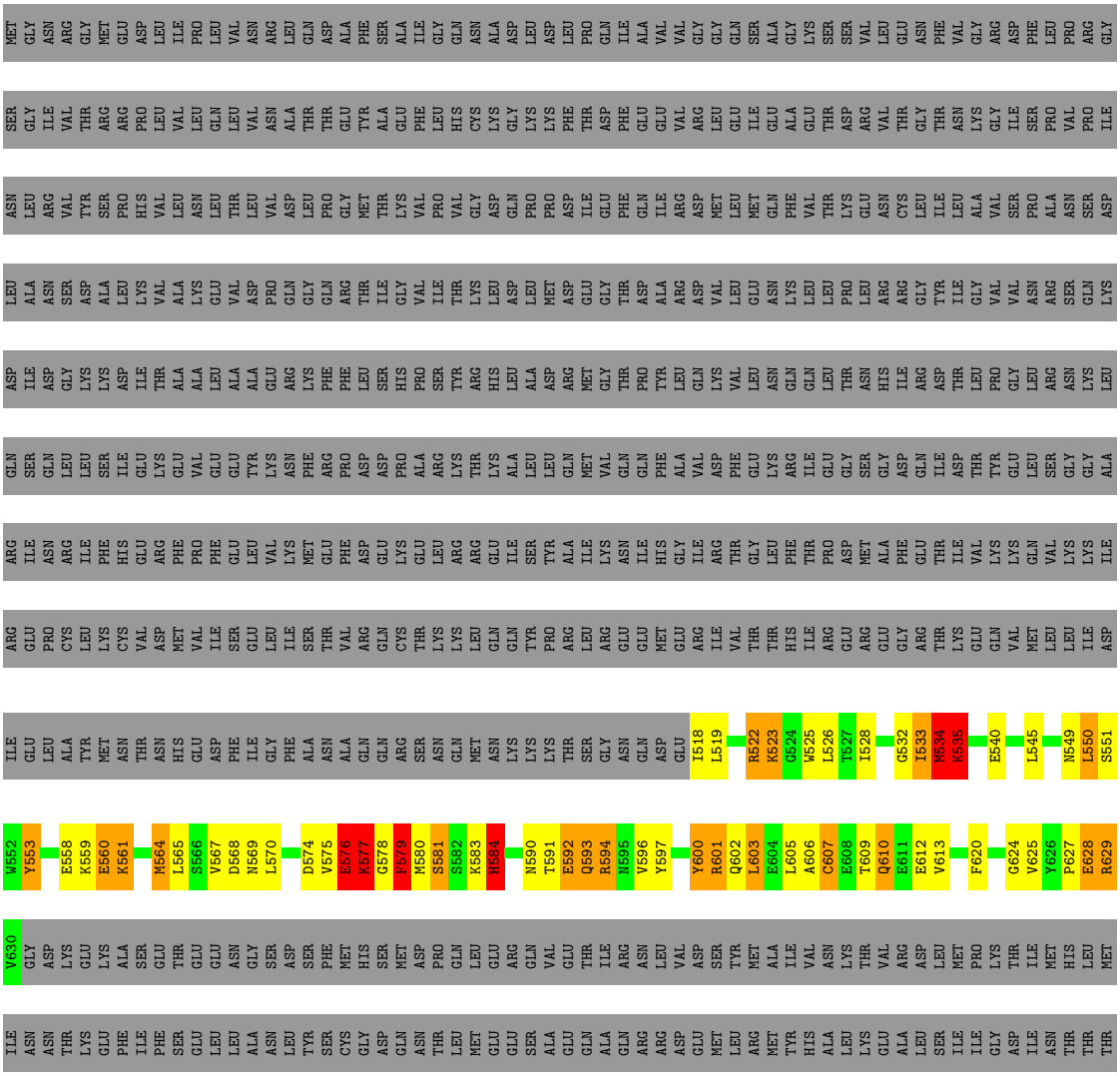
Chain B: 7% 8% 6% • 76%

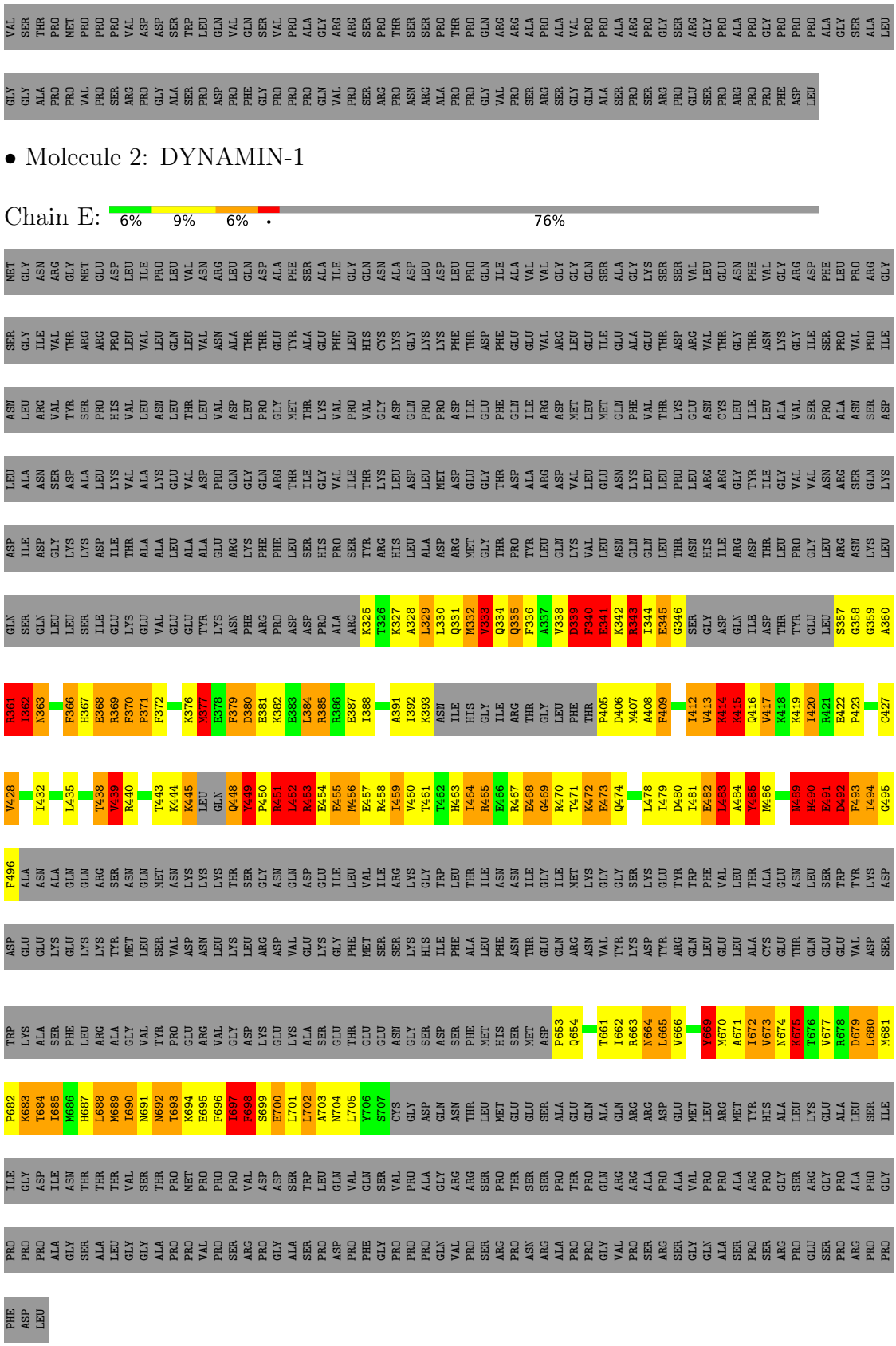




- Molecule 2: DYNAMIN-1

Chain C: 6% • •• 87%





• Molecule 2: DYNAMIN-1

Chain E: 6% 9% 6% • 76%

• Molecule 2: DYNAMIN-1

Chain F: 6% 5% ••

87%

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

SER GLY ILE VAL THR ARG ARG PRO LEU VAL LEU GLN LEU VAL ASN ALA THR THR GLU TYR ALA GLU PHE LEU HIS CYS LYS GLY LYS LYS PHE THR ASP PHE GLU GLU VAL ARG LEU GLU ILE GLU ALA GLU THR ASP ARG VAL THR GLY THR ASN LYS GLY ILE SER PRO VAL PRO ILE

ASN LEU ARG VAL TYR SER PRO HIS VAL LEU ASN LEU THR LEU VAL ASP PRO GLY MET THR LYS VAL PRO VAL GLY ASP GLN PRO PRO ASP ILE GLU PHE GLN ILE ARG ASP MET LEU MET GLN PHE VAL THR LYS GLU ASN CYS LEU ILE LEU ALA VAL SER PRO ALA ASN SER ASP

LEU ALA ASN SER ASP ALA LEU LYS VAL ALA ALA LYS GLU VAL ASP PRO GLN GLY GLN ARG THR ILE GLY VAL ILE THR LYS LEU ASP LEU MET ASP GLU GLY GLY THR ASP ALA ARG ASP VAL LEU GLU ASN LYS LEU LEU ARG ARG GLY TYR ILE GLY VAL VAL ASN ARG SER GLN LYS

ASP ILE ASP GLY LYS LYS ASP ILE THR ALA ALA LEU ALA GLU ARG LYS PHE PHE LEU SER HIS PRO SER TYR ARG HIS LEU ALA ASP ARG MET GLY THR PRO TYR LEU GLN LYS VAL LEU ASN GLN GLN LEU THR ASN HIS ILE ARG ASP THR LEU PRO GLY LEU ARG GLY ASN GLN LYS

GLN SER GLN LEU LEU SER ILE GLU LYS GLU VAL GLU GLU TYR LYS ASN PHE ARG PRO ASP ASP PRO ALA ARG LYS THR LYS ALA LEU LEU GLN MET VAL GLN GLN PHE ALA VAL ASP PHE GLU LYS ARG ILE ASP THR TYR GLY GLY GLN

ARG ILE ASN ARG ILE PHE HIS GLU ARG PHE PRO PHE GLU LEU VAL LYS MET GLU PHE ASP GLU LYS GLU LEU ARG ARG GLU ILE SER ARG LEU GLY GLU ILE ARG THR GLY LEU PHE THR PRO ASP ARG ILE ILE LYS ASN ILE HIS GLY ILE ARG ASN ILE ILE

ARG GLU PRO CYS LEU LYS CYS VAL ASP MET VAL ILE SER GLU LEU VAL ILE SER THR VAL ARG GLN CYS THR LYS LYS LEU GLN GLN TYR PRO ARG LEU ARG GLU GLU MET GLU ILE ILE ARG GLU VAL THR THR THR HIS ILE ARG GLU ARG GLU GLY ARG THR LYS GLU GLN VAL MET LEU LEU ILE ASP

ILE GLU LEU ALA TYR MET ASN HIS GLU ASP PHE ILE GLY PHE ALA ASN ALA GLN GLN ARG SER ASN GLN MET ASN LYS LYS THR SER GLY ASN GLN ASP GLU I518 L519 V520 I521 R522 K523 L526 T527 I528 I531 G532 I533 M534 K535 K539 E540 F543 V544

L550 S551 W552 Y553 D556 E557 E558 K559 E560 K561 K562 Y563 M564 L565 D568 N569 L570 K571 L572 R573 D574 V575 E576 K577 G578 F579 M580 S581 I585 F586 A587 L588 F589 R594 N595 V596 Y597 Y600 R601 Q602 L603 E604 L605 A606 C607 E612 L621 R622 A623 G624 V625 Y626 P627

E628 R629 V630 GLY ASP LYS GLU LYS ALA SER GLU THR GLU GLU ASN GLY SER ASP SER PHE MET HIS SER MET ASP PRO GLN LEU GLU ARG GLN VAL GLU THR ILE ARG ASN LEU VAL ASP SER TYR MET ALA ILE VAL ASN LYS THR VAL ARG ASP LEU MET ILE ALA HIS

LEU MET ILE ASN ASN THR LYS GLU PHE ILE PHE SER GLU LEU LEU ALA ASN LEU TYR SER CYS GLY ASP GLN ASN THR LEU MET GLU GLU SER ALA GLU GLN ALA ARG ARG ASP GLU MET LEU ARG MET TYR HIS ALA LEU LYS GLU ALA LEU SER ILE ILE GLY ASP ILE ASN THR

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

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

• Molecule 2: DYNAMIN-1

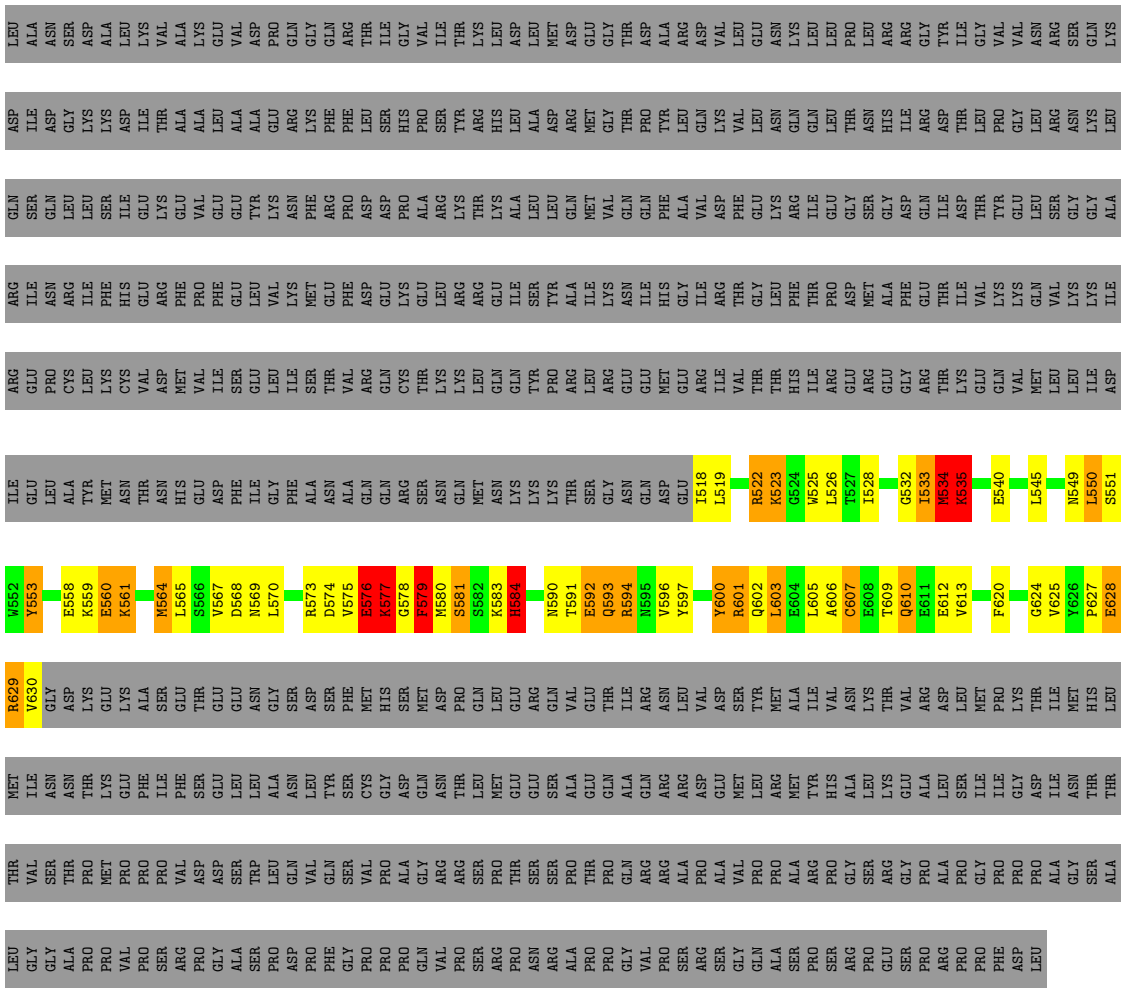
Chain H: 6% • ••

87%

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

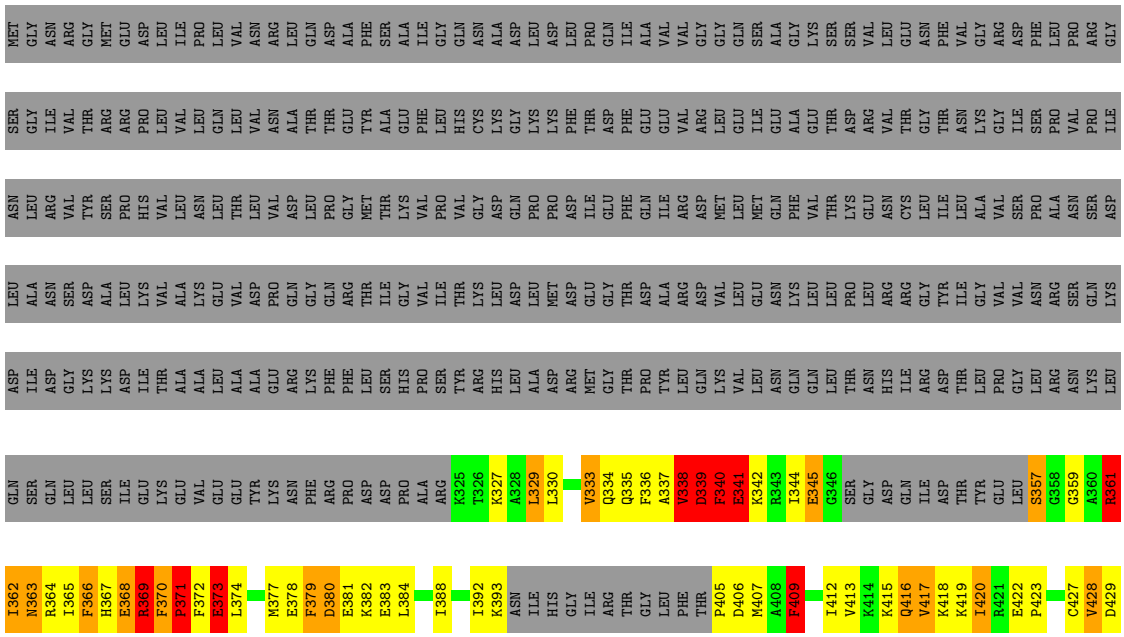
SER GLY ILE VAL THR ARG ARG PRO LEU VAL LEU GLN LEU VAL ASN ALA THR THR GLU TYR ALA GLU PHE LEU HIS CYS LYS GLY LYS LYS PHE THR ASP PHE GLU GLU VAL ARG LEU GLU ILE GLU ALA GLU THR ASP ARG VAL THR GLY THR ASN LYS GLY ILE SER PRO VAL PRO ILE

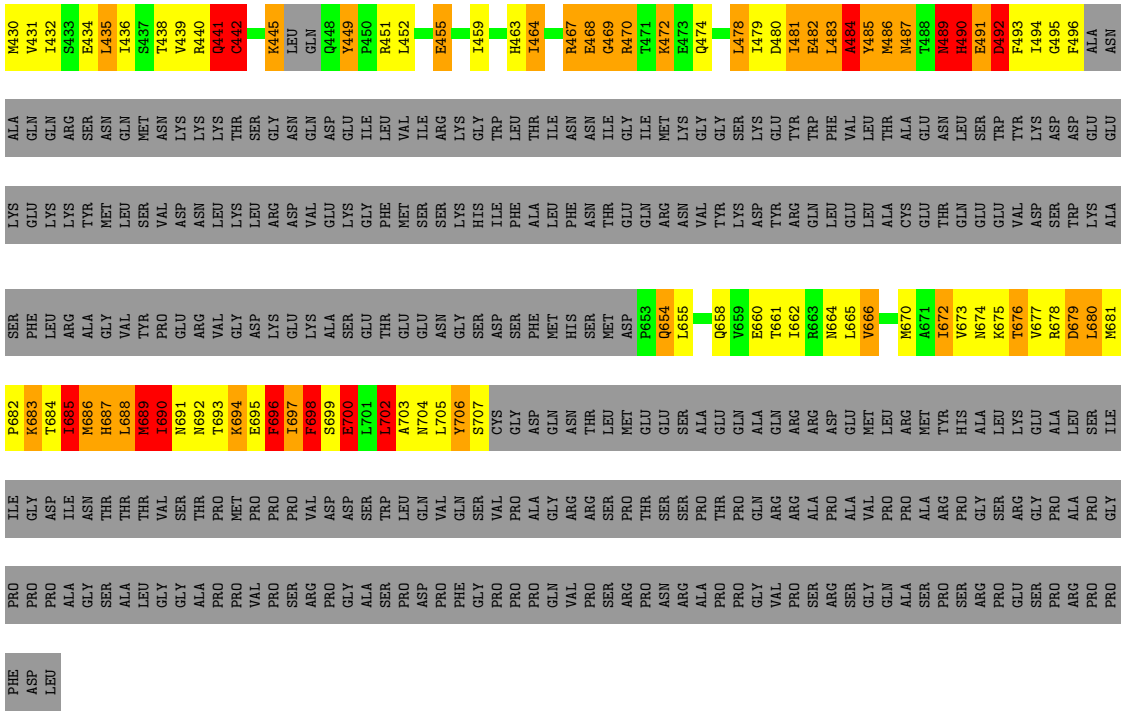
ASN LEU ARG VAL TYR SER PRO HIS VAL LEU ASN LEU THR LEU VAL ASP LEU PRO GLY MET THR LYS VAL PRO VAL GLY ASP GLN PRO PRO ASP ILE GLU PHE GLN ILE ARG ASP MET LEU MET GLN PHE VAL THR LYS GLU ASN CYS LEU ILE LEU ALA VAL SER PRO ALA ASN SER ASP



- Molecule 2: DYNAMIN-1

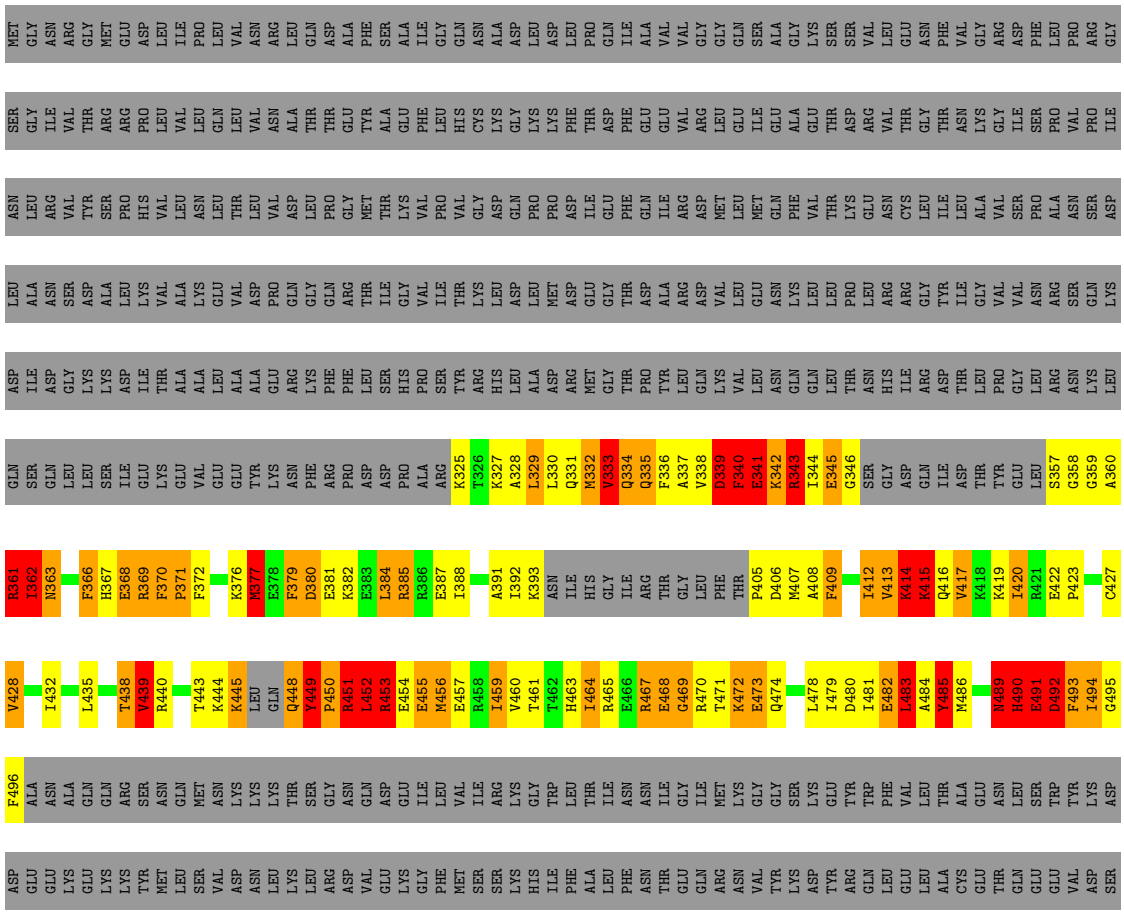
Chain I: 7% 9% 5% • 76%

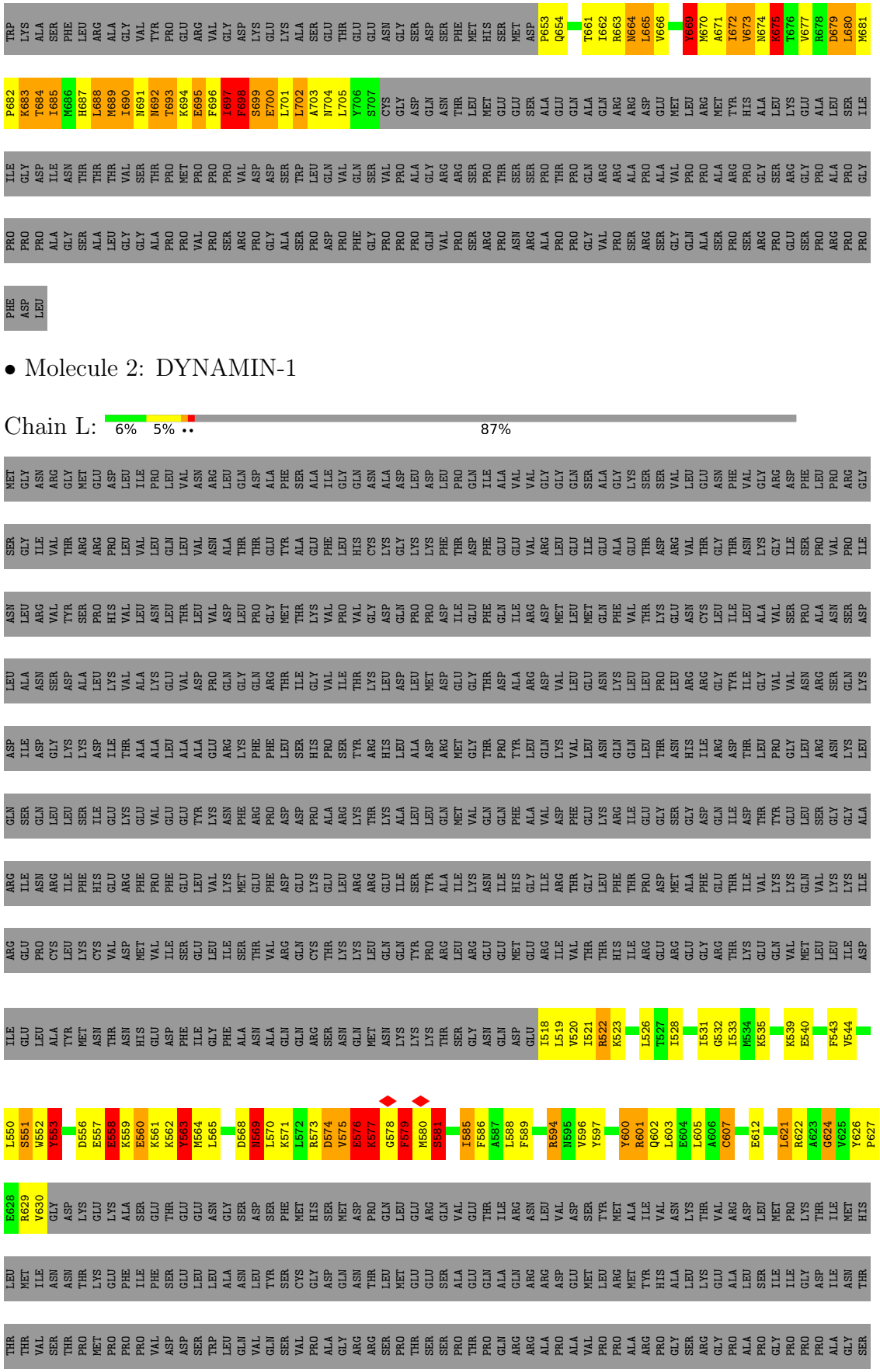




- Molecule 2: DYNAMIN-1

Chain J: 6% 9% 6% • 76%





• Molecule 2: DYNAMIN-1

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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	7525	Depositor
Resolution determination method	Not provided	
CTF correction method	INDIVIDUAL IMAGES	Depositor
Microscope	FEI/PHILIPS CM300FEG/HE	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	10	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	49000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	18.352	Depositor
Minimum map value	-18.065	Depositor
Average map value	0.361	Depositor
Map value standard deviation	3.624	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	510.0, 510.0, 510.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.55, 2.55, 2.55	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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.06	6/2604 (0.2%)	1.76	86/3524 (2.4%)
1	D	1.32	20/2683 (0.7%)	2.36	118/3630 (3.3%)
1	G	1.06	6/2604 (0.2%)	1.76	86/3524 (2.4%)
1	K	1.32	21/2683 (0.8%)	2.36	118/3630 (3.3%)
2	B	1.51	17/1718 (1.0%)	2.51	139/2293 (6.1%)
2	C	1.44	17/966 (1.8%)	2.52	79/1298 (6.1%)
2	E	1.55	20/1718 (1.2%)	2.63	170/2293 (7.4%)
2	F	1.42	14/966 (1.4%)	2.29	61/1298 (4.7%)
2	H	1.44	17/966 (1.8%)	2.52	79/1298 (6.1%)
2	I	1.51	18/1718 (1.0%)	2.51	141/2293 (6.1%)
2	J	1.55	20/1718 (1.2%)	2.64	170/2293 (7.4%)
2	L	1.42	14/966 (1.4%)	2.29	61/1298 (4.7%)
All	All	1.36	190/21310 (0.9%)	2.31	1308/28672 (4.6%)

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 (190) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	317	PHE	C-O	-20.01	1.05	1.24
1	D	317	PHE	C-O	-20.01	1.05	1.24
1	D	318	ARG	CA-C	-16.10	1.32	1.53
1	K	318	ARG	CA-C	-16.06	1.32	1.53
2	J	699	SER	CB-OG	-14.86	1.12	1.42
2	E	699	SER	CB-OG	-14.84	1.12	1.42
1	G	245	LYS	CA-CB	-14.09	1.32	1.53
1	A	245	LYS	CA-CB	-14.08	1.32	1.53
2	L	569	ASN	CA-CB	-13.88	1.35	1.53
2	F	569	ASN	CA-CB	-13.85	1.35	1.53
2	J	492	ASP	N-CA	-12.04	1.30	1.46
2	E	492	ASP	N-CA	-12.03	1.30	1.46
1	D	316	ASN	C-N	-11.25	1.17	1.33
1	K	316	ASN	C-N	-11.24	1.17	1.33
1	K	315	LYS	N-CA	-11.19	1.32	1.46
1	D	315	LYS	N-CA	-11.14	1.32	1.46
2	I	490	HIS	N-CA	-10.68	1.32	1.46
2	B	490	HIS	N-CA	-10.65	1.32	1.46
1	D	313	GLU	C-O	-9.71	1.10	1.24
1	K	313	GLU	C-O	-9.71	1.10	1.24
1	D	317	PHE	CA-C	-9.59	1.41	1.53
1	K	317	PHE	CA-C	-9.57	1.41	1.53
2	C	523	LYS	N-CA	-9.50	1.33	1.46
2	H	523	LYS	N-CA	-9.46	1.33	1.46
2	H	560	GLU	CA-C	-9.34	1.44	1.53
2	H	581	SER	N-CA	-9.28	1.32	1.45
2	C	560	GLU	CA-C	-9.27	1.44	1.53
2	C	581	SER	N-CA	-9.26	1.32	1.45
2	E	492	ASP	C-O	-8.76	1.12	1.24
2	J	492	ASP	C-O	-8.75	1.12	1.24
2	L	574	ASP	CA-CB	-8.70	1.42	1.52
2	F	581	SER	N-CA	-8.67	1.34	1.45
2	F	574	ASP	CA-CB	-8.66	1.42	1.52
2	L	581	SER	N-CA	-8.64	1.34	1.45
1	A	88	GLY	N-CA	-8.44	1.33	1.45
1	G	88	GLY	N-CA	-8.42	1.33	1.45
2	H	561	LYS	N-CA	-8.35	1.35	1.46
2	I	490	HIS	CD2-NE2	-8.33	1.28	1.37
2	C	561	LYS	N-CA	-8.31	1.35	1.46
2	B	490	HIS	CD2-NE2	-8.24	1.28	1.37
2	L	577	LYS	C-N	-8.24	1.24	1.33
2	F	577	LYS	C-N	-8.18	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	315	LYS	C-N	-7.87	1.19	1.33
1	K	315	LYS	C-N	-7.86	1.19	1.33
2	F	561	LYS	N-CA	-7.64	1.36	1.46
2	L	561	LYS	N-CA	-7.62	1.36	1.46
1	K	316	ASN	C-O	7.50	1.35	1.23
1	D	316	ASN	C-O	7.48	1.35	1.23
1	D	314	TYR	C-N	-7.34	1.24	1.33
1	K	314	TYR	C-N	-7.32	1.24	1.33
2	B	492	ASP	N-CA	-7.31	1.36	1.46
2	B	700	GLU	N-CA	-7.29	1.36	1.46
2	I	492	ASP	N-CA	-7.29	1.36	1.46
2	I	700	GLU	N-CA	-7.29	1.36	1.46
1	K	313	GLU	C-N	-7.25	1.24	1.33
1	D	313	GLU	C-N	-7.24	1.24	1.33
2	B	489	ASN	CA-C	-7.16	1.42	1.52
2	I	489	ASN	CA-C	-7.14	1.42	1.52
2	E	341	GLU	CA-C	-7.10	1.44	1.52
2	J	366	PHE	CA-CB	-7.09	1.41	1.53
2	E	366	PHE	CA-CB	-7.08	1.41	1.53
2	J	341	GLU	CA-C	-7.06	1.44	1.52
2	B	489	ASN	C-O	7.05	1.33	1.24
2	I	489	ASN	C-O	7.01	1.32	1.24
2	H	533	ILE	CA-CB	-7.00	1.46	1.54
1	D	245	LYS	CA-CB	-6.99	1.42	1.53
1	K	245	LYS	CA-CB	-6.97	1.43	1.53
2	C	533	ILE	CA-CB	-6.96	1.46	1.54
2	L	560	GLU	CA-C	-6.92	1.43	1.52
2	F	560	GLU	CA-C	-6.89	1.43	1.52
2	J	342	LYS	N-CA	-6.87	1.37	1.46
2	C	560	GLU	N-CA	-6.87	1.38	1.47
2	H	560	GLU	N-CA	-6.82	1.38	1.47
2	E	342	LYS	N-CA	-6.81	1.37	1.46
2	B	366	PHE	CA-CB	-6.75	1.42	1.53
2	I	366	PHE	CA-CB	-6.73	1.43	1.53
1	K	316	ASN	N-CA	-6.67	1.37	1.46
1	D	316	ASN	N-CA	-6.66	1.37	1.46
2	J	490	HIS	N-CA	-6.65	1.37	1.46
2	E	490	HIS	N-CA	-6.62	1.37	1.46
2	C	577	LYS	C-N	-6.61	1.25	1.32
2	F	558	GLU	CA-CB	-6.61	1.43	1.53
2	H	534	MET	N-CA	-6.59	1.37	1.46
2	H	577	LYS	C-N	-6.59	1.25	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	534	MET	N-CA	-6.56	1.37	1.46
2	L	558	GLU	CA-CB	-6.56	1.43	1.53
2	C	584	HIS	CA-CB	-6.51	1.44	1.53
2	H	584	HIS	CA-CB	-6.50	1.44	1.53
2	I	441	GLN	C-O	6.49	1.32	1.24
2	B	441	GLN	C-O	6.49	1.32	1.24
2	E	491	GLU	CA-C	-6.45	1.43	1.52
1	D	317	PHE	N-CA	-6.43	1.38	1.46
1	K	317	PHE	N-CA	-6.43	1.38	1.46
2	J	491	GLU	CA-C	-6.41	1.43	1.52
2	B	679	ASP	C-N	-6.31	1.25	1.33
2	I	679	ASP	C-N	-6.30	1.25	1.33
2	L	602	GLN	N-CA	-6.29	1.38	1.45
2	F	602	GLN	N-CA	-6.22	1.38	1.45
2	C	580	MET	CA-C	-6.20	1.46	1.53
2	C	592	GLU	N-CA	-6.16	1.38	1.46
2	H	592	GLU	N-CA	-6.16	1.38	1.46
1	K	311	VAL	N-CA	-6.12	1.39	1.46
2	C	522	ARG	CA-C	-6.09	1.44	1.52
2	I	693	THR	C-N	-6.09	1.26	1.33
2	B	693	THR	C-N	-6.09	1.26	1.33
2	H	522	ARG	CA-C	-6.08	1.44	1.52
1	D	311	VAL	N-CA	-6.08	1.39	1.46
2	E	449	TYR	CA-C	-6.07	1.46	1.53
2	H	601	ARG	C-N	-6.07	1.26	1.33
2	J	449	TYR	CA-C	-6.07	1.46	1.53
2	H	580	MET	CA-C	-6.06	1.46	1.53
2	E	453	ARG	C-O	-6.05	1.17	1.24
2	C	601	ARG	C-N	-6.04	1.26	1.33
2	F	601	ARG	C-N	-6.03	1.26	1.33
2	J	453	ARG	C-O	-6.03	1.17	1.24
2	J	452	LEU	CA-C	-6.00	1.45	1.52
2	L	601	ARG	C-N	-5.98	1.26	1.33
2	E	452	LEU	CA-C	-5.97	1.45	1.52
1	K	310	GLU	C-O	-5.96	1.16	1.24
2	E	340	PHE	N-CA	-5.92	1.39	1.46
1	D	310	GLU	C-O	-5.90	1.16	1.24
1	A	73	LEU	CA-CB	-5.89	1.45	1.53
2	J	489	ASN	CA-C	-5.89	1.44	1.52
2	J	340	PHE	N-CA	-5.88	1.39	1.46
2	E	489	ASN	CA-C	-5.88	1.44	1.52
1	G	73	LEU	CA-CB	-5.83	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	679	ASP	C-N	-5.82	1.26	1.33
2	J	698	PHE	CA-CB	-5.81	1.43	1.53
2	E	679	ASP	C-N	-5.81	1.26	1.33
2	E	698	PHE	CA-CB	-5.81	1.43	1.53
2	I	700	GLU	CA-CB	-5.80	1.43	1.53
1	A	234	VAL	N-CA	-5.77	1.39	1.46
2	B	700	GLU	CA-CB	-5.76	1.43	1.53
1	G	234	VAL	N-CA	-5.75	1.39	1.46
2	E	333	VAL	CA-CB	-5.73	1.46	1.54
1	D	179	SER	C-N	-5.73	1.25	1.33
1	D	310	GLU	C-N	-5.72	1.26	1.33
1	K	310	GLU	C-N	-5.72	1.26	1.33
2	J	333	VAL	CA-CB	-5.67	1.46	1.54
1	K	179	SER	C-N	-5.66	1.25	1.33
2	B	342	LYS	N-CA	-5.65	1.39	1.46
2	C	602	GLN	N-CA	-5.65	1.38	1.45
2	H	602	GLN	N-CA	-5.65	1.38	1.45
2	I	442	CYS	N-CA	-5.61	1.39	1.46
2	B	442	CYS	N-CA	-5.60	1.39	1.46
2	I	342	LYS	N-CA	-5.58	1.39	1.46
1	K	728	MET	N-CA	-5.55	1.39	1.46
1	D	728	MET	N-CA	-5.54	1.39	1.46
2	I	690	ILE	N-CA	-5.53	1.39	1.46
2	B	706	TYR	CA-CB	-5.53	1.44	1.53
2	J	492	ASP	C-N	-5.53	1.25	1.33
2	E	492	ASP	C-N	-5.52	1.25	1.33
2	C	578	GLY	N-CA	-5.52	1.40	1.45
2	B	690	ILE	N-CA	-5.51	1.39	1.46
2	H	578	GLY	N-CA	-5.51	1.40	1.45
2	C	610	GLN	C-N	-5.45	1.26	1.33
2	I	706	TYR	CA-CB	-5.45	1.44	1.53
2	L	580	MET	CA-C	-5.42	1.47	1.53
2	H	610	GLN	C-N	-5.41	1.26	1.33
2	F	580	MET	CA-C	-5.41	1.47	1.53
2	L	564	MET	C-O	-5.40	1.17	1.24
1	G	89	LYS	N-CA	-5.40	1.39	1.46
2	F	564	MET	C-O	-5.38	1.18	1.24
2	L	563	TYR	CA-CB	-5.37	1.44	1.53
1	A	89	LYS	N-CA	-5.35	1.39	1.46
2	I	698	PHE	C-O	-5.35	1.17	1.24
2	F	563	TYR	CA-CB	-5.35	1.44	1.53
1	A	87	LYS	CG-CD	-5.33	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	307	ILE	C-O	-5.33	1.17	1.24
2	B	698	PHE	C-O	-5.32	1.17	1.24
1	G	87	LYS	CG-CD	-5.32	1.36	1.52
1	K	307	ILE	C-O	-5.32	1.17	1.24
2	I	342	LYS	CA-CB	-5.29	1.44	1.53
2	J	451	ARG	CA-C	-5.26	1.48	1.53
2	B	342	LYS	CA-CB	-5.26	1.44	1.53
2	H	534	MET	CA-CB	-5.25	1.44	1.53
2	C	534	MET	CA-CB	-5.24	1.44	1.53
2	E	451	ARG	CA-C	-5.23	1.48	1.53
2	F	557	GLU	N-CA	-5.16	1.39	1.46
2	L	557	GLU	N-CA	-5.15	1.39	1.46
1	D	203	VAL	C-O	-5.12	1.18	1.24
2	E	484	ALA	N-CA	-5.10	1.39	1.46
2	J	377	MET	N-CA	-5.09	1.39	1.46
1	K	203	VAL	C-O	-5.08	1.18	1.24
2	L	520	VAL	C-N	-5.08	1.27	1.33
2	E	377	MET	N-CA	-5.07	1.39	1.46
2	J	484	ALA	N-CA	-5.06	1.39	1.46
2	F	520	VAL	C-N	-5.06	1.27	1.33
2	I	690	ILE	C-O	-5.02	1.18	1.24
1	K	304	LEU	C-O	-5.00	1.18	1.24

All (1308) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	314	TYR	CA-C-N	26.59	156.81	120.38
1	K	314	TYR	C-N-CA	26.59	156.81	120.38
1	D	314	TYR	CA-C-N	26.55	156.75	120.38
1	D	314	TYR	C-N-CA	26.55	156.75	120.38
2	F	569	ASN	CA-CB-CG	25.33	137.93	112.60
2	L	569	ASN	CA-CB-CG	25.31	137.91	112.60
1	K	317	PHE	O-C-N	-24.09	94.80	122.75
1	K	315	LYS	O-C-N	-24.09	96.58	122.12
1	D	317	PHE	O-C-N	-24.09	94.81	122.75
1	D	315	LYS	O-C-N	-24.08	96.59	122.12
1	K	318	ARG	NE-CZ-NH2	23.29	140.16	119.20
1	D	318	ARG	NE-CZ-NH2	23.20	140.08	119.20
1	K	316	ASN	CA-C-N	22.18	162.99	122.84
1	K	316	ASN	C-N-CA	22.18	162.99	122.84
1	D	316	ASN	CA-C-N	22.17	162.98	122.84
1	D	316	ASN	C-N-CA	22.17	162.98	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	315	LYS	CA-C-N	21.38	166.84	122.58
1	D	315	LYS	C-N-CA	21.38	166.84	122.58
1	K	315	LYS	CA-C-N	21.36	166.80	122.58
1	K	315	LYS	C-N-CA	21.36	166.80	122.58
1	K	316	ASN	O-C-N	-20.25	94.96	122.10
1	D	316	ASN	O-C-N	-20.25	94.97	122.10
2	C	577	LYS	CA-C-N	19.75	138.65	121.86
2	C	577	LYS	C-N-CA	19.75	138.65	121.86
2	B	492	ASP	CB-CG-OD2	19.72	163.76	118.40
2	I	492	ASP	CB-CG-OD2	19.68	163.68	118.40
2	H	577	LYS	CA-C-N	19.68	138.59	121.86
2	H	577	LYS	C-N-CA	19.68	138.59	121.86
1	K	318	ARG	CA-C-O	-19.57	100.48	120.64
1	D	318	ARG	CA-C-O	-19.55	100.50	120.64
2	B	362	ILE	N-CA-C	-19.31	93.16	110.74
2	I	362	ILE	N-CA-C	-19.24	93.23	110.74
1	D	317	PHE	N-CA-C	19.21	133.47	107.73
1	K	317	PHE	N-CA-C	19.19	133.44	107.73
2	E	362	ILE	N-CA-C	-18.51	93.89	110.74
2	J	362	ILE	N-CA-C	-18.49	93.91	110.74
1	K	314	TYR	O-C-N	-18.36	102.26	122.09
1	D	314	TYR	O-C-N	-18.29	102.33	122.09
2	I	492	ASP	CB-CG-OD1	-17.85	77.34	118.40
2	B	492	ASP	CB-CG-OD1	-17.84	77.37	118.40
1	K	318	ARG	NH1-CZ-NH2	-15.80	98.76	119.30
1	D	318	ARG	NH1-CZ-NH2	-15.79	98.78	119.30
2	J	368	GLU	N-CA-CB	15.69	133.47	110.56
2	E	368	GLU	N-CA-CB	15.67	133.44	110.56
1	K	316	ASN	N-CA-C	15.37	132.80	113.43
1	D	316	ASN	N-CA-C	15.35	132.78	113.43
1	K	87	LYS	CG-CD-CE	15.00	145.81	111.30
2	C	522	ARG	CA-C-N	14.99	150.18	121.54
2	C	522	ARG	C-N-CA	14.99	150.18	121.54
2	H	522	ARG	CA-C-N	14.99	150.17	121.54
2	H	522	ARG	C-N-CA	14.99	150.17	121.54
1	D	87	LYS	CG-CD-CE	14.98	145.76	111.30
2	I	366	PHE	N-CA-CB	14.52	131.57	109.94
2	B	366	PHE	N-CA-CB	14.44	131.45	109.94
1	K	313	GLU	O-C-N	-14.15	101.45	122.39
1	D	313	GLU	O-C-N	-14.12	101.50	122.39
1	K	228	ARG	CB-CG-CD	13.85	143.16	111.30
1	D	228	ARG	CB-CG-CD	13.82	143.10	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	449	TYR	CZ-CE2-CD2	-13.72	94.91	119.60
2	E	449	TYR	CZ-CE2-CD2	-13.71	94.93	119.60
2	B	338	VAL	CA-C-N	13.21	140.38	120.31
2	B	338	VAL	C-N-CA	13.21	140.38	120.31
2	I	338	VAL	CA-C-N	13.17	140.33	120.31
2	I	338	VAL	C-N-CA	13.17	140.33	120.31
2	J	343	ARG	NE-CZ-NH1	-13.15	108.35	121.50
2	E	343	ARG	NE-CZ-NH1	-13.12	108.38	121.50
2	J	451	ARG	CA-C-N	12.69	137.89	120.63
2	J	451	ARG	C-N-CA	12.69	137.89	120.63
2	E	451	ARG	CA-C-N	12.68	137.87	120.63
2	E	451	ARG	C-N-CA	12.68	137.87	120.63
2	E	340	PHE	N-CA-C	12.50	124.98	111.36
2	J	340	PHE	N-CA-C	12.47	124.95	111.36
2	E	699	SER	N-CA-CB	-12.20	89.88	110.49
2	J	699	SER	N-CA-CB	-12.20	89.88	110.49
2	J	342	LYS	CB-CG-CD	12.13	139.20	111.30
2	E	342	LYS	CB-CG-CD	12.12	139.18	111.30
2	C	523	LYS	N-CA-CB	12.00	130.77	110.49
2	H	523	LYS	N-CA-CB	11.99	130.76	110.49
2	C	591	THR	CA-C-N	11.92	142.00	121.14
2	C	591	THR	C-N-CA	11.92	142.00	121.14
2	H	591	THR	CA-C-N	11.91	141.99	121.14
2	H	591	THR	C-N-CA	11.91	141.99	121.14
2	B	489	ASN	O-C-N	-11.84	107.79	122.35
1	D	315	LYS	N-CA-C	11.82	125.64	111.33
2	I	489	ASN	O-C-N	-11.80	107.84	122.35
1	K	315	LYS	N-CA-C	11.76	125.56	111.33
2	B	440	ARG	CA-C-N	11.72	143.92	121.54
2	B	440	ARG	C-N-CA	11.72	143.92	121.54
2	I	440	ARG	CA-C-N	11.71	143.91	121.54
2	I	440	ARG	C-N-CA	11.71	143.91	121.54
1	K	310	GLU	CA-C-N	11.67	135.26	120.56
1	K	310	GLU	C-N-CA	11.67	135.26	120.56
1	D	310	GLU	CA-C-N	11.66	135.25	120.56
1	D	310	GLU	C-N-CA	11.66	135.25	120.56
2	E	449	TYR	CB-CG-CD1	11.48	138.03	120.80
2	J	449	TYR	CB-CG-CD1	11.44	137.96	120.80
2	B	490	HIS	CG-CD2-NE2	11.43	118.63	107.20
2	I	490	HIS	CG-CD2-NE2	11.42	118.62	107.20
1	D	260	LEU	N-CA-CB	11.29	126.44	110.07
1	A	228	ARG	CB-CG-CD	11.27	137.22	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	260	LEU	N-CA-CB	11.24	126.37	110.07
1	G	228	ARG	CB-CG-CD	11.23	137.12	111.30
2	H	610	GLN	CA-C-O	11.22	132.75	120.63
2	C	610	GLN	CA-C-O	11.20	132.72	120.63
2	C	580	MET	CA-C-N	11.18	146.12	123.20
2	C	580	MET	C-N-CA	11.18	146.12	123.20
2	H	580	MET	CA-C-N	11.16	146.09	123.20
2	H	580	MET	C-N-CA	11.16	146.09	123.20
2	E	449	TYR	CA-C-N	11.10	130.95	119.19
2	E	449	TYR	C-N-CA	11.10	130.95	119.19
2	J	449	TYR	CA-C-N	11.10	130.95	119.19
2	J	449	TYR	C-N-CA	11.10	130.95	119.19
2	B	679	ASP	CA-C-N	11.07	136.01	120.29
2	B	679	ASP	C-N-CA	11.07	136.01	120.29
2	I	679	ASP	CA-C-N	11.07	136.01	120.29
2	I	679	ASP	C-N-CA	11.07	136.01	120.29
2	J	366	PHE	N-CA-CB	10.98	129.04	110.49
2	E	366	PHE	N-CA-CB	10.95	129.00	110.49
2	L	577	LYS	CA-C-N	10.90	137.25	122.42
2	L	577	LYS	C-N-CA	10.90	137.25	122.42
2	F	577	LYS	CA-C-N	10.89	137.24	122.42
2	F	577	LYS	C-N-CA	10.89	137.24	122.42
2	L	580	MET	CA-C-N	10.88	143.40	123.27
2	L	580	MET	C-N-CA	10.88	143.40	123.27
2	F	580	MET	CA-C-N	10.85	143.34	123.27
2	F	580	MET	C-N-CA	10.85	143.34	123.27
2	F	569	ASN	OD1-CG-ND2	-10.82	111.78	122.60
2	I	340	PHE	N-CA-C	10.80	124.97	111.69
2	L	569	ASN	OD1-CG-ND2	-10.78	111.82	122.60
2	C	559	LYS	CA-C-N	10.78	136.69	121.71
2	C	559	LYS	C-N-CA	10.78	136.69	121.71
2	H	559	LYS	CA-C-N	10.78	136.69	121.71
2	H	559	LYS	C-N-CA	10.78	136.69	121.71
2	B	340	PHE	N-CA-C	10.77	124.93	111.69
2	L	569	ASN	CB-CG-ND2	-10.74	100.29	116.40
2	F	569	ASN	CB-CG-ND2	-10.72	100.32	116.40
2	B	487	ASN	CB-CG-ND2	-10.71	100.34	116.40
2	I	487	ASN	CB-CG-ND2	-10.68	100.38	116.40
2	H	610	GLN	O-C-N	-10.60	110.89	122.12
2	L	574	ASP	CA-CB-CG	10.58	123.18	112.60
2	C	610	GLN	O-C-N	-10.55	110.94	122.12
2	F	574	ASP	CA-CB-CG	10.54	123.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	601	ARG	CA-C-N	10.54	139.98	121.75
2	H	601	ARG	C-N-CA	10.54	139.98	121.75
2	C	601	ARG	CA-C-N	10.49	139.90	121.75
2	C	601	ARG	C-N-CA	10.49	139.90	121.75
1	A	245	LYS	CB-CA-C	10.47	126.60	111.73
1	G	245	LYS	CB-CA-C	10.47	126.60	111.73
2	E	449	TYR	CE1-CZ-CE2	-10.47	99.36	120.30
2	J	449	TYR	CE1-CZ-CE2	-10.45	99.40	120.30
2	B	441	GLN	N-CA-CB	10.44	128.13	110.49
2	I	441	GLN	N-CA-CB	10.43	128.11	110.49
2	C	600	TYR	N-CA-C	10.34	127.16	113.72
2	H	591	THR	O-C-N	-10.33	110.13	122.22
2	C	591	THR	O-C-N	-10.33	110.14	122.22
2	H	600	TYR	N-CA-C	10.32	127.13	113.72
2	B	369	ARG	NE-CZ-NH1	-10.28	111.22	121.50
2	I	369	ARG	NE-CZ-NH1	-10.27	111.23	121.50
1	D	310	GLU	O-C-N	-10.27	110.20	122.22
1	K	310	GLU	O-C-N	-10.26	110.22	122.22
2	I	700	GLU	N-CA-CB	10.14	127.62	110.49
2	B	700	GLU	N-CA-CB	10.12	127.60	110.49
2	E	452	LEU	N-CA-CB	10.10	124.62	109.98
2	H	560	GLU	CA-C-N	10.10	140.83	121.54
2	H	560	GLU	C-N-CA	10.10	140.83	121.54
2	J	452	LEU	N-CA-CB	10.10	124.62	109.98
2	C	560	GLU	CA-C-N	10.09	140.80	121.54
2	C	560	GLU	C-N-CA	10.09	140.80	121.54
2	J	697	ILE	O-C-N	-9.86	112.23	121.89
2	L	560	GLU	CA-C-N	9.86	140.37	121.54
2	L	560	GLU	C-N-CA	9.86	140.37	121.54
2	E	697	ILE	O-C-N	-9.84	112.25	121.89
2	F	560	GLU	CA-C-N	9.78	140.22	121.54
2	F	560	GLU	C-N-CA	9.78	140.22	121.54
2	L	601	ARG	CA-C-N	9.76	139.12	121.85
2	L	601	ARG	C-N-CA	9.76	139.12	121.85
2	F	601	ARG	CA-C-N	9.72	139.05	121.85
2	F	601	ARG	C-N-CA	9.72	139.05	121.85
1	A	87	LYS	CG-CD-CE	9.70	133.60	111.30
1	G	87	LYS	CG-CD-CE	9.69	133.60	111.30
2	E	449	TYR	CB-CG-CD2	-9.69	106.27	120.80
2	E	492	ASP	CB-CG-OD1	-9.68	96.14	118.40
2	J	492	ASP	CB-CG-OD1	-9.67	96.16	118.40
2	J	449	TYR	CB-CG-CD2	-9.66	106.31	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	581	SER	N-CA-C	9.62	123.80	109.95
2	F	581	SER	N-CA-C	9.60	123.78	109.95
1	D	180	ASP	CA-CB-CG	9.55	122.16	112.60
1	D	318	ARG	CB-CA-C	9.55	123.44	109.11
1	A	87	LYS	CA-C-N	9.54	140.11	121.41
1	A	87	LYS	C-N-CA	9.54	140.11	121.41
1	K	318	ARG	CB-CA-C	9.54	123.41	109.11
1	K	180	ASP	CA-CB-CG	9.53	122.13	112.60
2	I	699	SER	CA-C-N	9.51	139.71	121.54
2	I	699	SER	C-N-CA	9.51	139.71	121.54
1	G	87	LYS	CA-C-N	9.51	140.04	121.41
1	G	87	LYS	C-N-CA	9.51	140.04	121.41
2	B	699	SER	CA-C-N	9.50	139.68	121.54
2	B	699	SER	C-N-CA	9.50	139.68	121.54
2	I	372	PHE	O-C-N	-9.44	112.27	122.09
1	G	73	LEU	N-CA-CB	9.38	125.15	109.87
1	A	73	LEU	N-CA-CB	9.37	125.14	109.87
2	B	372	PHE	O-C-N	-9.37	112.35	122.09
1	A	245	LYS	CA-CB-CG	9.36	132.82	114.10
1	G	245	LYS	CA-CB-CG	9.36	132.81	114.10
2	C	581	SER	N-CA-C	9.34	124.72	109.96
2	H	581	SER	N-CA-C	9.34	124.72	109.96
2	I	372	PHE	CA-C-O	9.30	130.85	120.90
2	E	341	GLU	N-CA-CB	9.28	123.44	109.98
2	J	341	GLU	N-CA-CB	9.28	123.43	109.98
2	B	372	PHE	CA-C-O	9.26	130.81	120.90
2	B	341	GLU	N-CA-C	-9.21	100.81	111.03
2	I	341	GLU	N-CA-C	-9.21	100.81	111.03
2	F	574	ASP	N-CA-CB	9.19	124.40	109.88
2	L	574	ASP	N-CA-CB	9.19	124.39	109.88
2	E	489	ASN	O-C-N	-9.10	110.97	122.34
2	J	489	ASN	O-C-N	-9.09	110.97	122.34
2	I	409	PHE	CA-C-N	9.08	134.45	120.82
2	I	409	PHE	C-N-CA	9.08	134.45	120.82
2	B	409	PHE	CA-C-N	9.08	134.44	120.82
2	B	409	PHE	C-N-CA	9.08	134.44	120.82
2	H	592	GLU	CG-CD-OE2	-9.05	97.59	118.40
2	C	592	GLU	CG-CD-OE2	-9.05	97.59	118.40
2	L	600	TYR	N-CA-C	9.05	125.98	114.31
2	F	600	TYR	N-CA-C	9.04	125.97	114.31
2	J	679	ASP	CA-C-N	9.03	133.12	120.29
2	J	679	ASP	C-N-CA	9.03	133.12	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	679	ASP	CA-C-N	9.02	133.10	120.29
2	E	679	ASP	C-N-CA	9.02	133.10	120.29
2	F	574	ASP	CA-C-O	-8.98	110.69	121.02
2	E	338	VAL	CA-C-N	8.92	133.87	120.31
2	E	338	VAL	C-N-CA	8.92	133.87	120.31
2	L	574	ASP	CA-C-O	-8.92	110.76	121.02
2	B	706	TYR	N-CA-CB	8.90	125.52	110.49
2	I	706	TYR	N-CA-CB	8.86	125.46	110.49
2	J	338	VAL	CA-C-N	8.83	133.73	120.31
2	J	338	VAL	C-N-CA	8.83	133.73	120.31
1	D	316	ASN	CA-CB-CG	8.75	121.35	112.60
2	J	366	PHE	CA-CB-CG	8.72	122.52	113.80
2	E	366	PHE	CA-CB-CG	8.71	122.51	113.80
2	I	373	GLU	O-C-N	-8.71	111.66	122.20
1	K	316	ASN	CA-CB-CG	8.71	121.31	112.60
2	B	373	GLU	O-C-N	-8.69	111.69	122.20
2	E	483	LEU	CA-C-N	8.64	137.94	122.31
2	E	483	LEU	C-N-CA	8.64	137.94	122.31
2	J	483	LEU	CA-C-N	8.61	137.90	122.31
2	J	483	LEU	C-N-CA	8.61	137.90	122.31
2	J	483	LEU	O-C-N	-8.60	112.34	122.15
1	K	87	LYS	CB-CG-CD	-8.60	91.53	111.30
1	D	318	ARG	CG-CD-NE	8.59	130.89	112.00
1	D	87	LYS	CB-CG-CD	-8.59	91.55	111.30
1	K	318	ARG	CG-CD-NE	8.59	130.89	112.00
2	E	483	LEU	O-C-N	-8.58	112.36	122.15
2	C	592	GLU	N-CA-CB	8.53	124.30	110.40
2	H	592	GLU	N-CA-CB	8.52	124.30	110.40
1	K	313	GLU	CA-C-N	8.52	132.03	120.44
1	K	313	GLU	C-N-CA	8.52	132.03	120.44
1	D	289	ILE	CA-C-N	8.49	132.01	120.38
1	D	289	ILE	C-N-CA	8.49	132.01	120.38
1	D	313	GLU	CA-C-N	8.48	131.97	120.44
1	D	313	GLU	C-N-CA	8.48	131.97	120.44
1	D	178	ASN	CA-C-N	8.45	135.89	122.21
1	D	178	ASN	C-N-CA	8.45	135.89	122.21
2	C	535	LYS	CA-CB-CG	8.44	130.98	114.10
1	K	178	ASN	CA-C-N	8.44	135.88	122.21
1	K	178	ASN	C-N-CA	8.44	135.88	122.21
2	J	492	ASP	CB-CG-OD2	8.44	137.81	118.40
2	H	535	LYS	CA-CB-CG	8.43	130.96	114.10
2	E	492	ASP	CB-CG-OD2	8.43	137.79	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	289	ILE	CA-C-N	8.42	131.92	120.38
1	K	289	ILE	C-N-CA	8.42	131.92	120.38
2	J	416	GLN	CA-C-N	8.40	131.97	120.46
2	J	416	GLN	C-N-CA	8.40	131.97	120.46
2	B	441	GLN	CA-C-N	8.39	137.57	121.54
2	B	441	GLN	C-N-CA	8.39	137.57	121.54
2	H	533	ILE	O-C-N	-8.38	113.70	121.91
2	I	441	GLN	CA-C-N	8.37	137.53	121.54
2	I	441	GLN	C-N-CA	8.37	137.53	121.54
2	E	416	GLN	CA-C-N	8.37	131.92	120.46
2	E	416	GLN	C-N-CA	8.37	131.92	120.46
2	C	533	ILE	O-C-N	-8.35	113.73	121.91
2	F	558	GLU	CA-CB-CG	8.31	130.73	114.10
2	L	558	GLU	CA-CB-CG	8.29	130.69	114.10
2	I	700	GLU	CA-C-N	8.28	131.70	120.44
2	I	700	GLU	C-N-CA	8.28	131.70	120.44
2	J	376	LYS	CA-C-N	8.27	137.34	121.54
2	J	376	LYS	C-N-CA	8.27	137.34	121.54
2	B	366	PHE	CA-CB-CG	8.27	122.07	113.80
1	D	726	ASP	CA-C-N	8.27	132.03	120.29
1	D	726	ASP	C-N-CA	8.27	132.03	120.29
2	B	490	HIS	CE1-NE2-CD2	-8.27	100.73	109.00
2	I	440	ARG	O-C-N	-8.27	111.35	122.43
2	F	558	GLU	CB-CG-CD	8.27	126.65	112.60
2	B	700	GLU	CA-C-N	8.26	131.68	120.44
2	B	700	GLU	C-N-CA	8.26	131.68	120.44
2	B	440	ARG	O-C-N	-8.25	111.38	122.43
1	K	726	ASP	CA-C-N	8.25	132.00	120.29
1	K	726	ASP	C-N-CA	8.25	132.00	120.29
2	E	376	LYS	CA-C-N	8.24	137.28	121.54
2	E	376	LYS	C-N-CA	8.24	137.28	121.54
2	L	558	GLU	CB-CG-CD	8.23	126.58	112.60
2	I	490	HIS	CE1-NE2-CD2	-8.22	100.78	109.00
2	J	455	GLU	CA-C-N	8.22	133.15	120.82
2	J	455	GLU	C-N-CA	8.22	133.15	120.82
2	J	453	ARG	CG-CD-NE	-8.19	93.98	112.00
2	E	455	GLU	CA-C-N	8.19	133.10	120.82
2	E	455	GLU	C-N-CA	8.19	133.10	120.82
2	E	453	ARG	CG-CD-NE	-8.18	94.00	112.00
2	I	366	PHE	CA-CB-CG	8.17	121.97	113.80
1	G	270	ASP	CA-C-N	8.15	135.62	122.67
1	G	270	ASP	C-N-CA	8.15	135.62	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	270	ASP	CA-C-N	8.10	135.55	122.67
1	A	270	ASP	C-N-CA	8.10	135.55	122.67
2	H	580	MET	N-CA-CB	8.08	120.39	110.53
1	G	88	GLY	N-CA-C	8.07	132.31	113.18
2	H	584	HIS	CB-CG-CD2	-8.07	120.71	131.20
2	J	451	ARG	O-C-N	-8.06	113.67	122.38
1	A	88	GLY	N-CA-C	8.05	132.26	113.18
2	C	580	MET	N-CA-CB	8.05	120.35	110.53
2	E	451	ARG	O-C-N	-8.04	113.70	122.38
2	C	584	HIS	CB-CG-CD2	-8.03	120.76	131.20
1	K	266	ARG	CA-C-N	8.03	133.44	120.60
1	K	266	ARG	C-N-CA	8.03	133.44	120.60
1	D	266	ARG	CA-C-N	8.02	133.43	120.60
1	D	266	ARG	C-N-CA	8.02	133.43	120.60
2	B	484	ALA	N-CA-C	7.90	122.68	112.89
2	I	484	ALA	N-CA-C	7.87	122.65	112.89
2	E	377	MET	N-CA-CB	7.83	123.73	110.49
2	J	377	MET	N-CA-CB	7.83	123.72	110.49
2	F	569	ASN	CB-CG-OD1	7.72	136.24	120.80
2	L	569	ASN	CB-CG-OD1	7.71	136.23	120.80
1	A	741	ILE	CB-CG1-CD1	-7.68	97.67	113.80
1	G	741	ILE	CB-CG1-CD1	-7.68	97.68	113.80
1	K	312	GLU	O-C-N	-7.67	114.11	122.09
2	L	563	TYR	N-CA-CB	7.66	123.43	110.49
2	F	563	TYR	N-CA-CB	7.65	123.42	110.49
1	D	312	GLU	O-C-N	-7.63	114.15	122.09
1	D	180	ASP	N-CA-CB	7.63	123.39	110.49
1	K	180	ASP	N-CA-CB	7.63	123.38	110.49
2	E	473	GLU	CA-CB-CG	7.62	129.35	114.10
2	J	672	ILE	N-CA-C	7.61	118.38	110.62
2	J	473	GLU	CA-CB-CG	7.61	129.31	114.10
2	B	490	HIS	ND1-CG-CD2	-7.60	98.50	106.10
2	I	372	PHE	CA-C-N	7.60	133.27	121.19
2	I	372	PHE	C-N-CA	7.60	133.27	121.19
1	D	228	ARG	CG-CD-NE	7.58	128.68	112.00
1	G	303	GLN	CA-C-N	7.58	132.19	120.82
1	G	303	GLN	C-N-CA	7.58	132.19	120.82
2	B	372	PHE	CA-C-N	7.58	133.24	121.19
2	B	372	PHE	C-N-CA	7.58	133.24	121.19
2	I	490	HIS	ND1-CG-CD2	-7.57	98.53	106.10
1	K	228	ARG	CG-CD-NE	7.57	128.66	112.00
1	D	315	LYS	CA-C-O	-7.56	112.46	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	315	LYS	CA-C-O	-7.56	112.47	120.63
1	A	303	GLN	CA-C-N	7.55	132.15	120.82
1	A	303	GLN	C-N-CA	7.55	132.15	120.82
1	D	145	VAL	CG1-CB-CG2	-7.54	94.21	110.80
2	C	533	ILE	CB-CG1-CD1	-7.54	97.97	113.80
2	B	480	ASP	CA-C-N	7.54	135.53	121.97
2	B	480	ASP	C-N-CA	7.54	135.53	121.97
2	H	533	ILE	CB-CG1-CD1	-7.53	97.99	113.80
1	K	145	VAL	CG1-CB-CG2	-7.53	94.23	110.80
2	E	336	PHE	CA-C-N	7.53	130.70	120.54
2	E	336	PHE	C-N-CA	7.53	130.70	120.54
2	H	601	ARG	O-C-N	-7.52	112.59	122.59
2	I	480	ASP	CA-C-N	7.51	135.49	121.97
2	I	480	ASP	C-N-CA	7.51	135.49	121.97
1	A	282	ASN	CA-C-N	7.50	130.33	120.28
1	A	282	ASN	C-N-CA	7.50	130.33	120.28
2	I	449	TYR	CA-C-O	-7.50	112.17	119.51
2	I	490	HIS	CA-CB-CG	7.49	121.29	113.80
2	C	601	ARG	O-C-N	-7.49	112.63	122.59
2	J	336	PHE	CA-C-N	7.48	130.64	120.54
2	J	336	PHE	C-N-CA	7.48	130.64	120.54
2	B	449	TYR	CA-C-O	-7.48	112.18	119.51
2	J	492	ASP	CA-C-O	-7.47	109.82	120.51
2	E	492	ASP	CA-C-O	-7.46	109.84	120.51
1	G	282	ASN	CA-C-N	7.46	130.28	120.28
1	G	282	ASN	C-N-CA	7.46	130.28	120.28
2	B	490	HIS	CA-CB-CG	7.45	121.25	113.80
1	G	193	VAL	CA-C-N	7.44	129.29	122.37
1	G	193	VAL	C-N-CA	7.44	129.29	122.37
2	H	560	GLU	N-CA-C	7.44	125.00	110.56
2	C	560	GLU	N-CA-C	7.43	124.98	110.56
1	A	193	VAL	CA-C-N	7.43	129.28	122.37
1	A	193	VAL	C-N-CA	7.43	129.28	122.37
2	L	520	VAL	CA-C-N	7.41	130.94	120.42
2	L	520	VAL	C-N-CA	7.41	130.94	120.42
2	F	520	VAL	CA-C-N	7.41	130.94	120.42
2	F	520	VAL	C-N-CA	7.41	130.94	120.42
2	J	342	LYS	CA-CB-CG	7.38	128.86	114.10
2	E	342	LYS	CA-CB-CG	7.37	128.85	114.10
1	A	307	ILE	CA-C-N	7.35	130.00	120.44
1	A	307	ILE	C-N-CA	7.35	130.00	120.44
2	C	533	ILE	N-CA-CB	7.33	119.13	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	533	ILE	N-CA-CB	7.32	119.12	110.55
1	G	307	ILE	CA-C-N	7.30	129.93	120.44
1	G	307	ILE	C-N-CA	7.30	129.93	120.44
2	J	700	GLU	CA-C-N	7.30	131.77	120.82
2	J	700	GLU	C-N-CA	7.30	131.77	120.82
2	I	698	PHE	CA-C-N	7.29	135.47	121.54
2	I	698	PHE	C-N-CA	7.29	135.47	121.54
2	E	700	GLU	CA-C-N	7.29	131.75	120.82
2	E	700	GLU	C-N-CA	7.29	131.75	120.82
2	J	334	GLN	OE1-CD-NE2	7.28	129.88	122.60
2	B	698	PHE	CA-C-N	7.27	135.42	121.54
2	B	698	PHE	C-N-CA	7.27	135.42	121.54
1	A	285	LEU	CA-C-N	7.27	129.89	120.44
1	A	285	LEU	C-N-CA	7.27	129.89	120.44
2	J	367	HIS	O-C-N	-7.26	114.42	122.12
2	E	367	HIS	O-C-N	-7.26	114.42	122.12
1	K	270	ASP	CA-C-N	7.26	136.41	123.34
1	K	270	ASP	C-N-CA	7.26	136.41	123.34
1	D	270	ASP	CA-C-N	7.25	136.39	123.34
1	D	270	ASP	C-N-CA	7.25	136.39	123.34
2	E	334	GLN	OE1-CD-NE2	7.25	129.85	122.60
1	G	285	LEU	CA-C-N	7.25	129.86	120.44
1	G	285	LEU	C-N-CA	7.25	129.86	120.44
2	E	448	GLN	CA-C-N	7.25	131.69	120.60
2	E	448	GLN	C-N-CA	7.25	131.69	120.60
2	J	449	TYR	CE1-CZ-OH	7.24	141.61	119.90
2	E	449	TYR	CE1-CZ-OH	7.23	141.59	119.90
2	E	449	TYR	CA-C-O	-7.22	112.53	120.69
1	G	178	ASN	CA-C-N	7.22	134.20	122.29
1	G	178	ASN	C-N-CA	7.22	134.20	122.29
2	J	448	GLN	CA-C-N	7.22	131.64	120.60
2	J	448	GLN	C-N-CA	7.22	131.64	120.60
2	L	601	ARG	O-C-N	-7.21	112.99	122.59
2	J	449	TYR	CA-C-O	-7.20	112.55	120.69
2	L	559	LYS	CA-C-N	7.20	135.29	121.54
2	L	559	LYS	C-N-CA	7.20	135.29	121.54
2	E	492	ASP	N-CA-C	7.20	126.13	110.80
1	A	178	ASN	CA-C-N	7.19	134.16	122.29
1	A	178	ASN	C-N-CA	7.19	134.16	122.29
2	F	559	LYS	CA-C-N	7.19	135.28	121.54
2	F	559	LYS	C-N-CA	7.19	135.28	121.54
2	J	456	MET	CA-C-N	7.19	129.79	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	456	MET	C-N-CA	7.19	129.79	120.44
2	J	333	VAL	N-CA-CB	7.19	123.10	111.23
2	E	333	VAL	N-CA-CB	7.19	123.09	111.23
2	J	492	ASP	N-CA-C	7.18	126.09	110.80
2	E	456	MET	CA-C-N	7.17	129.76	120.44
2	E	456	MET	C-N-CA	7.17	129.76	120.44
2	F	601	ARG	O-C-N	-7.17	113.05	122.59
2	C	593	GLN	N-CA-C	7.16	119.74	108.79
2	H	593	GLN	N-CA-C	7.15	119.73	108.79
2	F	528	ILE	N-CA-CB	7.12	119.59	111.90
2	J	409	PHE	CA-C-N	7.12	130.13	120.38
2	J	409	PHE	C-N-CA	7.12	130.13	120.38
2	I	696	PHE	O-C-N	-7.12	113.12	122.59
1	D	140	MET	CA-CB-CG	7.11	128.32	114.10
2	I	696	PHE	CA-C-O	7.11	130.68	120.51
1	K	140	MET	CA-CB-CG	7.11	128.32	114.10
2	B	696	PHE	CA-C-O	7.10	130.66	120.51
2	E	409	PHE	CA-C-N	7.09	130.10	120.38
2	E	409	PHE	C-N-CA	7.09	130.10	120.38
2	B	362	ILE	N-CA-CB	7.09	119.15	110.64
2	B	696	PHE	O-C-N	-7.09	113.16	122.59
2	I	362	ILE	N-CA-CB	7.07	119.12	110.64
2	I	490	HIS	N-CA-CB	7.06	122.43	110.49
2	L	528	ILE	N-CA-CB	7.06	119.53	111.90
1	A	267	HIS	CA-C-N	7.05	134.08	122.73
1	A	267	HIS	C-N-CA	7.05	134.08	122.73
2	B	490	HIS	N-CA-CB	7.05	122.41	110.49
1	D	312	GLU	CA-C-O	7.04	128.43	120.90
1	G	267	HIS	CA-C-N	7.04	134.06	122.73
1	G	267	HIS	C-N-CA	7.04	134.06	122.73
1	K	312	GLU	CA-C-O	7.03	128.42	120.90
2	E	459	ILE	CA-C-N	7.03	130.40	120.42
2	E	459	ILE	C-N-CA	7.03	130.40	120.42
1	A	88	GLY	CA-C-N	7.02	134.11	121.97
1	A	88	GLY	C-N-CA	7.02	134.11	121.97
1	G	88	GLY	CA-C-N	7.02	134.11	121.97
1	G	88	GLY	C-N-CA	7.02	134.11	121.97
2	B	685	ILE	O-C-N	-7.00	113.83	122.57
1	G	296	LEU	CA-C-N	6.99	130.50	120.79
1	G	296	LEU	C-N-CA	6.99	130.50	120.79
2	J	459	ILE	CA-C-N	6.99	130.34	120.42
2	J	459	ILE	C-N-CA	6.99	130.34	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	685	ILE	O-C-N	-6.98	113.85	122.57
2	E	343	ARG	CG-CD-NE	6.96	127.31	112.00
2	J	343	ARG	CG-CD-NE	6.96	127.30	112.00
2	H	533	ILE	CA-C-N	6.95	134.81	121.54
2	H	533	ILE	C-N-CA	6.95	134.81	121.54
2	L	561	LYS	N-CA-CB	6.94	122.21	110.49
2	F	561	LYS	N-CA-CB	6.93	122.20	110.49
2	C	533	ILE	CA-C-N	6.92	134.75	121.54
2	C	533	ILE	C-N-CA	6.92	134.75	121.54
2	I	492	ASP	N-CA-CB	-6.90	98.82	110.49
1	A	296	LEU	CA-C-N	6.89	130.37	120.79
1	A	296	LEU	C-N-CA	6.89	130.37	120.79
2	J	460	VAL	CA-CB-CG2	-6.89	98.68	110.40
2	H	534	MET	N-CA-CB	6.89	122.14	110.49
2	H	561	LYS	N-CA-CB	6.89	122.14	110.49
2	J	413	VAL	N-CA-C	6.89	118.47	110.62
2	B	492	ASP	N-CA-CB	-6.89	98.85	110.49
2	C	561	LYS	N-CA-CB	6.88	122.12	110.49
2	E	413	VAL	N-CA-C	6.88	118.46	110.62
2	J	703	ALA	CA-C-N	6.88	129.82	120.54
2	J	703	ALA	C-N-CA	6.88	129.82	120.54
2	E	460	VAL	CA-CB-CG2	-6.87	98.72	110.40
2	C	534	MET	N-CA-CB	6.87	122.10	110.49
2	E	491	GLU	CA-C-O	-6.87	112.51	120.20
2	J	491	GLU	CA-C-O	-6.86	112.52	120.20
2	E	703	ALA	CA-C-N	6.85	129.79	120.54
2	E	703	ALA	C-N-CA	6.85	129.79	120.54
1	G	273	GLY	CA-C-N	6.85	132.37	121.62
1	G	273	GLY	C-N-CA	6.85	132.37	121.62
1	A	273	GLY	CA-C-N	6.85	132.37	121.62
1	A	273	GLY	C-N-CA	6.85	132.37	121.62
1	A	219	VAL	CB-CA-C	-6.83	103.22	111.97
2	J	385	ARG	CA-C-N	6.81	129.73	120.54
2	J	385	ARG	C-N-CA	6.81	129.73	120.54
2	E	385	ARG	CA-C-N	6.81	129.73	120.54
2	E	385	ARG	C-N-CA	6.81	129.73	120.54
1	G	219	VAL	CB-CA-C	-6.79	103.27	111.97
2	F	577	LYS	O-C-N	-6.79	113.56	122.59
2	L	577	LYS	O-C-N	-6.77	113.58	122.59
2	I	482	GLU	N-CA-C	6.77	119.52	111.33
1	D	318	ARG	N-CA-C	6.74	120.09	110.24
1	K	266	ARG	O-C-N	-6.74	114.97	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	482	GLU	N-CA-C	6.73	119.47	111.33
1	K	318	ARG	N-CA-C	6.73	120.06	110.24
2	B	686	MET	O-C-N	-6.71	115.11	122.09
2	I	363	ASN	N-CA-C	6.71	119.17	111.11
1	D	266	ARG	O-C-N	-6.71	115.01	122.12
2	B	363	ASN	N-CA-C	6.70	119.15	111.11
2	F	569	ASN	CB-CA-C	6.70	125.36	110.76
2	I	686	MET	O-C-N	-6.69	115.13	122.09
2	H	560	GLU	O-C-N	-6.69	115.16	122.38
2	L	569	ASN	CB-CA-C	6.67	125.31	110.76
2	C	560	GLU	O-C-N	-6.67	115.18	122.38
1	K	245	LYS	CB-CG-CD	-6.65	96.00	111.30
2	B	441	GLN	O-C-N	-6.65	113.74	122.59
1	K	30	ASP	CA-C-N	6.64	129.91	120.49
1	K	30	ASP	C-N-CA	6.64	129.91	120.49
2	J	491	GLU	N-CA-C	6.64	120.25	111.75
1	D	245	LYS	CB-CG-CD	-6.63	96.04	111.30
2	E	491	GLU	N-CA-C	6.63	120.23	111.75
2	H	575	VAL	CA-C-N	6.62	134.19	121.54
2	H	575	VAL	C-N-CA	6.62	134.19	121.54
2	H	610	GLN	OE1-CD-NE2	6.62	129.22	122.60
2	C	580	MET	O-C-N	-6.62	114.44	122.71
2	E	677	VAL	N-CA-C	6.61	118.16	110.62
2	J	415	LYS	CA-CB-CG	6.60	127.31	114.10
1	D	30	ASP	CA-C-N	6.60	129.86	120.49
1	D	30	ASP	C-N-CA	6.60	129.86	120.49
2	E	415	LYS	CA-CB-CG	6.60	127.30	114.10
1	G	738	ALA	CA-C-N	6.60	129.42	120.38
1	G	738	ALA	C-N-CA	6.60	129.42	120.38
2	C	575	VAL	CA-C-N	6.60	134.14	121.54
2	C	575	VAL	C-N-CA	6.60	134.14	121.54
1	A	738	ALA	CA-C-N	6.59	129.41	120.38
1	A	738	ALA	C-N-CA	6.59	129.41	120.38
2	H	592	GLU	N-CA-C	6.59	121.07	112.89
2	I	441	GLN	O-C-N	-6.59	113.82	122.59
2	B	489	ASN	CA-C-N	6.59	134.13	121.54
2	B	489	ASN	C-N-CA	6.59	134.13	121.54
2	J	677	VAL	N-CA-C	6.59	118.13	110.62
2	E	695	GLU	CG-CD-OE1	6.59	133.55	118.40
2	C	577	LYS	O-C-N	-6.59	113.83	122.59
2	F	581	SER	N-CA-CB	6.59	120.61	110.60
2	J	695	GLU	CG-CD-OE1	6.59	133.55	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	223	LYS	CB-CG-CD	6.58	126.44	111.30
2	C	592	GLU	N-CA-C	6.58	121.05	112.89
1	A	223	LYS	CB-CG-CD	6.58	126.43	111.30
2	C	533	ILE	CA-C-O	6.58	128.14	121.17
2	H	577	LYS	O-C-N	-6.58	113.84	122.59
2	H	533	ILE	CA-C-O	6.57	128.13	121.17
2	H	580	MET	O-C-N	-6.57	114.50	122.71
2	B	698	PHE	O-C-N	-6.57	115.16	122.12
2	C	610	GLN	OE1-CD-NE2	6.57	129.16	122.60
2	I	489	ASN	CA-C-N	6.56	134.08	121.54
2	I	489	ASN	C-N-CA	6.56	134.08	121.54
2	I	698	PHE	O-C-N	-6.56	115.16	122.12
2	B	416	GLN	CA-C-N	6.55	129.44	120.46
2	B	416	GLN	C-N-CA	6.55	129.44	120.46
2	L	581	SER	N-CA-CB	6.55	120.56	110.60
2	E	340	PHE	CA-C-N	-6.53	111.75	120.63
2	E	340	PHE	C-N-CA	-6.53	111.75	120.63
2	I	416	GLN	CA-C-N	6.53	129.41	120.46
2	I	416	GLN	C-N-CA	6.53	129.41	120.46
2	E	379	PHE	N-CA-C	6.53	119.10	109.24
2	J	379	PHE	N-CA-C	6.53	119.09	109.24
2	J	340	PHE	CA-C-N	-6.52	111.77	120.63
2	J	340	PHE	C-N-CA	-6.52	111.77	120.63
2	J	671	ALA	CA-C-N	6.51	129.37	120.46
2	J	671	ALA	C-N-CA	6.51	129.37	120.46
1	A	44	LYS	N-CA-C	6.50	118.91	111.11
2	J	699	SER	CA-C-N	6.49	130.18	120.31
2	J	699	SER	C-N-CA	6.49	130.18	120.31
2	H	549	ASN	CA-C-N	6.48	132.92	123.13
2	H	549	ASN	C-N-CA	6.48	132.92	123.13
2	C	610	GLN	N-CA-CB	6.48	119.78	110.06
2	E	468	GLU	N-CA-C	-6.47	104.08	112.23
2	E	472	LYS	CA-C-N	6.46	129.59	120.28
2	E	472	LYS	C-N-CA	6.46	129.59	120.28
2	H	610	GLN	N-CA-CB	6.46	119.76	110.06
2	E	699	SER	CA-C-N	6.46	130.13	120.31
2	E	699	SER	C-N-CA	6.46	130.13	120.31
2	J	468	GLU	N-CA-C	-6.46	104.09	112.23
1	K	727	GLU	N-CA-C	-6.46	104.32	111.36
2	B	361	ARG	CG-CD-NE	6.46	126.21	112.00
2	C	549	ASN	CA-C-N	6.46	132.88	123.13
2	C	549	ASN	C-N-CA	6.46	132.88	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	361	ARG	CG-CD-NE	6.45	126.20	112.00
1	G	44	LYS	N-CA-C	6.45	118.85	111.11
2	B	468	GLU	N-CA-C	-6.44	104.12	112.23
1	D	297	ARG	CB-CG-CD	6.44	126.11	111.30
1	K	297	ARG	CB-CG-CD	6.44	126.11	111.30
2	J	481	ILE	CA-C-N	6.43	129.19	120.38
2	J	481	ILE	C-N-CA	6.43	129.19	120.38
2	E	481	ILE	CA-C-N	6.43	129.19	120.38
2	E	481	ILE	C-N-CA	6.43	129.19	120.38
2	I	340	PHE	CA-C-N	-6.43	111.89	120.63
2	I	340	PHE	C-N-CA	-6.43	111.89	120.63
2	J	472	LYS	CA-C-N	6.43	129.53	120.28
2	J	472	LYS	C-N-CA	6.43	129.53	120.28
2	B	340	PHE	CA-C-N	-6.42	111.89	120.63
2	B	340	PHE	C-N-CA	-6.42	111.89	120.63
2	H	576	GLU	CA-C-N	6.42	133.81	121.54
2	H	576	GLU	C-N-CA	6.42	133.81	121.54
2	E	387	GLU	CA-C-N	6.42	129.58	120.53
2	E	387	GLU	C-N-CA	6.42	129.58	120.53
2	C	576	GLU	CA-C-N	6.42	133.79	121.54
2	C	576	GLU	C-N-CA	6.42	133.79	121.54
1	D	727	GLU	N-CA-C	-6.41	104.37	111.36
2	E	449	TYR	CB-CA-C	6.41	119.97	109.46
2	J	387	GLU	CA-C-N	6.41	129.57	120.53
2	J	387	GLU	C-N-CA	6.41	129.57	120.53
2	J	449	TYR	CB-CA-C	6.41	119.97	109.46
2	I	468	GLU	N-CA-C	-6.41	104.16	112.23
2	J	372	PHE	CA-C-N	6.41	129.19	120.54
2	J	372	PHE	C-N-CA	6.41	129.19	120.54
1	K	171	ILE	N-CA-C	6.39	117.70	107.73
1	D	171	ILE	N-CA-C	6.37	117.67	107.73
2	J	492	ASP	CA-CB-CG	-6.37	106.23	112.60
2	E	492	ASP	CA-CB-CG	-6.37	106.23	112.60
2	J	484	ALA	N-CA-CB	6.37	121.52	109.93
2	E	484	ALA	N-CA-CB	6.36	121.51	109.93
1	G	741	ILE	CA-CB-CG1	-6.36	99.58	110.40
2	E	372	PHE	CA-C-N	6.36	129.13	120.54
2	E	372	PHE	C-N-CA	6.36	129.13	120.54
1	K	254	ALA	CA-C-N	6.36	129.09	120.38
1	K	254	ALA	C-N-CA	6.36	129.09	120.38
2	J	690	ILE	N-CA-C	6.35	116.84	110.23
2	E	697	ILE	CB-CG1-CD1	6.35	127.13	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	690	ILE	N-CA-C	6.34	116.83	110.23
2	J	697	ILE	CB-CG1-CD1	6.34	127.12	113.80
1	A	741	ILE	CA-CB-CG1	-6.34	99.62	110.40
1	A	272	MET	CA-C-N	6.33	132.28	121.39
1	A	272	MET	C-N-CA	6.33	132.28	121.39
1	K	276	TYR	CA-C-N	6.33	128.76	120.28
1	K	276	TYR	C-N-CA	6.33	128.76	120.28
2	H	590	ASN	O-C-N	-6.33	115.63	123.04
2	J	362	ILE	N-CA-CB	6.33	118.23	110.64
1	D	317	PHE	CA-C-O	-6.33	114.36	120.94
1	K	317	PHE	CA-C-O	-6.32	114.37	120.94
2	L	580	MET	O-C-N	-6.32	114.81	122.71
2	E	450	PRO	N-CA-CB	-6.32	96.82	103.52
1	D	276	TYR	CA-C-N	6.31	128.74	120.28
1	D	276	TYR	C-N-CA	6.31	128.74	120.28
1	D	254	ALA	CA-C-N	6.31	129.02	120.38
1	D	254	ALA	C-N-CA	6.31	129.02	120.38
2	J	450	PRO	N-CA-CB	-6.31	96.83	103.52
2	F	580	MET	O-C-N	-6.31	114.83	122.71
1	G	272	MET	CA-C-N	6.31	132.24	121.39
1	G	272	MET	C-N-CA	6.31	132.24	121.39
2	E	704	ASN	OD1-CG-ND2	-6.30	116.30	122.60
2	I	696	PHE	N-CA-CB	6.30	121.14	110.49
2	E	362	ILE	N-CA-CB	6.30	118.20	110.64
2	J	704	ASN	OD1-CG-ND2	-6.30	116.30	122.60
2	C	590	ASN	O-C-N	-6.29	115.68	123.04
1	G	299	LYS	CA-C-N	6.29	128.70	120.28
1	G	299	LYS	C-N-CA	6.29	128.70	120.28
2	B	696	PHE	N-CA-CB	6.28	121.11	110.49
2	J	490	HIS	CA-C-N	6.28	129.54	120.38
2	J	490	HIS	C-N-CA	6.28	129.54	120.38
1	A	67	ARG	NE-CZ-NH2	6.27	124.84	119.20
1	G	67	ARG	NE-CZ-NH2	6.27	124.85	119.20
2	E	415	LYS	CB-CG-CD	6.27	125.72	111.30
2	E	490	HIS	CA-C-N	6.27	129.53	120.38
2	E	490	HIS	C-N-CA	6.27	129.53	120.38
2	J	415	LYS	CB-CG-CD	6.26	125.70	111.30
2	C	522	ARG	N-CA-CB	6.26	121.06	110.49
2	H	522	ARG	N-CA-CB	6.25	121.05	110.49
1	A	299	LYS	CA-C-N	6.23	128.63	120.28
1	A	299	LYS	C-N-CA	6.23	128.63	120.28
2	I	342	LYS	CB-CG-CD	6.21	125.59	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	584	HIS	CA-CB-CG	6.21	120.01	113.80
2	B	342	LYS	CB-CG-CD	6.20	125.57	111.30
2	B	489	ASN	N-CA-CB	6.19	119.92	110.70
2	H	584	HIS	CA-CB-CG	6.17	119.97	113.80
1	D	282	ASN	CA-C-N	6.15	128.53	120.28
1	D	282	ASN	C-N-CA	6.15	128.53	120.28
2	B	377	MET	CA-C-N	6.15	132.39	121.75
2	B	377	MET	C-N-CA	6.15	132.39	121.75
2	I	693	THR	CA-C-N	6.15	130.97	121.19
2	I	693	THR	C-N-CA	6.15	130.97	121.19
2	F	575	VAL	CA-C-N	6.15	133.28	121.54
2	F	575	VAL	C-N-CA	6.15	133.28	121.54
2	J	494	ILE	CA-CB-CG1	6.15	120.85	110.40
2	B	693	THR	CA-C-N	6.14	130.95	121.19
2	B	693	THR	C-N-CA	6.14	130.95	121.19
2	I	377	MET	CA-C-N	6.13	132.36	121.75
2	I	377	MET	C-N-CA	6.13	132.36	121.75
1	K	282	ASN	CA-C-N	6.13	128.49	120.28
1	K	282	ASN	C-N-CA	6.13	128.49	120.28
2	J	480	ASP	CA-C-N	6.12	128.50	120.60
2	J	480	ASP	C-N-CA	6.12	128.50	120.60
2	L	575	VAL	CA-C-N	6.12	133.23	121.54
2	L	575	VAL	C-N-CA	6.12	133.23	121.54
2	I	489	ASN	N-CA-CB	6.12	119.81	110.70
2	E	339	ASP	N-CA-CB	6.11	119.75	110.28
2	E	480	ASP	CA-C-N	6.11	128.48	120.60
2	E	480	ASP	C-N-CA	6.11	128.48	120.60
2	E	494	ILE	CA-CB-CG1	6.11	120.78	110.40
1	A	120	ILE	N-CA-C	-6.10	99.08	107.99
1	D	131	ASN	CA-C-N	6.10	132.16	122.59
1	D	131	ASN	C-N-CA	6.10	132.16	122.59
2	J	460	VAL	N-CA-C	6.09	116.87	110.72
2	E	460	VAL	N-CA-C	6.09	116.87	110.72
1	K	131	ASN	CA-C-N	6.08	132.14	122.59
1	K	131	ASN	C-N-CA	6.08	132.14	122.59
1	G	120	ILE	N-CA-C	-6.08	99.11	107.99
2	J	417	VAL	CA-C-N	6.07	128.41	120.28
2	J	417	VAL	C-N-CA	6.07	128.41	120.28
2	E	468	GLU	CA-C-N	6.06	127.77	120.13
2	E	468	GLU	C-N-CA	6.06	127.77	120.13
2	H	580	MET	CA-CB-CG	6.06	126.22	114.10
2	C	580	MET	CA-CB-CG	6.05	126.21	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	361	ARG	CA-C-N	-6.05	113.50	120.88
2	E	361	ARG	C-N-CA	-6.05	113.50	120.88
2	E	417	VAL	CA-C-N	6.05	128.39	120.28
2	E	417	VAL	C-N-CA	6.05	128.39	120.28
2	H	575	VAL	N-CA-CB	6.05	118.43	111.90
2	J	339	ASP	N-CA-CB	6.05	119.65	110.28
2	C	584	HIS	N-CA-CB	6.04	120.33	110.37
2	H	584	HIS	N-CA-CB	6.04	120.33	110.37
2	C	575	VAL	N-CA-CB	6.04	118.42	111.90
1	D	730	ARG	CA-C-N	6.03	128.37	120.28
1	D	730	ARG	C-N-CA	6.03	128.37	120.28
1	K	311	VAL	N-CA-CB	6.03	117.61	110.55
2	J	361	ARG	CA-C-N	-6.03	113.53	120.88
2	J	361	ARG	C-N-CA	-6.03	113.53	120.88
2	J	468	GLU	CA-C-N	6.02	127.72	120.13
2	J	468	GLU	C-N-CA	6.02	127.72	120.13
1	A	87	LYS	CA-C-O	-6.02	111.91	120.51
1	D	311	VAL	N-CA-CB	6.01	117.58	110.55
2	B	368	GLU	CA-C-N	6.00	131.66	122.24
2	B	368	GLU	C-N-CA	6.00	131.66	122.24
1	K	730	ARG	CA-C-N	6.00	128.32	120.28
1	K	730	ARG	C-N-CA	6.00	128.32	120.28
2	F	585	ILE	N-CA-C	5.99	118.26	108.97
1	K	102	GLU	CA-C-N	5.99	128.31	120.28
1	K	102	GLU	C-N-CA	5.99	128.31	120.28
1	G	87	LYS	CA-C-O	-5.98	111.96	120.51
2	I	683	LYS	O-C-N	-5.98	115.81	122.03
2	B	689	MET	CA-C-N	5.98	132.73	121.97
2	B	689	MET	C-N-CA	5.98	132.73	121.97
2	C	534	MET	CA-C-N	5.98	130.88	121.08
2	C	534	MET	C-N-CA	5.98	130.88	121.08
1	D	102	GLU	CA-C-N	5.97	128.29	120.28
1	D	102	GLU	C-N-CA	5.97	128.29	120.28
2	F	553	TYR	N-CA-CB	5.97	119.60	110.70
2	I	674	ASN	O-C-N	-5.97	115.92	122.07
2	I	655	LEU	CA-C-N	5.97	128.56	120.38
2	I	655	LEU	C-N-CA	5.97	128.56	120.38
2	L	576	GLU	CA-C-N	5.97	132.95	121.54
2	L	576	GLU	C-N-CA	5.97	132.95	121.54
2	I	415	LYS	CA-C-N	5.97	128.76	120.29
2	I	415	LYS	C-N-CA	5.97	128.76	120.29
2	J	449	TYR	CA-CB-CG	5.97	124.64	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	689	MET	CA-C-N	5.96	132.71	121.97
2	I	689	MET	C-N-CA	5.96	132.71	121.97
2	B	683	LYS	O-C-N	-5.96	115.83	122.03
2	L	553	TYR	N-CA-CB	5.96	119.58	110.70
2	F	560	GLU	N-CA-C	5.96	123.49	110.80
2	L	585	ILE	N-CA-C	5.96	118.20	108.97
2	I	683	LYS	CA-C-N	5.95	132.91	121.54
2	I	683	LYS	C-N-CA	5.95	132.91	121.54
2	B	674	ASN	O-C-N	-5.95	115.94	122.07
2	B	683	LYS	CA-C-N	5.95	132.90	121.54
2	B	683	LYS	C-N-CA	5.95	132.90	121.54
2	I	368	GLU	CA-C-N	5.95	131.58	122.24
2	I	368	GLU	C-N-CA	5.95	131.58	122.24
2	H	534	MET	CA-C-N	5.95	130.84	121.08
2	H	534	MET	C-N-CA	5.95	130.84	121.08
2	I	702	LEU	CA-C-N	5.95	128.57	120.54
2	I	702	LEU	C-N-CA	5.95	128.57	120.54
2	C	560	GLU	N-CA-CB	5.95	119.55	110.39
2	B	415	LYS	CA-C-N	5.95	128.73	120.29
2	B	415	LYS	C-N-CA	5.95	128.73	120.29
2	E	449	TYR	CA-CB-CG	5.94	124.60	113.90
2	H	560	GLU	N-CA-CB	5.94	119.54	110.39
2	L	560	GLU	N-CA-C	5.93	123.44	110.80
2	B	655	LEU	CA-C-N	5.93	128.50	120.38
2	B	655	LEU	C-N-CA	5.93	128.50	120.38
2	F	576	GLU	CA-C-N	5.92	132.85	121.54
2	F	576	GLU	C-N-CA	5.92	132.85	121.54
2	E	439	VAL	CG1-CB-CG2	-5.92	97.78	110.80
2	H	609	THR	CA-C-N	5.92	128.48	120.38
2	H	609	THR	C-N-CA	5.92	128.48	120.38
2	J	439	VAL	CG1-CB-CG2	-5.92	97.79	110.80
2	I	699	SER	CA-C-O	-5.91	112.06	120.51
2	B	702	LEU	CA-C-N	5.91	128.51	120.54
2	B	702	LEU	C-N-CA	5.91	128.51	120.54
2	C	609	THR	CA-C-N	5.91	128.47	120.38
2	C	609	THR	C-N-CA	5.91	128.47	120.38
1	D	142	LYS	N-CA-CB	-5.91	102.73	110.88
1	K	142	LYS	N-CA-CB	-5.91	102.73	110.88
2	B	699	SER	CA-C-O	-5.90	112.07	120.51
1	K	64	VAL	O-C-N	5.90	126.33	121.85
2	I	694	LYS	CA-C-N	5.90	130.57	121.19
2	I	694	LYS	C-N-CA	5.90	130.57	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	29	LEU	CA-C-N	5.90	132.80	121.54
1	K	29	LEU	C-N-CA	5.90	132.80	121.54
2	I	666	VAL	CA-C-N	5.89	129.66	120.82
2	I	666	VAL	C-N-CA	5.89	129.66	120.82
2	J	339	ASP	CA-C-N	5.89	128.66	120.29
2	J	339	ASP	C-N-CA	5.89	128.66	120.29
2	B	418	LYS	CA-C-N	5.89	130.56	120.72
2	B	418	LYS	C-N-CA	5.89	130.56	120.72
2	C	581	SER	N-CA-CB	5.89	120.27	110.14
2	J	699	SER	N-CA-C	5.88	123.33	110.80
2	E	699	SER	N-CA-C	5.88	123.33	110.80
2	E	672	ILE	N-CA-C	5.88	118.40	111.05
2	E	339	ASP	CA-C-N	5.87	128.63	120.29
2	E	339	ASP	C-N-CA	5.87	128.63	120.29
2	H	581	SER	N-CA-CB	5.87	120.24	110.14
1	D	29	LEU	CA-C-N	5.87	132.75	121.54
1	D	29	LEU	C-N-CA	5.87	132.75	121.54
1	G	244	GLY	O-C-N	-5.87	114.40	122.68
2	C	584	HIS	CB-CA-C	5.86	120.16	110.78
2	L	621	LEU	CA-C-N	5.86	128.72	120.28
2	L	621	LEU	C-N-CA	5.86	128.72	120.28
2	F	621	LEU	CA-C-N	5.86	128.72	120.28
2	F	621	LEU	C-N-CA	5.86	128.72	120.28
1	D	64	VAL	O-C-N	5.86	126.30	121.85
2	B	694	LYS	CA-C-N	5.86	130.50	121.19
2	B	694	LYS	C-N-CA	5.86	130.50	121.19
2	J	339	ASP	O-C-N	-5.85	115.07	122.27
2	J	341	GLU	CG-CD-OE2	-5.85	104.94	118.40
2	I	418	LYS	CA-C-N	5.85	130.49	120.72
2	I	418	LYS	C-N-CA	5.85	130.49	120.72
2	H	584	HIS	CB-CA-C	5.85	120.14	110.78
2	E	339	ASP	O-C-N	-5.84	115.08	122.27
1	D	285	LEU	CA-C-N	5.84	128.10	120.28
1	D	285	LEU	C-N-CA	5.84	128.10	120.28
1	G	67	ARG	NE-CZ-NH1	-5.84	115.66	121.50
1	A	67	ARG	NE-CZ-NH1	-5.83	115.67	121.50
2	B	666	VAL	CA-C-N	5.83	129.57	120.82
2	B	666	VAL	C-N-CA	5.83	129.57	120.82
1	A	244	GLY	O-C-N	-5.81	114.48	122.68
2	E	341	GLU	CG-CD-OE2	-5.81	105.03	118.40
2	B	694	LYS	N-CA-CB	5.81	119.59	109.72
1	K	285	LEU	CA-C-N	5.80	128.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	285	LEU	C-N-CA	5.80	128.06	120.28
2	E	384	LEU	CA-C-N	5.80	128.84	120.38
2	E	384	LEU	C-N-CA	5.80	128.84	120.38
2	I	379	PHE	N-CA-C	5.79	117.99	109.24
1	G	131	ASN	CA-C-N	5.79	133.28	122.74
1	G	131	ASN	C-N-CA	5.79	133.28	122.74
1	K	228	ARG	CD-NE-CZ	5.79	132.50	124.40
2	I	694	LYS	N-CA-CB	5.78	119.55	109.72
2	B	379	PHE	N-CA-C	5.78	117.97	109.24
2	J	469	GLY	CA-C-O	-5.78	114.56	120.45
2	B	472	LYS	CA-C-N	5.77	128.02	120.28
2	B	472	LYS	C-N-CA	5.77	128.02	120.28
2	I	455	GLU	CA-C-N	5.77	128.29	120.38
2	I	455	GLU	C-N-CA	5.77	128.29	120.38
2	J	490	HIS	O-C-N	-5.77	114.91	122.59
1	A	190	ALA	CA-C-N	5.77	129.83	120.60
1	A	190	ALA	C-N-CA	5.77	129.83	120.60
1	G	190	ALA	CA-C-N	5.77	129.83	120.60
1	G	190	ALA	C-N-CA	5.77	129.83	120.60
1	A	131	ASN	CA-C-N	5.77	133.24	122.74
1	A	131	ASN	C-N-CA	5.77	133.24	122.74
1	G	244	GLY	CA-C-O	5.77	128.54	119.31
2	E	490	HIS	O-C-N	-5.76	114.93	122.59
2	J	384	LEU	CA-C-N	5.76	128.79	120.38
2	J	384	LEU	C-N-CA	5.76	128.79	120.38
2	J	464	ILE	CB-CG1-CD1	5.76	125.90	113.80
2	L	560	GLU	N-CA-CB	5.76	120.22	110.49
2	I	677	VAL	N-CA-C	5.76	117.18	110.62
2	E	469	GLY	CA-C-O	-5.75	114.58	120.45
2	E	464	ILE	CB-CG1-CD1	5.75	125.88	113.80
2	B	455	GLU	CA-C-N	5.75	128.26	120.38
2	B	455	GLU	C-N-CA	5.75	128.26	120.38
2	E	683	LYS	CA-C-N	5.75	132.52	121.54
2	E	683	LYS	C-N-CA	5.75	132.52	121.54
2	J	683	LYS	CA-C-N	5.75	132.53	121.54
2	J	683	LYS	C-N-CA	5.75	132.53	121.54
2	I	472	LYS	CA-C-N	5.75	127.98	120.28
2	I	472	LYS	C-N-CA	5.75	127.98	120.28
1	D	228	ARG	CD-NE-CZ	5.75	132.44	124.40
1	A	89	LYS	N-CA-CB	5.74	118.03	109.19
1	K	38	GLY	CA-C-O	-5.74	116.02	121.87
1	A	244	GLY	CA-C-O	5.73	128.47	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	560	GLU	N-CA-CB	5.72	120.16	110.49
1	G	89	LYS	N-CA-CB	5.72	118.00	109.19
2	B	492	ASP	OD1-CG-OD2	-5.71	109.20	122.90
1	K	296	LEU	CA-C-N	5.71	128.25	120.54
1	K	296	LEU	C-N-CA	5.71	128.25	120.54
1	D	38	GLY	CA-C-O	-5.71	116.05	121.87
2	L	528	ILE	CA-C-N	5.71	128.98	120.31
2	L	528	ILE	C-N-CA	5.71	128.98	120.31
1	G	170	LEU	CA-C-N	5.70	129.61	122.43
1	G	170	LEU	C-N-CA	5.70	129.61	122.43
2	B	383	GLU	CA-C-N	5.69	128.18	120.38
2	B	383	GLU	C-N-CA	5.69	128.18	120.38
2	B	677	VAL	N-CA-C	5.69	117.11	110.62
1	K	727	GLU	CA-C-N	5.69	132.41	121.54
1	K	727	GLU	C-N-CA	5.69	132.41	121.54
1	A	170	LEU	CA-C-N	5.69	129.60	122.43
1	A	170	LEU	C-N-CA	5.69	129.60	122.43
2	J	368	GLU	CA-C-N	5.69	131.17	122.24
2	J	368	GLU	C-N-CA	5.69	131.17	122.24
1	D	256	ARG	CA-C-N	5.68	128.22	120.54
1	D	256	ARG	C-N-CA	5.68	128.22	120.54
2	L	575	VAL	CA-C-O	-5.68	113.67	120.78
1	K	256	ARG	CA-C-N	5.68	128.21	120.54
1	K	256	ARG	C-N-CA	5.68	128.21	120.54
1	D	296	LEU	CA-C-N	5.68	128.21	120.54
1	D	296	LEU	C-N-CA	5.68	128.21	120.54
2	I	383	GLU	CA-C-N	5.68	128.16	120.38
2	I	383	GLU	C-N-CA	5.68	128.16	120.38
2	F	528	ILE	CA-C-N	5.68	128.94	120.31
2	F	528	ILE	C-N-CA	5.68	128.94	120.31
2	J	377	MET	CA-C-N	5.67	131.66	122.53
2	J	377	MET	C-N-CA	5.67	131.66	122.53
2	F	581	SER	CA-CB-OG	-5.67	99.76	111.10
2	I	492	ASP	OD1-CG-OD2	-5.67	109.30	122.90
2	E	485	TYR	CE1-CZ-CE2	-5.66	108.97	120.30
2	H	624	GLY	CA-C-N	5.66	129.56	122.48
2	H	624	GLY	C-N-CA	5.66	129.56	122.48
2	J	485	TYR	CE1-CZ-CE2	-5.66	108.98	120.30
2	L	581	SER	CA-CB-OG	-5.66	99.78	111.10
1	D	727	GLU	CA-C-N	5.65	132.33	121.54
1	D	727	GLU	C-N-CA	5.65	132.33	121.54
1	G	741	ILE	CA-CB-CG2	5.65	120.10	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	575	VAL	CA-C-O	-5.65	113.72	120.78
2	E	377	MET	CA-C-N	5.63	131.60	122.53
2	E	377	MET	C-N-CA	5.63	131.60	122.53
2	F	568	ASP	N-CA-C	5.63	118.75	110.30
2	C	624	GLY	CA-C-N	5.63	129.52	122.48
2	C	624	GLY	C-N-CA	5.63	129.52	122.48
2	L	568	ASP	N-CA-C	5.63	118.74	110.30
2	E	368	GLU	CA-C-N	5.62	131.07	122.24
2	E	368	GLU	C-N-CA	5.62	131.07	122.24
1	D	281	LEU	CA-C-N	5.62	128.08	120.38
1	D	281	LEU	C-N-CA	5.62	128.08	120.38
1	A	741	ILE	CA-CB-CG2	5.62	120.05	110.50
2	E	671	ALA	CA-C-N	5.62	129.34	120.47
2	E	671	ALA	C-N-CA	5.62	129.34	120.47
2	H	564	MET	CA-C-N	5.62	130.47	122.72
2	H	564	MET	C-N-CA	5.62	130.47	122.72
1	K	281	LEU	CA-C-N	5.62	128.07	120.38
1	K	281	LEU	C-N-CA	5.62	128.07	120.38
1	D	219	VAL	CA-C-N	5.61	128.36	120.28
1	D	219	VAL	C-N-CA	5.61	128.36	120.28
1	A	169	CYS	CA-C-N	5.61	129.85	121.72
1	A	169	CYS	C-N-CA	5.61	129.85	121.72
2	H	528	ILE	N-CA-CB	5.61	117.96	111.90
2	C	564	MET	CA-C-N	5.60	130.45	122.72
2	C	564	MET	C-N-CA	5.60	130.45	122.72
2	I	469	GLY	CA-C-O	-5.60	114.35	120.40
1	K	90	LYS	CA-C-N	5.60	128.83	120.87
1	K	90	LYS	C-N-CA	5.60	128.83	120.87
2	B	469	GLY	CA-C-O	-5.60	114.35	120.40
1	D	90	LYS	CA-C-N	5.60	128.82	120.87
1	D	90	LYS	C-N-CA	5.60	128.82	120.87
1	G	169	CYS	CA-C-N	5.60	129.84	121.72
1	G	169	CYS	C-N-CA	5.60	129.84	121.72
2	C	528	ILE	N-CA-CB	5.59	117.94	111.90
2	J	414	LYS	CA-C-O	-5.58	114.92	120.90
1	G	80	TYR	CA-C-N	5.58	131.73	121.85
1	G	80	TYR	C-N-CA	5.58	131.73	121.85
1	K	219	VAL	CA-C-N	5.58	128.31	120.28
1	K	219	VAL	C-N-CA	5.58	128.31	120.28
2	B	478	LEU	CA-C-N	5.57	127.58	120.56
2	B	478	LEU	C-N-CA	5.57	127.58	120.56
1	G	248	ILE	N-CA-C	5.57	116.30	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	248	ILE	N-CA-C	5.57	116.30	110.62
2	I	685	ILE	CA-C-N	5.57	128.05	120.54
2	I	685	ILE	C-N-CA	5.57	128.05	120.54
2	B	335	GLN	CA-C-N	5.56	127.72	120.28
2	B	335	GLN	C-N-CA	5.56	127.72	120.28
2	E	414	LYS	CA-C-O	-5.56	114.95	120.90
2	I	478	LEU	CA-C-N	5.55	127.55	120.56
2	I	478	LEU	C-N-CA	5.55	127.55	120.56
2	J	457	GLU	CA-C-N	5.55	127.71	120.28
2	J	457	GLU	C-N-CA	5.55	127.71	120.28
2	E	485	TYR	CG-CD2-CE2	-5.55	112.88	121.20
1	A	80	TYR	CA-C-N	5.54	131.66	121.85
1	A	80	TYR	C-N-CA	5.54	131.66	121.85
2	I	335	GLN	CA-C-N	5.54	127.71	120.28
2	I	335	GLN	C-N-CA	5.54	127.71	120.28
2	B	685	ILE	CA-C-N	5.54	128.02	120.54
2	B	685	ILE	C-N-CA	5.54	128.02	120.54
2	J	485	TYR	CG-CD2-CE2	-5.53	112.91	121.20
2	L	560	GLU	O-C-N	-5.52	115.25	122.59
2	B	449	TYR	CA-CB-CG	5.51	123.81	113.90
2	E	457	GLU	CA-C-N	5.50	127.65	120.28
2	E	457	GLU	C-N-CA	5.50	127.65	120.28
1	A	123	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	G	123	ARG	NE-CZ-NH1	-5.46	116.03	121.50
2	F	560	GLU	O-C-N	-5.46	115.33	122.59
2	I	449	TYR	CA-CB-CG	5.46	123.72	113.90
1	K	277	LEU	CA-C-N	5.46	127.53	120.44
1	K	277	LEU	C-N-CA	5.46	127.53	120.44
2	F	564	MET	CA-C-N	5.45	130.16	122.09
2	F	564	MET	C-N-CA	5.45	130.16	122.09
2	I	687	HIS	CA-C-N	5.45	131.95	121.54
2	I	687	HIS	C-N-CA	5.45	131.95	121.54
1	D	280	VAL	CA-C-N	5.44	127.88	120.54
1	D	280	VAL	C-N-CA	5.44	127.88	120.54
2	B	687	HIS	CA-C-N	5.44	131.92	121.54
2	B	687	HIS	C-N-CA	5.44	131.92	121.54
1	D	160	LEU	CA-C-N	5.42	128.09	120.28
1	D	160	LEU	C-N-CA	5.42	128.09	120.28
1	A	270	ASP	O-C-N	-5.42	114.98	122.46
1	G	270	ASP	O-C-N	-5.42	114.98	122.46
2	E	704	ASN	N-CA-CB	5.42	118.01	109.94
1	G	113	LYS	N-CA-C	5.42	119.84	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	704	ASN	N-CA-CB	5.41	118.00	109.94
1	A	85	HIS	CA-C-N	5.41	132.20	123.33
1	A	85	HIS	C-N-CA	5.41	132.20	123.33
1	K	160	LEU	CA-C-N	5.41	128.07	120.28
1	K	160	LEU	C-N-CA	5.41	128.07	120.28
2	H	528	ILE	CA-C-N	5.41	128.53	120.31
2	H	528	ILE	C-N-CA	5.41	128.53	120.31
2	L	564	MET	CA-C-N	5.41	130.09	122.09
2	L	564	MET	C-N-CA	5.41	130.09	122.09
1	K	300	LEU	CA-C-N	5.41	127.84	120.54
1	K	300	LEU	C-N-CA	5.41	127.84	120.54
2	E	673	VAL	CA-C-N	5.40	127.78	120.38
2	E	673	VAL	C-N-CA	5.40	127.78	120.38
1	D	300	LEU	CA-C-N	5.40	127.83	120.54
1	D	300	LEU	C-N-CA	5.40	127.83	120.54
1	A	106	ASP	CA-C-N	5.40	128.92	120.82
1	A	106	ASP	C-N-CA	5.40	128.92	120.82
2	C	609	THR	CA-C-O	5.40	127.42	121.11
1	G	736	LYS	CA-C-N	5.40	127.46	120.44
1	G	736	LYS	C-N-CA	5.40	127.46	120.44
1	K	731	MET	CA-C-N	5.40	127.83	120.54
1	K	731	MET	C-N-CA	5.40	127.83	120.54
2	C	528	ILE	CA-C-N	5.39	128.51	120.31
2	C	528	ILE	C-N-CA	5.39	128.51	120.31
2	I	342	LYS	CA-CB-CG	5.39	124.89	114.10
2	J	699	SER	O-C-N	-5.39	115.42	122.59
2	F	568	ASP	CA-C-O	5.39	126.62	120.80
1	G	85	HIS	CA-C-N	5.39	132.17	123.33
1	G	85	HIS	C-N-CA	5.39	132.17	123.33
2	J	673	VAL	CA-C-N	5.39	127.77	120.38
2	J	673	VAL	C-N-CA	5.39	127.77	120.38
1	G	106	ASP	CA-C-N	5.39	128.91	120.82
1	G	106	ASP	C-N-CA	5.39	128.91	120.82
2	H	609	THR	CA-C-O	5.39	127.42	121.11
2	E	367	HIS	CA-C-N	5.38	131.26	122.65
2	E	367	HIS	C-N-CA	5.38	131.26	122.65
2	E	699	SER	O-C-N	-5.38	115.44	122.59
1	A	736	LYS	CA-C-N	5.38	127.43	120.44
1	A	736	LYS	C-N-CA	5.38	127.43	120.44
2	B	342	LYS	CA-CB-CG	5.38	124.86	114.10
2	J	363	ASN	N-CA-C	5.38	120.25	111.37
1	D	277	LEU	CA-C-N	5.38	127.43	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	277	LEU	C-N-CA	5.38	127.43	120.44
2	J	367	HIS	CA-C-N	5.38	131.25	122.65
2	J	367	HIS	C-N-CA	5.38	131.25	122.65
1	K	280	VAL	CA-C-N	5.38	127.80	120.54
1	K	280	VAL	C-N-CA	5.38	127.80	120.54
2	H	629	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	D	731	MET	CA-C-N	5.37	127.79	120.54
1	D	731	MET	C-N-CA	5.37	127.79	120.54
2	J	343	ARG	CD-NE-CZ	5.37	131.92	124.40
2	L	568	ASP	CA-C-O	5.36	126.59	120.80
2	E	363	ASN	N-CA-C	5.36	120.21	111.37
2	E	343	ARG	CD-NE-CZ	5.36	131.90	124.40
2	I	440	ARG	CA-C-O	5.35	125.96	119.38
1	A	113	LYS	N-CA-C	5.35	119.75	113.23
2	C	581	SER	CA-CB-OG	-5.33	100.43	111.10
2	B	440	ARG	CA-C-O	5.33	125.94	119.38
2	J	333	VAL	CA-CB-CG2	5.33	119.46	110.40
2	J	461	THR	CA-C-N	5.33	127.95	120.28
2	J	461	THR	C-N-CA	5.33	127.95	120.28
1	D	207	LEU	N-CA-C	-5.33	105.92	112.90
2	E	333	VAL	CA-CB-CG2	5.33	119.45	110.40
2	E	461	THR	CA-C-N	5.33	127.95	120.28
2	E	461	THR	C-N-CA	5.33	127.95	120.28
1	K	207	LEU	N-CA-C	-5.32	105.93	112.90
2	J	474	GLN	CA-C-N	5.32	127.26	120.56
2	J	474	GLN	C-N-CA	5.32	127.26	120.56
2	H	581	SER	CA-CB-OG	-5.32	100.46	111.10
2	E	474	GLN	CA-C-N	5.32	127.26	120.56
2	E	474	GLN	C-N-CA	5.32	127.26	120.56
2	J	335	GLN	CA-C-N	5.31	127.40	120.28
2	J	335	GLN	C-N-CA	5.31	127.40	120.28
2	C	629	ARG	NE-CZ-NH1	-5.31	116.19	121.50
2	C	568	ASP	N-CA-C	5.31	117.87	109.96
2	E	456	MET	CG-SD-CE	5.31	112.58	100.90
2	E	693	THR	CB-CA-C	-5.30	101.66	110.68
2	J	341	GLU	N-CA-C	-5.30	105.15	111.03
2	J	693	THR	CB-CA-C	-5.30	101.67	110.68
2	B	364	ARG	CB-CG-CD	5.29	123.48	111.30
1	K	286	THR	CA-C-N	5.29	127.37	120.28
1	K	286	THR	C-N-CA	5.29	127.37	120.28
2	I	483	LEU	CA-C-N	5.29	130.40	121.14
2	I	483	LEU	C-N-CA	5.29	130.40	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	85	HIS	O-C-N	-5.29	114.56	122.39
2	H	568	ASP	N-CA-C	5.29	117.84	109.96
1	D	286	THR	CA-C-N	5.28	127.36	120.28
1	D	286	THR	C-N-CA	5.28	127.36	120.28
1	G	266	ARG	N-CA-C	5.28	117.95	111.82
2	J	456	MET	CG-SD-CE	5.28	112.53	100.90
2	J	483	LEU	N-CA-CB	5.28	117.98	110.16
2	E	696	PHE	CA-CB-CG	5.28	119.08	113.80
2	E	341	GLU	N-CA-C	-5.28	105.17	111.03
2	J	675	LYS	N-CA-CB	5.28	117.62	109.91
2	E	483	LEU	N-CA-CB	5.27	117.96	110.16
2	E	675	LYS	N-CA-CB	5.27	117.60	109.91
2	I	364	ARG	CB-CG-CD	5.26	123.40	111.30
1	G	85	HIS	O-C-N	-5.26	114.61	122.39
2	E	335	GLN	CA-C-N	5.26	127.32	120.28
2	E	335	GLN	C-N-CA	5.26	127.32	120.28
2	J	456	MET	CB-CG-SD	-5.25	96.95	112.70
1	A	266	ARG	N-CA-C	5.25	117.91	111.82
2	B	483	LEU	CA-C-N	5.25	130.32	121.14
2	B	483	LEU	C-N-CA	5.25	130.32	121.14
1	K	84	LEU	O-C-N	-5.25	116.67	122.07
2	L	553	TYR	CB-CG-CD1	5.25	128.67	120.80
1	D	734	ALA	CA-C-N	5.24	127.31	120.28
1	D	734	ALA	C-N-CA	5.24	127.31	120.28
2	E	456	MET	CB-CG-SD	-5.24	96.97	112.70
2	F	553	TYR	CB-CG-CD1	5.24	128.67	120.80
1	A	242	ILE	CA-C-N	5.24	127.25	120.44
1	A	242	ILE	C-N-CA	5.24	127.25	120.44
2	I	361	ARG	CA-C-N	-5.24	114.49	120.88
2	I	361	ARG	C-N-CA	-5.24	114.49	120.88
2	B	704	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	G	242	ILE	CA-C-N	5.23	127.24	120.44
1	G	242	ILE	C-N-CA	5.23	127.24	120.44
2	I	449	TYR	O-C-N	5.22	125.86	121.31
2	J	696	PHE	CA-CB-CG	5.22	119.02	113.80
2	B	361	ARG	CA-C-N	-5.22	114.51	120.88
2	B	361	ARG	C-N-CA	-5.22	114.51	120.88
2	F	522	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	D	84	LEU	O-C-N	-5.22	116.69	122.07
2	L	522	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	K	734	ALA	CA-C-N	5.21	127.26	120.28
1	K	734	ALA	C-N-CA	5.21	127.26	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	575	VAL	N-CA-CB	5.21	119.82	111.23
2	B	467	ARG	N-CA-C	5.20	119.47	113.18
2	I	467	ARG	N-CA-C	5.20	119.47	113.18
2	F	575	VAL	N-CA-CB	5.20	119.81	111.23
2	B	365	ILE	N-CA-CB	5.20	119.80	111.23
2	I	417	VAL	CA-C-N	5.19	127.24	120.28
2	I	417	VAL	C-N-CA	5.19	127.24	120.28
2	I	420	ILE	CA-CB-CG2	5.19	119.33	110.50
2	B	449	TYR	O-C-N	5.19	125.83	121.31
1	D	267	HIS	CG-CD2-NE2	5.19	112.39	107.20
2	I	696	PHE	CA-C-N	5.19	127.85	120.53
2	I	696	PHE	C-N-CA	5.19	127.85	120.53
1	G	87	LYS	O-C-N	5.19	129.49	122.59
2	B	435	LEU	CA-C-N	5.18	127.56	120.46
2	B	435	LEU	C-N-CA	5.18	127.56	120.46
2	J	699	SER	CA-CB-OG	5.18	121.47	111.10
2	I	365	ILE	N-CA-CB	5.18	119.78	111.23
2	J	420	ILE	CA-CB-CG2	5.18	119.31	110.50
2	J	438	THR	N-CA-C	5.18	116.92	111.28
2	E	699	SER	CA-CB-OG	5.17	121.44	111.10
1	A	87	LYS	O-C-N	5.17	129.46	122.59
2	C	592	GLU	OE1-CD-OE2	5.17	135.30	122.90
2	E	420	ILE	CA-CB-CG2	5.16	119.28	110.50
1	D	92	THR	N-CA-C	-5.16	107.65	114.31
2	J	696	PHE	CA-C-N	5.16	127.81	120.53
2	J	696	PHE	C-N-CA	5.16	127.81	120.53
2	B	696	PHE	CA-C-N	5.16	127.81	120.53
2	B	696	PHE	C-N-CA	5.16	127.81	120.53
2	E	438	THR	N-CA-C	5.16	116.90	111.28
2	H	592	GLU	OE1-CD-OE2	5.16	135.29	122.90
1	A	102	GLU	CA-C-N	5.16	127.19	120.28
1	A	102	GLU	C-N-CA	5.16	127.19	120.28
1	G	92	THR	N-CA-C	-5.16	107.02	113.72
2	J	492	ASP	CA-C-N	5.16	132.43	122.07
2	J	492	ASP	C-N-CA	5.16	132.43	122.07
2	B	420	ILE	CA-CB-CG2	5.15	119.26	110.50
1	G	102	GLU	CA-C-N	5.15	127.18	120.28
1	G	102	GLU	C-N-CA	5.15	127.18	120.28
1	K	267	HIS	CG-CD2-NE2	5.15	112.35	107.20
2	I	435	LEU	CA-C-N	5.15	127.51	120.46
2	I	435	LEU	C-N-CA	5.15	127.51	120.46
1	A	92	THR	N-CA-C	-5.15	107.03	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	690	ILE	N-CA-CB	5.14	119.71	111.23
2	E	696	PHE	CA-C-N	5.14	127.78	120.53
2	E	696	PHE	C-N-CA	5.14	127.78	120.53
1	K	92	THR	N-CA-C	-5.14	107.68	114.31
1	K	221	GLU	O-C-N	-5.14	115.11	122.41
2	E	492	ASP	CA-C-N	5.14	132.40	122.07
2	E	492	ASP	C-N-CA	5.14	132.40	122.07
2	H	610	GLN	CA-C-N	5.13	127.41	120.38
2	H	610	GLN	C-N-CA	5.13	127.41	120.38
2	B	417	VAL	CA-C-N	5.13	127.15	120.28
2	B	417	VAL	C-N-CA	5.13	127.15	120.28
2	I	704	ASN	OD1-CG-ND2	-5.13	117.47	122.60
2	B	464	ILE	CA-C-N	5.12	127.46	120.54
2	B	464	ILE	C-N-CA	5.12	127.46	120.54
2	I	690	ILE	N-CA-CB	5.12	119.69	111.23
2	B	673	VAL	CA-C-N	5.12	127.10	120.44
2	B	673	VAL	C-N-CA	5.12	127.10	120.44
1	D	221	GLU	O-C-N	-5.12	115.14	122.41
2	J	694	LYS	CA-C-N	5.11	129.32	121.19
2	J	694	LYS	C-N-CA	5.11	129.32	121.19
2	H	575	VAL	CA-C-O	-5.11	114.00	120.89
2	I	464	ILE	CA-C-N	5.11	127.44	120.54
2	I	464	ILE	C-N-CA	5.11	127.44	120.54
2	C	610	GLN	CA-C-N	5.11	127.38	120.38
2	C	610	GLN	C-N-CA	5.11	127.38	120.38
2	J	669	TYR	O-C-N	-5.10	116.71	122.12
2	H	550	LEU	N-CA-CB	5.10	119.11	110.69
2	B	373	GLU	CA-C-O	5.10	126.98	121.02
2	E	694	LYS	CA-C-N	5.09	129.29	121.19
2	E	694	LYS	C-N-CA	5.09	129.29	121.19
2	I	673	VAL	CA-C-N	5.09	127.06	120.44
2	I	673	VAL	C-N-CA	5.09	127.06	120.44
1	G	194	ASP	CA-C-N	5.09	125.37	119.47
1	G	194	ASP	C-N-CA	5.09	125.37	119.47
2	I	373	GLU	CA-C-O	5.09	126.97	121.02
2	C	575	VAL	CA-C-O	-5.08	114.03	120.89
2	F	586	PHE	O-C-N	-5.08	117.25	123.10
1	D	316	ASN	N-CA-CB	5.08	119.15	110.51
2	F	553	TYR	CA-C-O	-5.08	115.28	121.78
1	A	21	SER	CA-C-N	5.08	127.08	120.28
1	A	21	SER	C-N-CA	5.08	127.08	120.28
2	C	578	GLY	O-C-N	-5.08	119.78	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	456	MET	CB-CA-C	-5.08	102.31	110.74
2	C	550	LEU	N-CA-CB	5.08	119.07	110.69
2	F	574	ASP	O-C-N	5.07	129.38	122.48
2	E	456	MET	CB-CA-C	-5.07	102.32	110.74
2	F	553	TYR	CB-CG-CD2	-5.07	113.19	120.80
1	K	316	ASN	N-CA-CB	5.07	119.13	110.51
2	L	553	TYR	CA-C-O	-5.07	115.29	121.78
2	B	413	VAL	N-CA-C	5.07	117.38	111.05
1	A	194	ASP	CA-C-N	5.07	125.35	119.47
1	A	194	ASP	C-N-CA	5.07	125.35	119.47
1	G	21	SER	CA-C-N	5.06	127.06	120.28
1	G	21	SER	C-N-CA	5.06	127.06	120.28
2	L	553	TYR	CB-CG-CD2	-5.06	113.21	120.80
2	E	490	HIS	ND1-CE1-NE2	-5.06	103.34	108.40
1	A	41	SER	CA-CB-OG	5.06	121.22	111.10
2	E	669	TYR	O-C-N	-5.06	116.76	122.12
1	G	41	SER	CA-CB-OG	5.06	121.22	111.10
1	A	124	VAL	CA-C-N	5.06	129.57	122.09
1	A	124	VAL	C-N-CA	5.06	129.57	122.09
2	I	413	VAL	N-CA-C	5.05	117.37	111.05
2	E	449	TYR	CG-CD2-CE2	-5.05	113.62	121.20
2	J	704	ASN	N-CA-C	5.05	117.17	111.11
2	L	533	ILE	CA-C-N	5.05	131.19	121.54
2	L	533	ILE	C-N-CA	5.05	131.19	121.54
2	F	533	ILE	CA-C-N	5.05	131.19	121.54
2	F	533	ILE	C-N-CA	5.05	131.19	121.54
1	G	124	VAL	CA-C-N	5.05	129.56	122.09
1	G	124	VAL	C-N-CA	5.05	129.56	122.09
1	D	247	ASP	N-CA-C	5.05	117.19	110.53
2	B	339	ASP	CA-C-N	5.04	129.21	120.58
2	B	339	ASP	C-N-CA	5.04	129.21	120.58
1	G	87	LYS	CB-CG-CD	5.04	122.90	111.30
2	J	449	TYR	CG-CD2-CE2	-5.04	113.63	121.20
2	I	371	PRO	CA-C-N	5.04	127.35	120.54
2	I	371	PRO	C-N-CA	5.04	127.35	120.54
1	K	311	VAL	CA-C-N	5.04	127.34	120.54
1	K	311	VAL	C-N-CA	5.04	127.34	120.54
1	K	303	GLN	CA-C-N	5.04	127.30	120.65
1	K	303	GLN	C-N-CA	5.04	127.30	120.65
2	J	332	MET	N-CA-CB	5.04	117.52	110.12
1	A	282	ASN	O-C-N	-5.03	116.78	122.12
1	D	303	GLN	CA-C-N	5.03	127.30	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	303	GLN	C-N-CA	5.03	127.30	120.65
2	E	332	MET	N-CA-CB	5.03	117.52	110.12
2	E	704	ASN	N-CA-C	5.03	117.15	111.11
2	L	586	PHE	O-C-N	-5.03	117.32	123.10
1	D	221	GLU	CA-C-N	5.03	129.28	122.19
1	D	221	GLU	C-N-CA	5.03	129.28	122.19
2	J	490	HIS	ND1-CE1-NE2	-5.03	103.37	108.40
1	A	87	LYS	CB-CG-CD	5.03	122.86	111.30
2	H	578	GLY	O-C-N	-5.03	119.81	123.08
1	K	221	GLU	CA-C-N	5.03	129.28	122.19
1	K	221	GLU	C-N-CA	5.03	129.28	122.19
1	D	311	VAL	CA-C-N	5.02	127.32	120.54
1	D	311	VAL	C-N-CA	5.02	127.32	120.54
2	I	339	ASP	CA-C-N	5.02	129.17	120.58
2	I	339	ASP	C-N-CA	5.02	129.17	120.58
2	L	574	ASP	O-C-N	5.02	129.31	122.48
1	G	282	ASN	O-C-N	-5.02	116.80	122.12
2	I	344	ILE	CB-CA-C	-5.02	105.54	111.97
2	F	556	ASP	CA-C-N	5.02	130.49	121.66
2	F	556	ASP	C-N-CA	5.02	130.49	121.66
1	K	247	ASP	N-CA-C	5.01	117.15	110.53
2	L	556	ASP	CA-C-N	5.01	130.48	121.66
2	L	556	ASP	C-N-CA	5.01	130.48	121.66
2	C	575	VAL	N-CA-C	5.01	114.49	107.37
2	H	575	VAL	N-CA-C	5.01	114.48	107.37
2	B	371	PRO	CA-C-N	5.01	127.30	120.54
2	B	371	PRO	C-N-CA	5.01	127.30	120.54
1	D	304	LEU	CA-C-N	5.01	127.30	120.54
1	D	304	LEU	C-N-CA	5.01	127.30	120.54
1	K	304	LEU	CA-C-N	5.00	127.30	120.54
1	K	304	LEU	C-N-CA	5.00	127.30	120.54
2	I	339	ASP	O-C-N	-5.00	116.11	122.27

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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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
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	Mainchain,Sidechain
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	Peptide,Mainchain
2	B	490	HIS	Mainchain
2	B	654	GLN	Mainchain
2	B	686	MET	Mainchain

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Mol	Chain	Res	Type	Group
2	B	698	PHE	Sidechain
2	B	706	TYR	Sidechain
2	C	522	ARG	Mainchain,Sidechain
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
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	Peptide,Mainchain
1	D	317	PHE	Mainchain,Sidechain
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	Mainchain,Sidechain
2	E	341	GLU	Mainchain,Sidechain
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	Peptide,Mainchain,Sidechain
2	E	451	ARG	Mainchain

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Mol	Chain	Res	Type	Group
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
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	Mainchain,Sidechain
2	F	558	GLU	Sidechain
2	F	563	TYR	Mainchain,Sidechain
2	F	569	ASN	Mainchain,Sidechain
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

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Mol	Chain	Res	Type	Group
2	H	522	ARG	Mainchain,Sidechain
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
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	Mainchain,Sidechain
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	Peptide,Mainchain
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	Mainchain,Sidechain
2	J	341	GLU	Mainchain,Sidechain

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Mol	Chain	Res	Type	Group
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
2	J	449	TYR	Peptide,Mainchain,Sidechain
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	Peptide,Mainchain
1	K	317	PHE	Mainchain,Sidechain
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

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Mol	Chain	Res	Type	Group
2	L	522	ARG	Sidechain
2	L	532	GLY	Mainchain
2	L	553	TYR	Mainchain,Sidechain
2	L	558	GLU	Sidechain
2	L	563	TYR	Mainchain,Sidechain
2	L	569	ASN	Mainchain,Sidechain
2	L	576	GLU	Mainchain
2	L	579	PHE	Sidechain
2	L	581	SER	Mainchain
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	76	0
1	D	2643	0	2693	118	0
1	G	2567	0	2629	77	0
1	K	2643	0	2693	130	0
2	B	1697	0	1753	131	0
2	C	946	0	938	23	0
2	E	1697	0	1751	175	0
2	F	946	0	939	30	0
2	H	946	0	938	24	0
2	I	1697	0	1752	167	0
2	J	1697	0	1751	201	0
2	L	946	0	939	29	0
All	All	20992	0	21405	1013	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 24.

All (1013) 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	1.09
2:J:448:GLN:HE22	1:K:315:LYS:C	1.60	1.09
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:317:PHE:CZ	2:E:332:MET:C	2.32	1.01
2:I:341:GLU:CD	2:J:341:GLU:OE2	2.04	1.00
1:D:318:ARG:NE	2:E:449:TYR:CB	2.23	0.99
2:J:448:GLN:NE2	1:K:315:LYS:C	2.21	0.99
2:E:465:ARG:HH12	1:K:198:GLN:NE2	1.58	0.99
2:J:332:MET:C	1:K:317:PHE:CZ	2.32	0.99
2:J:449:TYR:CB	1:K:318:ARG:NE	2.23	0.98
1:D:315:LYS:C	2:E:448:GLN:NE2	2.21	0.98
2:J:332:MET:O	1:K:317:PHE:HZ	1.38	0.97
2:E:393:LYS:HE3	2:J:361:ARG:HD2	1.47	0.96
2:I:341:GLU:HG2	2:J:341:GLU:OE2	1.65	0.96
1:D:317:PHE:HZ	2:E:332:MET:O	1.38	0.96
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:H	2:I:702:LEU:HD23	1.34	0.91
1:A:12:LEU:HB3	1:A:745:ILE:HG12	1.52	0.91
1:D:316:ASN:N	2:E:448:GLN:NE2	2.19	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:E:465:ARG:NH1	1:K:198:GLN:NE2	2.18	0.90
2:J:448:GLN:NE2	1:K:316:ASN:N	2.19	0.90
1:A:207:LEU:HB2	1:A:235:VAL:HG22	1.52	0.89
1:K:137:LEU:HB3	1:K:160:LEU:HD22	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:331:GLN:CD	1:K:316:ASN:HD21	1.80	0.88
2:B:653:PRO:CD	2:I:345:GLU:O	2.21	0.88
1:D:316:ASN:HD21	2:E:331:GLN:CD	1.80	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
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
1:A:31:LEU:HG	1:A:285:LEU:HD22	1.58	0.85
2:E:459:ILE:HD12	2:E:705: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:F:523:LYS:HE2	2:F:544:VAL:HG13	1.58	0.85
2:I:392:ILE:HD13	2:I:662:ILE:HG13	1.57	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
1:D:16:LEU:HD23	1:D:29:LEU:HD11	1.58	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:HD23	2:E:702:LEU:N	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:12:LEU:HD23	1:D:745:ILE:HG12	1.64	0.79
1:D:36:VAL:HG22	1:D:48:LEU:HD22	1.64	0.79
1:D:318:ARG:O	2:E:444:LYS:HB3	1.82	0.79
2:B:661:THR:HG23	2:J:675:LYS:HE2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:36:VAL:HG22	1:K:48:LEU:HD22	1.64	0.79
2:I:341:GLU:CD	2:J:341:GLU:CD	2.50	0.79
2:E:675:LYS:HE2	2:I:661:THR:HG23	1.63	0.79
1:D:40:GLN:HB2	1:D:141:THR:HG22	1.62	0.78
1:K:12:LEU:HD23	1:K:745:ILE:HG12	1.64	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
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:E:384:LEU:HB3	2:E:666:VAL:HG13	1.65	0.78
2:I:702:LEU:HD23	2:I:702:LEU:N	2.00	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
1:A:206:LYS:HE2	1:A:238:SER:HA	1.66	0.77
2:J:449:TYR:HB3	1:K:318:ARG:HE	1.47	0.77
1:G:206:LYS:HE2	1:G:238:SER:HA	1.66	0.77
2:I:422:GLU:HB3	2:I:423:PRO:HD3	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:HD23	2:B:702:LEU:N	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
1:A:59:ARG:HB3	1:A:242:ILE:HG23	1.67	0.76
2:I:463:HIS:CE1	2:J:334:GLN:NE2	2.54	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:A:191:LYS:HA	1:A:195:PRO:HA	1.69	0.75
1:G:27:ALA:HB1	1:G:296:LEU:HD12	1.68	0.75
2:E:661:THR:HG22	2:E:665:LEU:HD21	1.69	0.75
1:D:181:LEU:HD23	1:D:219:VAL:HG21	1.67	0.75
1:G:191:LYS:HA	1:G:195:PRO:HA	1.69	0.75
2:J:661:THR:HG22	2:J:665:LEU:HD21	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:454:GLU:CD	1:K:271:ARG:NH1	2.45	0.74
2:E:465:ARG:NH2	1:K:198:GLN:NE2	2.35	0.74
2:J:449:TYR:HB2	1:K:318:ARG:HE	1.43	0.74
2:I:695:GLU:HG3	2:J:337:ALA:C	2.13	0.74
2:L:531:ILE:HD12	2:L:535:LYS:HD3	1.68	0.74
2:E:422:GLU:HB3	2:E:423:PRO:HD3	1.69	0.73
2:I:459:ILE:HD12	2:I:705:LEU:HD13	1.70	0.73
1:A:27:ALA:HB1	1:A:296:LEU:HD12	1.68	0.73
2:F:531:ILE:HD12	2:F:535:LYS:HD3	1.68	0.73
1:D:316:ASN:ND2	2:E:331:GLN:CD	2.47	0.73
2:I:696:PHE:HA	2:I:700:GLU:HG3	1.70	0.73
2:J:331:GLN:CD	1:K:316:ASN:ND2	2.47	0.73
2:B:459:ILE:HD12	2:B:705:LEU:HD13	1.70	0.72
2:B:688:LEU:HD23	2:B:688:LEU:N	2.03	0.72
2:B:696:PHE:HA	2:B:700:GLU:HG3	1.70	0.72
2:E:490:HIS:CG	2:E:491:GLU:H	2.07	0.72
1:A:48:LEU:HG	1:A:134:LEU:HD23	1.72	0.72
2:I:463:HIS:HE1	2:J:334:GLN:NE2	1.87	0.72
2:J:453:ARG:H	1:K:318:ARG:CD	1.98	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:I:694:LYS:NZ	2:J:341:GLU:OE2	2.23	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:B:380:ASP:HA	2:B:670:MET:HB3	1.72	0.71
2:I:707:SER:HA	2:J:702:LEU:HB2	1.72	0.71
1:G:48:LEU:HG	1:G:134:LEU:HD23	1.72	0.71
2:I:688:LEU:N	2:I:688:LEU:HD23	2.03	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
1:G:140:MET:HE2	1:G:160:LEU:HD21	1.73	0.70
2:J:702:LEU:HD23	2:J:702:LEU:H	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
2:C:518:ILE:HG13	2:C:519:LEU:H	1.56	0.70
1:D:318:ARG:CD	2:E:449:TYR:HB2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:LEU:HD22	1:G:136:ASP:HB2	1.73	0.70
1:A:29:LEU:HD23	1:A:289:ILE:HG12	1.74	0.70
2:B:442:CYS:HB3	2:B:445:LYS:HZ2	1.57	0.70
2:I:442:CYS:HB3	2:I:445:LYS:HZ2	1.57	0.70
2:I:687:HIS:CD2	2:I:688:LEU:HD21	2.27	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: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:B:687:HIS:CD2	2:B:688:LEU:HD21	2.27	0.69
2:J:449:TYR:HB2	1:K:318:ARG:CD	2.21	0.69
1:A:140:MET:HE2	1:A:160:LEU:HD21	1.73	0.69
1:D:316:ASN:HB3	2:E:332:MET:HG2	1.73	0.69
2:I:439:VAL:HG12	2:I:697:ILE:HB	1.74	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
1:G:12:LEU:HD13	1:G:745:ILE:HA	1.75	0.69
2:J:332:MET:HG2	1:K:316:ASN:HB3	1.73	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:HD23	2:E:702:LEU:H	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:G:29:LEU:HD23	1:G:289:ILE:HG12	1.74	0.68
2:J:384:LEU:HD11	2:J:412:ILE:HG23	1.74	0.68
2:J:392:ILE:HA	2:J:408:ALA:HB2	1.75	0.68
2:J:448:GLN:HE22	1:K:315:LYS:CA	2.07	0.68
2:E:417:VAL:HB	2:E:479:ILE:HG23	1.74	0.68
2:I:334:GLN:OE1	2:J:695:GLU:HG3	1.94	0.68
2:I:388:ILE:HG21	2:I:666:VAL:HG21	1.76	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:E:692:ASN:C	2:E:692:ASN:HD22	2.00	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:J:692:ASN:C	2:J:692:ASN:HD22	2.00	0.67
2:B:333:VAL:HG12	2:B:333:VAL:O	1.93	0.67
2:B:692:ASN:C	2:B:692:ASN:HD22	2.02	0.67
1:D:207:LEU:HD22	1:D:220:LEU:HD11	1.77	0.67
2:E:392:ILE:HA	2:E:408:ALA:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:694:LYS:HE2	2:J:341:GLU:HG3	1.76	0.67
1:K:13:VAL:HG11	1:K:31:LEU:HD21	1.75	0.67
1:K:207:LEU:HD22	1:K:220:LEU:HD11	1.77	0.67
2:B:388:ILE:HG12	2:B:666:VAL:HG11	1.77	0.67
2:E:465:ARG:CZ	1:K:198:GLN:NE2	2.58	0.67
2:F:518:ILE:HG13	2:F:519:LEU:H	1.60	0.67
2:F:552:TRP:HH2	2:F:565:LEU:HD13	1.59	0.67
1:D:318:ARG:H	2:E:453:ARG:HB3	1.59	0.67
2:I:692:ASN:C	2:I:692:ASN:HD22	2.02	0.67
2:I:388:ILE:HG12	2:I:666:VAL:HG11	1.77	0.67
1:K:40:GLN:HG3	1:K:63:ILE:HB	1.76	0.67
1:D:40:GLN:HG3	1:D:63:ILE:HB	1.76	0.67
2:J:453:ARG:HB3	1:K:318:ARG:H	1.59	0.67
2:J:688:LEU:N	2:J:688:LEU:HD23	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:333:VAL:HG12	2:I:333:VAL:O	1.93	0.67
2:I:703:ALA:HA	2:J:699:SER:HA	1.75	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:I:452:LEU:HD13	2:I:452:LEU:C	2.19	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:452:LEU:HD13	2:B:452:LEU:C	2.19	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
1:D:67:ARG:HH21	1:D:120:ILE:HG12	1.61	0.66
2:J:414:LYS:HG2	2:J:483:LEU:HB3	1.78	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:E:681:MET:HB2	2:E:682:PRO:HD3	1.77	0.65
2:J:681:MET:HB2	2:J:682:PRO:HD3	1.78	0.65
2:B:665:LEU:HD21	2:J:675:LYS:HD3	1.79	0.65
2:B:388:ILE:HG12	2:B:666:VAL:HG21	1.78	0.65
1:K:13:VAL:HG13	1:K:29:LEU:HD13	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:217:ARG:HG3	1:A:265:TYR:HE1	1.62	0.64
2:B:384:LEU:HD22	2:B:670:MET:HG2	1.79	0.64
1:G:56:PHE:HB3	1:G:94:PHE:HB3	1.78	0.64
1:D:171:ILE:HD12	1:D:193:VAL:HG21	1.80	0.64
1:G:217:ARG:HG3	1:G:265:TYR:HE1	1.62	0.64
2:I:384:LEU:HD22	2:I:670:MET:HG2	1.79	0.64
1:A:56:PHE:HB3	1:A:94:PHE:HB3	1.78	0.64
1:K:40:GLN:HE22	1:K:145:VAL:HG11	1.63	0.64
2:I:687:HIS:HE1	2:J:342:LYS:HD3	1.63	0.64
2:B:329:LEU:HG	2:B:702:LEU:HA	1.79	0.63
2:I:695:GLU:HG3	2:J:337:ALA:O	1.96	0.63
1:K:171:ILE:HD12	1:K:193:VAL:HG21	1.80	0.63
1:D:40:GLN:HE22	1:D:145:VAL:HG11	1.63	0.63
2:I:329:LEU:HG	2:I:702:LEU:HA	1.79	0.63
2:C:607:CYS:HB3	2:C:612:GLU:HB3	1.81	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
2:E:690:ILE:HG22	2:E:691:ASN:N	2.12	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
1:K:87:LYS:HB2	1:K:87:LYS:HZ2	1.65	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:D:87:LYS:HZ3	1:D:87:LYS:HB2	1.64	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:D:208:ASP:HB3	1:D:258:PHE:HB2	1.82	0.61
1:K:208:ASP:HB3	1:K:258:PHE:HB2	1.83	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:570:LEU:HD13	2:L:588:LEU:HD13	1.82	0.61
2:L:573:ARG:HB2	2:L:630:VAL:HA	1.80	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
1:G:23:ILE:HG22	1:G:25:GLN:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:385:ARG:HH12	2:J:663:ARG:HA	1.66	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:A:209:LEU:HD11	1:A:238:SER:HB3	1.83	0.61
1:D:135:VAL:HG12	1:D:137:LEU:HG	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
2:I:702:LEU:H	2:I:702:LEU:CD2	2.09	0.60
2:E:494:ILE:HG13	2:I:675:LYS:HE2	1.84	0.60
2:F:570:LEU:HD13	2:F:588:LEU:HD13	1.82	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: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
1:A:232:ILE:HG21	1:A:277:LEU:HA	1.82	0.60
2:I:698:PHE:CZ	2:J:691:ASN:ND2	2.70	0.60
2:L:518:ILE:HG13	2:L:519:LEU:N	2.16	0.60
2:E:491:GLU:OE2	2:E:492:ASP:HA	2.02	0.59
2:J:452:LEU:HD13	2:J:452:LEU:C	2.27	0.59
2:B:489:ASN:N	2:B:489:ASN:OD1	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
1:D:201:ILE:HD12	1:D:277:LEU:HD12	1.83	0.59
2:I:694:LYS:HE2	2:J:341:GLU:CG	2.32	0.59
1:A:94:PHE:HZ	1:A:124:VAL:HG11	1.68	0.59
2:E:452:LEU:HD13	2:E:452:LEU:C	2.27	0.59
2:B:374:LEU:HD13	2:B:423:PRO:HB2	1.84	0.59
2:E:379:PHE:HE1	2:E:419:LYS:HB2	1.68	0.59
1:G:94:PHE:HZ	1:G:124:VAL:HG11	1.68	0.59
2:I:374:LEU:HD13	2:I:423:PRO:HB2	1.84	0.59
2:J:491:GLU:OE2	2:J:492:ASP:HA	2.02	0.59
2:I:698:PHE:CE1	2:J:691:ASN:CG	2.81	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
2:F:579:PHE:N	2:F:579:PHE:HD1	2.01	0.59
1:G:70:VAL:HG23	1:G:119:PRO:HB3	1.85	0.59
2:J:379:PHE:HE1	2:J:419:LYS:HB2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:10:ILE:HB	1:K:11:PRO:HD3	1.85	0.59
1:A:70:VAL:HG23	1:A:119:PRO:HB3	1.85	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
2:B:690:ILE:HG22	2:B:691:ASN:N	2.17	0.58
1:D:319:PRO:O	2:E:444:LYS:NZ	2.30	0.58
2:B:392:ILE:HG13	2:B:393:LYS:HG2	1.85	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
2:I:489:ASN:OD1	2:I:489:ASN:N	2.35	0.58
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
1:D:42:ALA:HB1	1:D:174:VAL:HG12	1.84	0.58
2:I:681:MET:HB2	2:I:682:PRO:HD3	1.86	0.58
2:C:579:PHE:CD1	2:C:579:PHE:N	2.70	0.58
1:D:229:ARG:HG3	1:D:280:VAL:HG11	1.85	0.58
2:I:690:ILE:HG22	2:I:691:ASN:N	2.17	0.58
2:J:702:LEU:N	2:J:702:LEU:CD2	2.67	0.58
2:F:579:PHE:N	2:F:579:PHE:CD1	2.72	0.58
2:I:338:VAL:HG11	2:J:687:HIS:ND1	2.18	0.58
2:H:579:PHE:N	2:H:579:PHE:CD1	2.70	0.58
2:F:531:ILE:HG23	2:F:535:LYS:HD3	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:N	2:L:579:PHE:CD1	2.71	0.57
2:I:698:PHE:HE1	2:J:691:ASN:CG	2.12	0.57
2:I:341:GLU:OE2	2:J:341:GLU:OE2	2.22	0.57
2:J:332:MET:SD	1:K:317:PHE:CD1	2.97	0.57
2:J:489:ASN:N	2:J:489:ASN:OD1	2.35	0.57
2:L:531:ILE:HG23	2:L:535:LYS:HD3	1.86	0.57
2:C:579:PHE:N	2:C:579:PHE:HD1	2.03	0.57
2:E:428:VAL:HG11	2:E:472:LYS:HG3	1.86	0.57
1:G:13:VAL:HG11	1:G:289:ILE:HD13	1.87	0.57
2:H:579:PHE:N	2:H:579:PHE:HD1	2.03	0.57
1:A:13:VAL:HG11	1:A:289:ILE:HD13	1.87	0.57
2:E:432:ILE:HG12	2:E:689:MET:HE1	1.86	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:I:687:HIS:CE1	2:J:342:LYS:HD3	2.40	0.57
2:J:432:ILE:HG12	2:J:689:MET:HE1	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:444:LYS:O	1:K:318:ARG:N	2.15	0.57
2:J:444:LYS:NZ	1:K:319:PRO:O	2.30	0.57
2:B:681:MET:HB2	2:B:682:PRO:HD3	1.86	0.56
2:B:702:LEU:N	2:B:702:LEU:CD2	2.65	0.56
2:C:565:LEU:HD11	2:C:570:LEU:HD21	1.85	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:J:428:VAL:HG11	2:J:472:LYS:HG3	1.86	0.56
2:L:577:LYS:HE3	2:L:577:LYS:H	1.70	0.56
1:A:69:LEU:HD13	1:A:101:ILE:HG12	1.86	0.56
2:B:481:ILE:HG22	2:B:482:GLU:OE1	2.05	0.56
2:E:489:ASN:N	2:E:489:ASN:OD1	2.35	0.56
2:J:391:ALA:HB1	2:J:408:ALA:HA	1.87	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:B:687:HIS:CG	2:B:688:LEU:HD23	2.41	0.56
1:D:83:PHE:HZ	1:D:97:VAL:HG13	1.70	0.56
2:E:344:ILE:HD13	2:E:690:ILE:HG13	1.88	0.56
2:E:465:ARG:NH2	1:K:228:ARG:HH21	2.04	0.56
2:E:687:HIS:CG	2:E:688:LEU:HD23	2.41	0.56
2:F:521:ILE:HD13	2:F:622:ARG:HB3	1.87	0.56
2:F:577:LYS:HE3	2:F:577:LYS:H	1.71	0.56
2:I:379:PHE:HE2	2:I:419:LYS:HD3	1.71	0.56
2:J:478:LEU:HD12	2:J:680:LEU:HD23	1.88	0.56
2:L:521:ILE:HD13	2:L:622:ARG:HB3	1.87	0.56
2:E:346:GLY:HA3	2:E:360:ALA:HB1	1.87	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: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:B:495:GLY:O	2:B:496:PHE:HB2	2.05	0.56
2:E:392:ILE:HG13	2:E:393:LYS:HG2	1.87	0.56
2:I:702:LEU:N	2:I:702:LEU:CD2	2.65	0.56
2:I:694:LYS:HE2	2:J:341:GLU:CD	2.31	0.56
2:J:384:LEU:HD13	2:J:670:MET:HE3	1.87	0.56
2:H:535:LYS:O	2:H:535:LYS:HG3	2.06	0.55
2:B:379:PHE:HE2	2:B:419:LYS:HD3	1.71	0.55
2:E:702:LEU:N	2:E:702:LEU:CD2	2.67	0.55
2:I:495:GLY:O	2:I:496:PHE:HB2	2.05	0.55
1:D:170:LEU:HD21	1:D:281:LEU:HD22	1.89	0.55
2:E:458:ARG:HG3	1:K:229:ARG:HH22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:235:VAL:HB	1:G:255:GLU:HB2	1.87	0.55
2:I:334:GLN:CD	2:J:695:GLU:HG3	2.31	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:E:384:LEU:HD13	2:E:670:MET:HE3	1.87	0.55
2:B:688:LEU:O	2:B:689:MET:C	2.48	0.55
2:I:698:PHE:HZ	2:J:691:ASN:ND2	2.03	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
1:K:140:MET:HE2	1:K:157:ARG:HA	1.89	0.54
1:A:271:ARG:O	1:A:272:MET:HE2	2.08	0.54
2:B:329:LEU:HD21	2:B:705:LEU:HG	1.89	0.54
2:C:535:LYS:O	2:C:535:LYS:HG3	2.06	0.54
2:E:662:ILE:HD13	2:E:665:LEU:HD12	1.90	0.54
2:E:688:LEU:O	2:E:689:MET:C	2.46	0.54
2:I:329:LEU:HD21	2:I:705:LEU:HG	1.90	0.54
1:D:140:MET:HE2	1:D:157:ARG:HA	1.89	0.54
2:J:662:ILE:HD13	2:J:665:LEU:HD12	1.90	0.54
2:J:444:LYS:HE3	1:K:319:PRO:C	2.33	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:I:369:ARG:HH12	2:I:430:MET:HE1	1.73	0.54
2:J:449:TYR:HD1	1:K:317:PHE:O	1.89	0.54
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.71	0.54
1:D:17:GLN:HG3	1:D:29:LEU:HD12	1.90	0.54
1:D:316:ASN:N	2:E:448:GLN:HE21	2.02	0.54
2:E:495:GLY:O	2:E:496:PHE:HB2	2.08	0.54
1:K:17:GLN:HG3	1:K:29:LEU:HD12	1.90	0.54
2:B:494:ILE:HG23	2:J:675:LYS:HD2	1.90	0.54
1:D:319:PRO:C	2:E:444:LYS:HE3	2.33	0.54
2:E:675:LYS:HD2	2:I:494:ILE:HG23	1.90	0.54
1:G:15:ARG:HG3	1:G:15:ARG:HH11	1.71	0.54
1:G:33:GLN:HB2	1:G:133:THR:HB	1.90	0.54
1:A:33:GLN:HB2	1:A:133:THR:HB	1.89	0.53
2:B:379:PHE:CZ	2:B:416:GLN:HG2	2.44	0.53
2:J:362:ILE:CG2	2:J:363:ASN:N	2.71	0.53
2:I:362:ILE:CG2	2:I:363:ASN:N	2.72	0.53
2:B:362:ILE:CG2	2:B:363:ASN:N	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:459:ILE:HG21	2:I:705:LEU:HD22	1.90	0.53
2:I:688:LEU:O	2:I:689:MET:C	2.47	0.53
1:G:271:ARG:O	1:G:272:MET:HE2	2.08	0.53
2:J:345:GLU:OE1	2:J:345:GLU:CA	2.55	0.53
2:J:495:GLY:O	2:J:496:PHE:HB2	2.08	0.53
2:J:688:LEU:O	2:J:689:MET:C	2.46	0.53
2:H:596:VAL:HG11	2:H:603:LEU:HB2	1.89	0.53
1:A:274:THR:HB	1:A:275:PRO:HD3	1.90	0.53
2:B:369:ARG:HH12	2:B:430:MET:HE1	1.73	0.53
2:I:703:ALA:CA	2:J:699:SER:HA	2.39	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:OE1	2:I:345:GLU:CA	2.55	0.53
2:B:361:ARG:O	2:B:362:ILE:C	2.52	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
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
2:I:388:ILE:HG13	2:I:409:PHE:HA	1.90	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:340:PHE:CD2	2:B:694:LYS:HG3	2.45	0.52
2:B:370:PHE:N	2:B:371:PRO:HD2	2.25	0.52
2:B:345:GLU:OE1	2:B:345:GLU:CA	2.55	0.52
2:I:370:PHE:N	2:I:371:PRO:HD2	2.25	0.51
2:J:332:MET:SD	1:K:317:PHE:CA	2.88	0.51
2:E:333:VAL:HG23	2:E:333:VAL:O	2.10	0.51
2:I:340:PHE:CD2	2:I:694:LYS:HG3	2.45	0.51
1:D:316:ASN:CB	2:E:445:LYS:HG3	2.34	0.51
1:A:300:LEU:HB3	1:A:735:LEU:HD22	1.93	0.51
2:C:553:TYR:CG	2:C:558:GLU:HG2	2.45	0.51
2:C:577:LYS:HE3	2:C:577:LYS:H	1.76	0.51
1:G:300:LEU:HB3	1:G:735:LEU:HD22	1.93	0.51
2:J:361:ARG:O	2:J:362:ILE:C	2.51	0.51
2:L:578:GLY:HA3	2:L:585:ILE:HD12	1.90	0.51
1:D:62:GLY:HA3	1:D:113:LYS:HE2	1.93	0.51
2:F:607:CYS:HB3	2:F:612:GLU:HB3	1.91	0.51
2:I:340:PHE:O	2:I:341:GLU:C	2.50	0.51
2:J:333:VAL:HG23	2:J:333:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:672:ILE:HD13	2:J:491:GLU:HA	1.93	0.50
2:B:496:PHE:CE2	2:B:660:GLU:HG2	2.46	0.50
2:I:367:HIS:CG	2:I:682:PRO:HB3	2.47	0.50
2:B:340:PHE:O	2:B:341:GLU:C	2.50	0.50
2:I:698:PHE:HZ	2:J:691:ASN:HD21	1.59	0.50
1:D:140:MET:HE3	1:D:160:LEU:HD12	1.94	0.50
1:D:310:GLU:HA	1:D:313:GLU:HG2	1.94	0.50
1:G:83:PHE:HB2	1:G:86:CYS:HB2	1.94	0.50
2:I:496:PHE:CE2	2:I:660:GLU:HG2	2.46	0.50
1:A:83:PHE:HB2	1:A:86:CYS:HB2	1.94	0.50
2:B:369:ARG:CD	2:B:369:ARG:C	2.84	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
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
2:I:369:ARG:C	2:I:369:ARG:CD	2.84	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:E:345:GLU:OE1	2:E:345:GLU:CA	2.55	0.50
2:I:703:ALA:CB	2:J:699:SER:HA	2.41	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:E:361:ARG:O	2:E:362:ILE:C	2.51	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
2:J:392:ILE:HG22	2:J:408:ALA:HB1	1.93	0.49
1:K:117:PRO:HB3	1:K:159:MET:HE1	1.93	0.49
2:E:370:PHE:N	2:E:371:PRO:HD2	2.26	0.49
2:I:374:LEU:HG	2:I:678:ARG:HB3	1.94	0.49
2:B:367:HIS:CG	2:B:682:PRO:HB3	2.46	0.49
1:D:318:ARG:N	2:E:444:LYS:O	2.15	0.49
2:E:392:ILE:HG22	2:E:408:ALA:HB1	1.93	0.49
2:F:526:LEU:HD13	2:F:605:LEU:HD22	1.94	0.49
2:J:340:PHE:CZ	2:J:439:VAL:HG12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:449:TYR:HB2	2:J:453:ARG:H	1.77	0.49
1:D:307:ILE:HB	1:D:728:MET:HG3	1.95	0.49
2:I:359:GLY:HA2	2:I:362:ILE:HG22	1.93	0.49
2:J:453:ARG:HG3	2:J:454:GLU:N	2.27	0.49
2:L:562:LYS:O	2:L:563:TYR:HB3	2.12	0.49
1:A:217:ARG:HD2	1:A:264:SER:HB3	1.94	0.49
1:D:117:PRO:HB3	1:D:159:MET:HE1	1.94	0.49
2:E:449:TYR:HB2	2:E:453:ARG:H	1.78	0.49
1:K:43:GLY:HA3	1:K:236:ASN:HD22	1.78	0.49
1:K:191:LYS:HZ1	1:K:225:LEU:HG	1.78	0.49
1:K:307:ILE:HB	1:K:728:MET:HG3	1.95	0.49
1:A:33:GLN:CB	1:A:133:THR:HB	2.43	0.49
2:B:336:PHE:CD2	2:B:697:ILE:HD11	2.48	0.49
2:B:494:ILE:HG23	2:J:675:LYS:CD	2.43	0.49
1:D:173:ALA:HB2	1:D:190:ALA:HB2	1.94	0.49
2:E:453:ARG:HG3	2:E:454:GLU:N	2.27	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
2:E:340:PHE:HZ	2:E:439:VAL:HG12	1.78	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:B:362:ILE:HG23	2:B:363:ASN:N	2.28	0.48
2:I:362:ILE:HG23	2:I:363:ASN:N	2.28	0.48
1:A:40:GLN:O	1:A:41:SER:HB3	2.13	0.48
2:I:490:HIS:NE2	2:I:672:ILE:HG21	2.28	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
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
1:D:43:GLY:HA3	1:D:236:ASN:HD22	1.78	0.48
2:J:413:VAL:HG21	2:J:486:MET:H	1.79	0.48
2:J:417:VAL:HB	2:J:479:ILE:CG2	2.43	0.48
1:A:37:VAL:HG22	1:A:171:ILE:HG23	1.94	0.48
1:D:43:GLY:HA3	1:D:236:ASN:ND2	2.29	0.48
1:D:161:MET:HA	1:D:164:VAL:HG22	1.95	0.48
2:E:340:PHE:CZ	2:E:439:VAL:HG12	2.47	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:C:525:TRP:HB3	2:C:540:GLU:HG2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:HD11	1:D:281:LEU:HD22	1.96	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: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
1:A:9:LEU:HG	1:A:286:THR:HG23	1.95	0.48
2:B:378:GLU:HG2	2:B:420:ILE:HD13	1.95	0.48
2:E:675:LYS:CD	2:I:494:ILE:HG23	2.43	0.48
2:F:526:LEU:HD13	2:F:605:LEU:HB3	1.95	0.48
1:G:9:LEU:HG	1:G:286:THR:HG23	1.96	0.48
1:G:83:PHE:CZ	1:G:97:VAL:HG13	2.43	0.48
2:I:378:GLU:HG2	2:I:420:ILE:HD13	1.95	0.48
2:L:526:LEU:HD13	2:L:605:LEU:HB3	1.95	0.48
2:J:435:LEU:HD12	2:J:690:ILE:HD12	1.96	0.48
1:K:83:PHE:CE2	1:K:122:LEU:HD22	2.49	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:B:370:PHE:CE1	2:B:427:CYS:HB2	2.49	0.47
2:E:452:LEU:C	2:E:452:LEU:CD1	2.87	0.47
2:E:485:TYR:CD1	2:I:484:ALA:HB3	2.49	0.47
2:J:340:PHE:HZ	2:J:439:VAL:HG12	1.78	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
2:J:448:GLN:CD	1:K:314:TYR:O	2.57	0.47
2:J:452:LEU:C	2:J:452:LEU:CD1	2.87	0.47
1:K:235:VAL:HG11	1:K:254:ALA:HB3	1.97	0.47
2:I:670:MET:HE2	2:I:670:MET:HA	1.96	0.47
2:J:409:PHE:CE2	2:J:490:HIS:HB3	2.50	0.47
2:J:490:HIS:CG	2:J:491:GLU:N	2.75	0.47
2:J:697:ILE:HD13	2:J:697:ILE:O	2.14	0.47
1:K:59:ARG:HA	1:K:64:VAL:HG13	1.96	0.47
1:D:55:ASP:HB3	1:D:98:ARG:HD3	1.96	0.47
2:E:413:VAL:HG21	2:E:486:MET:H	1.79	0.47
2:I:463:HIS:HE1	2:J:334:GLN:CD	2.20	0.47
2:J:379:PHE:CE1	2:J:419:LYS:HB2	2.49	0.47
1:K:83:PHE:CZ	1:K:97:VAL:HG13	2.50	0.47
2:B:432:ILE:CD1	2:B:472:LYS:HE3	2.45	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
2:E:369:ARG:C	2:E:369:ARG:CD	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:435:LEU:HD12	2:E:690:ILE:HD12	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
1:K:149:PRO:HD2	1:K:152:ILE:HD13	1.96	0.47
2:B:439:VAL:HA	2:B:697:ILE:HG13	1.97	0.47
2:E:697:ILE:HD13	2:E:697:ILE:O	2.14	0.47
2:I:439:VAL:HA	2:I:697:ILE:HG13	1.97	0.47
2:J:331:GLN:NE2	1:K:316:ASN:ND2	2.51	0.47
1:K:55:ASP:HB3	1:K:98:ARG:HD3	1.96	0.47
1:A:173:ALA:HB1	1:A:187:LEU:HD23	1.97	0.47
2:B:678:ARG:HD2	2:J:494:ILE:CD1	2.45	0.47
1:D:191:LYS:HZ1	1:D:225:LEU:HG	1.80	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
2:J:369:ARG:C	2:J:369:ARG:CD	2.87	0.47
2:J:692:ASN:C	2:J:692:ASN:ND2	2.70	0.47
2:B:478:LEU:HD11	2:B:680:LEU:HD23	1.96	0.47
2:E:465:ARG:CZ	1:K:198:GLN:HE21	2.28	0.47
1:G:173:ALA:HB1	1:G:187:LEU:HD23	1.97	0.47
2:I:370:PHE:CE1	2:I:427:CYS:HB2	2.50	0.47
2:I:452:LEU:HD13	2:I:452:LEU:O	2.15	0.47
2:I:688:LEU:N	2:I:688:LEU:CD2	2.74	0.47
2:J:687:HIS:C	2:J:688:LEU:HD23	2.40	0.47
2:B:670:MET:HE2	2:B:670:MET:HA	1.96	0.47
1:D:149:PRO:HD2	1:D:152:ILE:HD13	1.96	0.47
1:D:314:TYR:O	2:E:448:GLN:CD	2.57	0.47
2:E:449:TYR:CD2	2:E:452:LEU:HB3	2.50	0.47
2:E:670:MET:HE2	2:E:670:MET:HA	1.97	0.47
2:E:682:PRO:HB3	2:I:654:GLN:NE2	2.30	0.47
2:F:571:LYS:HB3	2:F:589:PHE:CZ	2.49	0.47
2:I:361:ARG:O	2:I:362:ILE:C	2.52	0.47
2:J:670:MET:HE2	2:J:670:MET:HA	1.97	0.46
2:L:571:LYS:HB3	2:L:589:PHE:CZ	2.49	0.46
2:E:687:HIS:C	2:E:688:LEU:HD23	2.40	0.46
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
1:A:205:THR:HG22	1:A:236:ASN:HD22	1.81	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
2:B:431:VAL:HG21	2:B:685:ILE:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:654:GLN:NE2	2:J:682:PRO:HB3	2.30	0.46
2:E:444:LYS:HD2	2:E:453:ARG:CD	2.45	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: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:325:LYS:HA	2:E:328:ALA:HB3	1.98	0.46
2:J:444:LYS:HD2	2:J:453:ARG:CD	2.45	0.46
2:B:484:ALA:HB3	2:J:485:TYR:HD1	1.80	0.46
1:G:29:LEU:N	1:G:29:LEU:HD12	2.31	0.46
2:J:325:LYS:HA	2:J:328:ALA:HB3	1.98	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
1:D:289:ILE:HG21	1:D:745:ILE:HD13	1.96	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:G:259:PHE:HB3	1:G:272:MET:HB3	1.98	0.46
1:K:61:SER:HA	1:K:242:ILE:CD1	2.46	0.46
2:I:687:HIS:C	2:I:688:LEU:HD23	2.41	0.46
2:J:384:LEU:HB2	2:J:670:MET:HE3	1.97	0.46
2:B:452:LEU:HD13	2:B:452:LEU:O	2.15	0.46
2:I:337:ALA:HB1	2:I:698:PHE:CD1	2.51	0.46
2:J:449:TYR:CD2	2:J:452:LEU:HB3	2.50	0.46
1:A:9:LEU:HD23	1:A:290:ARG:CZ	2.46	0.45
1:A:29:LEU:HD12	1:A:29:LEU:N	2.31	0.45
2:E:485:TYR:HD1	2:I:484:ALA:HB3	1.80	0.45
2:F:579:PHE:HD1	2:F:579:PHE:H	1.62	0.45
2:I:687:HIS:HD2	2:I:688:LEU:HD21	1.77	0.45
1:K:23:ILE:HG22	1:K:25:GLN:HE21	1.82	0.45
1:K:229:ARG:HD2	1:K:280:VAL:HG21	1.99	0.45
1:A:170:LEU:HD22	1:A:201:ILE:CG1	2.46	0.45
1:A:259:PHE:HB3	1:A:272:MET:HB3	1.98	0.45
1:D:229:ARG:HD2	1:D:280:VAL:HG21	1.99	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
2:B:688:LEU:N	2:B:688:LEU:CD2	2.74	0.45
1:D:61:SER:HA	1:D:242:ILE:CD1	2.46	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
2:I:490:HIS:CD2	2:I:491:GLU:N	2.83	0.45
2:J:384:LEU:HD21	2:J:412:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ARG:HA	1:A:101:ILE:HD12	1.99	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
2:B:692:ASN:C	2:B:692:ASN:ND2	2.72	0.45
2:E:384:LEU:HB2	2:E:670:MET:HE3	1.97	0.45
2:B:490:HIS:CD2	2:B:491:GLU:N	2.83	0.45
2:B:491:GLU:CD	2:B:491:GLU:C	2.84	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
1:D:140:MET:HE3	1:D:160:LEU:CD1	2.47	0.45
2:E:384:LEU:HD21	2:E:412:ILE:HG23	1.98	0.45
2:E:417:VAL:HB	2:E:479:ILE:CG2	2.43	0.45
2:E:675:LYS:CD	2:I:665:LEU:HD21	2.45	0.45
2:E:683:LYS:HE2	2:I:658:GLN:HE21	1.82	0.45
2:I:452:LEU:C	2:I:452:LEU:CD1	2.88	0.45
2:I:491:GLU:C	2:I:491:GLU:CD	2.84	0.45
2:I:687:HIS:CD2	2:I:688:LEU:HD23	2.52	0.45
2:J:329:LEU:HD23	2:J:702:LEU:HB3	1.99	0.45
2:J:388:ILE:HD11	2:J:412:ILE:HD11	1.98	0.45
2:B:367:HIS:CD2	2:B:682:PRO:HB3	2.52	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
2:B:470:ARG:HH11	2:B:470:ARG:HG3	1.82	0.45
2:B:676:THR:HG22	2:B:680:LEU:HD22	1.99	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:H:545:LEU:HB2	2:H:550:LEU:HD13	1.98	0.45
2:I:676:THR:HG22	2:I:680:LEU:HD22	1.99	0.45
2:J:489:ASN:C	2:J:490:HIS:O	2.59	0.45
2:B:428:VAL:HG13	2:B:689:MET:CE	2.47	0.45
2:I:374:LEU:HD13	2:I:423:PRO:CB	2.47	0.45
2:J:340:PHE:O	2:J:341:GLU:C	2.53	0.45
2:J:380:ASP:OD1	2:J:380:ASP:N	2.49	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
1:A:51:PHE:CD1	1:A:281:LEU:HD12	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
2:C:545:LEU:HB2	2:C:550:LEU:HD13	1.98	0.45
1:D:83:PHE:CZ	1:D:97:VAL:HG13	2.50	0.45
2:E:329:LEU:HD23	2:E:702:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:369:ARG:C	2:B:369:ARG:HD3	2.42	0.45
2:B:405:PRO:HA	2:B:662:ILE:CD1	2.47	0.45
2:E:380:ASP:OD1	2:E:380:ASP:N	2.49	0.45
2:E:493:PHE:CZ	2:E:665:LEU:HD23	2.52	0.45
1:G:309:LYS:NZ	1:G:309:LYS:HB3	2.31	0.45
2:I:369:ARG:C	2:I:369:ARG:HD3	2.42	0.45
2:I:370:PHE:CZ	2:I:374:LEU:HD21	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:A:80:TYR:HB2	1:A:90:LYS:HB3	1.98	0.45
1:A:234:VAL:CG1	1:A:277:LEU:HD22	2.47	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:D:23:ILE:HG22	1:D:25:GLN:HE21	1.82	0.45
2:E:379:PHE:CE1	2:E:419:LYS:HB2	2.49	0.45
2:I:409:PHE:CD1	2:I:666:VAL:HG13	2.51	0.45
2:J:680:LEU:HD12	2:J:680:LEU:HA	1.88	0.45
1:K:113:LYS:HD2	1:K:113:LYS:N	2.32	0.45
1:A:309:LYS:NZ	1:A:309:LYS:HB3	2.31	0.44
2:B:474:GLN:HG2	2:B:688:LEU:CD1	2.47	0.44
2:B:687:HIS:C	2:B:688:LEU:HD23	2.41	0.44
1:G:80:TYR:HB2	1:G:90:LYS:HB3	1.98	0.44
1:G:234:VAL:CG1	1:G:277:LEU:HD22	2.47	0.44
2:I:429:ASP:HA	2:I:432:ILE:HD12	1.99	0.44
2:I:470:ARG:HG3	2:I:470:ARG:HH11	1.82	0.44
2:I:703:ALA:HA	2:J:699:SER:CA	2.45	0.44
2:J:406:ASP:OD1	2:J:407:MET:N	2.50	0.44
1:K:235:VAL:HG23	1:K:255:GLU:HA	1.99	0.44
2:B:409:PHE:HD1	2:B:666:VAL:HG13	1.81	0.44
2:I:367:HIS:CD2	2:I:682:PRO:HB3	2.52	0.44
2:I:428:VAL:HG13	2:I:689:MET:CE	2.47	0.44
2:I:490:HIS:CG	2:I:491:GLU:N	2.81	0.44
2:J:662:ILE:HA	2:J:665:LEU:CD1	2.46	0.44
2:B:452:LEU:C	2:B:452:LEU:CD1	2.88	0.44
1:D:113:LYS:HD2	1:D:113:LYS:N	2.32	0.44
1:D:140:MET:CE	1:D:157:ARG:HA	2.46	0.44
2:E:406:ASP:OD1	2:E:407:MET:N	2.50	0.44
2:E:464:ILE:HG13	2:E:693:THR:HG23	1.98	0.44
2:E:485:TYR:CE2	2:I:485:TYR:HB3	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:464:ILE:HG13	2:J:693:THR:HG23	1.98	0.44
2:B:665:LEU:HD21	2:J:675:LYS:CD	2.46	0.44
1:D:317:PHE:CE2	2:E:332:MET:HA	2.52	0.44
2:E:340:PHE:O	2:E:341:GLU:C	2.53	0.44
2:I:409:PHE:HD1	2:I:666:VAL:HG13	1.81	0.44
2:H:600:TYR:O	2:H:601:ARG:HB2	2.18	0.44
1:K:58:PRO:HG3	1:K:101:ILE:CG2	2.47	0.44
1:K:140:MET:HE3	1:K:160:LEU:CD1	2.47	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
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
2:J:370:PHE:CE1	2:J:427:CYS:HB2	2.53	0.44
1:K:84:LEU:HD13	1:K:121:ASN:HD22	1.82	0.44
1:D:84:LEU:HD13	1:D:121:ASN:HD22	1.82	0.44
2:I:341:GLU:HG3	2:J:341:GLU:OE2	2.09	0.44
1:K:140:MET:CE	1:K:157:ARG:HA	2.46	0.44
2:I:417:VAL:HB	2:I:479:ILE:HG23	2.00	0.44
1:G:46:SER:HA	1:G:237:ARG:HH21	1.82	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
2:B:380:ASP:OD1	2:B:380:ASP:N	2.49	0.43
2:J:491:GLU:CD	2:J:491:GLU:C	2.86	0.43
1:K:235:VAL:CG2	1:K:255:GLU:HA	2.48	0.43
1:A:46:SER:HA	1:A:237:ARG:HH21	1.82	0.43
1:A:83:PHE:CZ	1:A:122:LEU:HD22	2.53	0.43
1:A:299:LYS:HD3	1:A:299:LYS:C	2.43	0.43
2:B:490:HIS:CG	2:B:491:GLU:N	2.81	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
2:I:380:ASP:OD1	2:I:380:ASP:N	2.49	0.43
2:I:474:GLN:HG2	2:I:688:LEU:HD12	2.00	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
1:A:232:ILE:CG1	1:A:280:VAL:HG21	2.49	0.43
2:E:491:GLU:O	2:E:491:GLU:HG2	2.18	0.43
1:G:232:ILE:CG1	1:G:280:VAL:HG21	2.49	0.43
2:J:344:ILE:HG21	2:J:690:ILE:HD11	2.01	0.43
2:J:449:TYR:HA	2:J:450:PRO:HD2	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:489:ASN:C	2:B:490:HIS:O	2.62	0.43
2:C:526:LEU:HD13	2:C:605:LEU:HB3	2.00	0.43
2:E:344:ILE:HG21	2:E:690:ILE:HD11	2.01	0.43
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
1:G:16:LEU:HD21	1:G:742:ILE:HG12	2.00	0.43
2:B:474:GLN:HG2	2:B:688:LEU:HD12	2.00	0.43
1:G:176:PRO:CB	1:G:206:LYS:HD2	2.46	0.43
2:I:459:ILE:HD13	2:I:705:LEU:HA	2.00	0.43
2:L:621:LEU:HD23	2:L:627:PRO:HD3	2.01	0.43
2:C:600:TYR:O	2:C:601:ARG:HB2	2.18	0.43
2:F:621:LEU:HD23	2:F:627:PRO:HD3	2.01	0.43
2:I:381:GLU:HG2	2:I:382:LYS:HG3	2.00	0.43
2:L:573:ARG:CD	2:L:575:VAL:HG22	2.48	0.43
1:A:9:LEU:CD1	1:A:286:THR:HG23	2.49	0.43
1:A:67:ARG:HH22	1:A:107:ARG:HH21	1.67	0.43
1:D:191:LYS:NZ	1:D:225:LEU:HG	2.33	0.43
2:E:664:ASN:HD22	2:E:664:ASN:HA	1.62	0.43
1:G:63:ILE:HG21	1:G:148:GLN:HE22	1.84	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:H:596:VAL:HG13	2:H:597:TYR:HD1	1.83	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
1:G:66:ARG:HB2	1:G:105:THR:CG2	2.48	0.43
1:G:299:LYS:HD3	1:G:299:LYS:C	2.43	0.43
2:I:489:ASN:C	2:I:490:HIS:O	2.61	0.43
2:L:624:GLY:HA2	2:L:626:TYR:CZ	2.54	0.43
1:A:209:LEU:HD11	1:A:238:SER:CB	2.47	0.43
2:E:329:LEU:CG	2:E:702:LEU:HD22	2.45	0.43
2:E:381:GLU:HG2	2:E:382:LYS:HG3	2.00	0.43
2:I:694:LYS:HE2	2:J:341:GLU:OE2	2.19	0.43
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
2:E:489:ASN:C	2:E:490:HIS:O	2.59	0.42
2:F:573:ARG:CD	2:F:575:VAL:HG22	2.48	0.42
1:G:56:PHE:CB	1:G:94:PHE:HB3	2.48	0.42
1:K:48:LEU:HB3	1:K:57:LEU:CD1	2.49	0.42
1:K:170:LEU:HD11	1:K:281:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:HB2	1:A:105:THR:CG2	2.48	0.42
2:B:374:LEU:H	2:B:374:LEU:HD22	1.84	0.42
2:C:567:VAL:HG13	2:C:625:VAL:CG2	2.50	0.42
1:D:48:LEU:HB3	1:D:57:LEU:CD1	2.49	0.42
2:E:491:GLU:CD	2:E:491:GLU:C	2.86	0.42
2:E:684:THR:HG22	2:E:685:ILE:N	2.34	0.42
2:H:567:VAL:HG13	2:H:625:VAL:CG2	2.50	0.42
2:J:467:ARG:HA	2:J:467:ARG:HD3	1.86	0.42
1:K:289:ILE:HG21	1:K:745:ILE:HG21	2.02	0.42
2:B:329:LEU:HD12	2:B:329:LEU:HA	1.87	0.42
2:B:357:SER:N	2:B:434:GLU:HG3	2.33	0.42
2:B:381:GLU:HG2	2:B:382:LYS:HG3	2.01	0.42
2:B:459:ILE:HD13	2:B:705:LEU:HA	2.00	0.42
2:C:627:PRO:O	2:C:628:GLU:HB2	2.20	0.42
2:E:405:PRO:CB	2:I:683:LYS:HD3	2.49	0.42
1:G:31:LEU:CD2	1:G:130:LEU:HD12	2.48	0.42
2:I:463:HIS:CE1	2:J:334:GLN:CD	2.96	0.42
2:I:374:LEU:H	2:I:374:LEU:HD22	1.84	0.42
1:K:13:VAL:HG13	1:K:29:LEU:CD1	2.49	0.42
2:B:371:PRO:HA	2:B:374:LEU:HD23	2.02	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:664:ASN:HD22	2:J:664:ASN:HA	1.62	0.42
2:I:371:PRO:HA	2:I:374:LEU:HD23	2.02	0.42
2:J:381:GLU:HG2	2:J:382:LYS:HG3	2.00	0.42
2:J:491:GLU:O	2:J:491:GLU:HG2	2.18	0.42
1:K:191:LYS:NZ	1:K:225:LEU:HG	2.33	0.42
1:A:167:GLU:O	1:A:168:ASN:HB2	2.19	0.42
1:D:55:ASP:HB3	1:D:98:ARG:CD	2.50	0.42
1:D:237:ARG:HG3	1:D:251:ALA:HB2	2.02	0.42
1:G:167:GLU:O	1:G:168:ASN:HB2	2.19	0.42
2:J:420:ILE:HD11	2:J:673:VAL:HG11	2.02	0.42
2:B:388:ILE:CG1	2:B:409:PHE:HA	2.50	0.42
2:E:654:GLN:HG2	2:E:654:GLN:O	2.20	0.42
2:H:627:PRO:O	2:H:628:GLU:HB2	2.20	0.42
2:I:388:ILE:CG1	2:I:409:PHE:HA	2.50	0.42
2:I:406:ASP:OD1	2:I:407:MET:N	2.52	0.42
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:467:ARG:HA	2:B:467:ARG:HD3	1.87	0.42
1:D:170:LEU:HD11	1:D:281:LEU:CD2	2.50	0.42
1:D:316:ASN:HB3	2:E:332:MET:CG	2.47	0.42
2:F:600:TYR:O	2:F:601:ARG:HB2	2.18	0.42
1:G:23:ILE:HG12	1:G:734:ALA:HB1	2.02	0.42
2:J:684:THR:HG22	2:J:685:ILE:N	2.34	0.42
2:C:579:PHE:HD1	2:C:579:PHE:H	1.62	0.41
2:F:535:LYS:O	2:F:535:LYS:HG2	2.20	0.41
2:I:707:SER:HA	2:J:702:LEU:CB	2.47	0.41
1:A:135:VAL:HG12	1:A:137:LEU:HG	2.02	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:D:289:ILE:HG21	1:D:745:ILE:HG21	2.01	0.41
2:E:329:LEU:HD12	2:E:329:LEU:HA	1.86	0.41
1:G:135:VAL:HG12	1:G:137:LEU:HG	2.02	0.41
1:K:34:ILE:HG22	1:K:48:LEU:HD11	2.01	0.41
1:K:55:ASP:HB3	1:K:98:ARG:CD	2.50	0.41
2:L:535:LYS:HG2	2:L:535:LYS:O	2.20	0.41
1:A:23:ILE:HG12	1:A:734:ALA:HB1	2.02	0.41
1:D:66:ARG:O	1:D:67:ARG:HG3	2.20	0.41
2:E:478:LEU:CD1	2:E:680:LEU:HD23	2.50	0.41
2:E:493:PHE:CZ	2:E:664:ASN:HB3	2.55	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
1:D:78:THR:HB	1:D:80:TYR:CE1	2.56	0.41
1:G:134:LEU:N	1:G:134:LEU:HD12	2.36	0.41
2:J:345:GLU:O	2:J:346:GLY:C	2.64	0.41
2:J:377:MET:HE3	2:J:422:GLU:HG2	2.02	0.41
2:J:455:GLU:HG2	2:J:705:LEU:CD1	2.50	0.41
2:J:478:LEU:CD1	2:J:680:LEU:HD23	2.50	0.41
2:J:493:PHE:CZ	2:J:664:ASN:HB3	2.55	0.41
2:L:596:VAL:HG13	2:L:597:TYR:HD1	1.85	0.41
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:E:456:MET:SD	2:E:701:LEU:HD21	2.60	0.41
2:J:329:LEU:HD11	2:J:456:MET:HE1	2.03	0.41
1:K:66:ARG:O	1:K:67:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:654:GLN:HG2	2:B:654:GLN:O	2.20	0.41
1:D:13:VAL:HG13	1:D:29:LEU:CD1	2.49	0.41
1:D:204:ILE:HB	1:D:207:LEU:HD11	2.03	0.41
2:E:377:MET:HE3	2:E:422:GLU:HG2	2.02	0.41
2:F:551:SER:HB2	2:F:553:TYR:HE1	1.85	0.41
1:G:63:ILE:HG21	1:G:148:GLN:NE2	2.36	0.41
1:G:301:GLN:HE21	1:G:301:GLN:HA	1.85	0.41
2:H:583:LYS:HD2	2:H:606:ALA:HB1	2.03	0.41
2:I:435:LEU:HD23	2:I:436:ILE:N	2.36	0.41
2:I:439:VAL:HA	2:I:697:ILE:HB	2.03	0.41
1:K:78:THR:HB	1:K:80:TYR:CE1	2.56	0.41
1:K:135:VAL:HG21	1:K:163:PHE:CD1	2.56	0.41
1:A:134:LEU:N	1:A:134:LEU:HD12	2.35	0.41
2:B:333:VAL:O	2:B:333:VAL:CG1	2.66	0.41
2:B:680:LEU:HD11	2:J:406:ASP:HB3	2.02	0.41
2:B:684:THR:HG22	2:B:685:ILE:N	2.35	0.41
2:E:345:GLU:O	2:E:346:GLY:C	2.64	0.41
2:E:406:ASP:HB3	2:I:680:LEU:HD11	2.02	0.41
2:I:384:LEU:HG	2:I:666:VAL:HG12	2.03	0.41
2:I:490:HIS:CE1	2:I:672:ILE:HG21	2.56	0.41
2:I:654:GLN:O	2:I:654:GLN:HG2	2.20	0.41
2:J:687:HIS:CD2	2:J:688:LEU:HD23	2.53	0.41
1:K:204:ILE:HB	1:K:207:LEU:HD11	2.03	0.41
1:A:307:ILE:HG21	1:A:728:MET:HB3	2.03	0.41
2:B:340:PHE:HD2	2:B:694:LYS:HG3	1.85	0.41
2:B:439:VAL:HA	2:B:697:ILE:HB	2.03	0.41
1:G:138:PRO:HG2	1:G:159:MET:SD	2.61	0.41
2:H:607:CYS:HB2	2:H:613:VAL:HG23	2.03	0.41
2:I:329:LEU:HD12	2:I:329:LEU:HA	1.88	0.41
2:I:340:PHE:HD2	2:I:694:LYS:HG3	1.85	0.41
2:I:684:THR:HG22	2:I:685:ILE:N	2.35	0.41
1:K:274:THR:HB	1:K:275:PRO:HD3	2.03	0.41
2:L:543:PHE:CD2	2:L:550:LEU:HD21	2.56	0.41
2:B:345:GLU:O	2:B:346:GLY:C	2.64	0.40
2:B:435:LEU:HD23	2:B:436:ILE:N	2.35	0.40
2:C:583:LYS:HD2	2:C:606:ALA:HB1	2.03	0.40
1:D:170:LEU:HD12	1:D:170:LEU:HA	1.94	0.40
1:D:274:THR:HB	1:D:275:PRO:HD3	2.03	0.40
1:D:315:LYS:HA	2:E:448:GLN:HE22	1.86	0.40
2:E:329:LEU:HD11	2:E:456:MET:HE1	2.03	0.40
1:G:262:HIS:HA	1:G:263:PRO:HD2	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HG21	1:A:148:GLN:NE2	2.36	0.40
1:A:164:VAL:HG21	1:A:193:VAL:HG11	2.03	0.40
2:B:409:PHE:CD2	2:B:486:MET:HE3	2.55	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:539:LYS:HG2	2:F:540:GLU:H	1.85	0.40
2:F:573:ARG:HD2	2:F:575:VAL:HG22	2.04	0.40
1:K:201:ILE:HD12	1:K:277:LEU:CD1	2.51	0.40
2:B:330:LEU:HD22	2:B:330:LEU:HA	1.89	0.40
2:C:553:TYR:CD1	2:C:558:GLU:HG2	2.56	0.40
2:E:391:ALA:CB	2:E:408:ALA:HA	2.50	0.40
1:G:307:ILE:HG21	1:G:728:MET:HB3	2.03	0.40
2:I:409:PHE:CD2	2:I:486:MET:HE3	2.56	0.40
2:J:384:LEU:HD21	2:J:412:ILE:CG2	2.52	0.40
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.91	0.40
1:A:138:PRO:HG2	1:A:159:MET:SD	2.62	0.40
1:A:170:LEU:HD22	1:A:201:ILE:HG12	2.02	0.40
1:A:301:GLN:HE21	1:A:301:GLN:HA	1.85	0.40
2:B:384:LEU:HG	2:B:666:VAL:HG12	2.03	0.40
1:D:135:VAL:HG21	1:D:163:PHE:CD1	2.56	0.40
1:G:87:LYS:O	1:G:87:LYS:HG3	2.20	0.40
2:J:456:MET:HE2	2:J:456:MET:HB2	2.03	0.40
1:A:87:LYS:O	1:A:87:LYS:HG3	2.20	0.40
2:B:384:LEU:HD22	2:B:670:MET:CG	2.50	0.40
1:G:66:ARG:HB3	1:G:115:ILE:HG22	2.04	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
2:I:384:LEU:HD22	2:I:670:MET:CG	2.50	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%)	21	59
1	D	333/864 (38%)	319 (96%)	13 (4%)	1 (0%)	36	72
1	G	325/864 (38%)	313 (96%)	10 (3%)	2 (1%)	21	59
1	K	333/864 (38%)	319 (96%)	13 (4%)	1 (0%)	36	72
2	B	194/864 (22%)	158 (81%)	28 (14%)	8 (4%)	2	18
2	C	111/864 (13%)	94 (85%)	12 (11%)	5 (4%)	2	17
2	E	194/864 (22%)	166 (86%)	23 (12%)	5 (3%)	4	25
2	F	111/864 (13%)	93 (84%)	16 (14%)	2 (2%)	6	34
2	H	111/864 (13%)	94 (85%)	12 (11%)	5 (4%)	2	17
2	I	194/864 (22%)	158 (81%)	29 (15%)	7 (4%)	2	20
2	J	194/864 (22%)	166 (86%)	23 (12%)	5 (3%)	4	25
2	L	111/864 (13%)	93 (84%)	16 (14%)	2 (2%)	6	34
All	All	2536/10368 (24%)	2286 (90%)	205 (8%)	45 (2%)	9	34

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
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

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Mol	Chain	Res	Type
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%)	272 (95%)	15 (5%)	21 42
1	D	295/761 (39%)	282 (96%)	13 (4%)	25 47
1	G	287/761 (38%)	272 (95%)	15 (5%)	21 42
1	K	295/761 (39%)	282 (96%)	13 (4%)	25 47
2	B	191/761 (25%)	155 (81%)	36 (19%)	1 8
2	C	102/761 (13%)	89 (87%)	13 (13%)	4 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	191/761 (25%)	152 (80%)	39 (20%)	1 7
2	F	102/761 (13%)	90 (88%)	12 (12%)	5 18
2	H	102/761 (13%)	89 (87%)	13 (13%)	4 16
2	I	191/761 (25%)	155 (81%)	36 (19%)	1 8
2	J	191/761 (25%)	152 (80%)	39 (20%)	1 7
2	L	102/761 (13%)	90 (88%)	12 (12%)	5 18
All	All	2336/9132 (26%)	2080 (89%)	256 (11%)	8 20

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	73	LEU
1	A	79	GLU
1	A	87	LYS
1	A	121	ASN
1	A	172	LEU
1	A	175	SER
1	A	228	ARG
1	A	240	LYS
1	A	245	LYS
1	A	248	ILE
1	A	301	GLN
1	A	309	LYS
1	A	727	GLU
1	A	741	ILE
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
2	B	373	GLU
2	B	380	ASP
2	B	428	VAL
2	B	438	THR

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Mol	Chain	Res	Type
2	B	441	GLN
2	B	445	LYS
2	B	449	TYR
2	B	451	ARG
2	B	464	ILE
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	672	ILE
2	B	676	THR
2	B	679	ASP
2	B	680	LEU
2	B	685	ILE
2	B	688	LEU
2	B	697	ILE
2	B	700	GLU
2	B	702	LEU
2	C	533	ILE
2	C	534	MET
2	C	535	LYS
2	C	551	SER
2	C	560	GLU
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	140	MET
1	D	160	LEU
1	D	225	LEU

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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	333	VAL
2	E	339	ASP
2	E	340	PHE
2	E	345	GLU
2	E	357	SER
2	E	366	PHE
2	E	368	GLU
2	E	369	ARG
2	E	380	ASP
2	E	415	LYS
2	E	428	VAL
2	E	438	THR
2	E	439	VAL
2	E	443	THR
2	E	445	LYS
2	E	449	TYR
2	E	451	ARG
2	E	452	LEU
2	E	468	GLU
2	E	473	GLU
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	679	ASP
2	E	680	LEU
2	E	684	THR
2	E	685	ILE
2	E	688	LEU
2	E	692	ASN

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Mol	Chain	Res	Type
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	574	ASP
2	F	577	LYS
2	F	579	PHE
2	F	581	SER
2	F	594	ARG
2	F	603	LEU
1	G	69	LEU
1	G	73	LEU
1	G	79	GLU
1	G	87	LYS
1	G	121	ASN
1	G	172	LEU
1	G	175	SER
1	G	228	ARG
1	G	240	LYS
1	G	245	LYS
1	G	248	ILE
1	G	301	GLN
1	G	309	LYS
1	G	727	GLU
1	G	741	ILE
2	H	533	ILE
2	H	534	MET
2	H	535	LYS
2	H	551	SER
2	H	560	GLU
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

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Mol	Chain	Res	Type
2	H	610	GLN
2	I	327	LYS
2	I	329	LEU
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	428	VAL
2	I	438	THR
2	I	441	GLN
2	I	445	LYS
2	I	449	TYR
2	I	451	ARG
2	I	464	ILE
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	672	ILE
2	I	676	THR
2	I	679	ASP
2	I	680	LEU
2	I	685	ILE
2	I	688	LEU
2	I	697	ILE
2	I	700	GLU
2	I	702	LEU
2	J	327	LYS
2	J	329	LEU
2	J	330	LEU
2	J	333	VAL
2	J	339	ASP

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Mol	Chain	Res	Type
2	J	340	PHE
2	J	345	GLU
2	J	357	SER
2	J	366	PHE
2	J	368	GLU
2	J	369	ARG
2	J	380	ASP
2	J	415	LYS
2	J	428	VAL
2	J	438	THR
2	J	439	VAL
2	J	443	THR
2	J	445	LYS
2	J	449	TYR
2	J	451	ARG
2	J	452	LEU
2	J	468	GLU
2	J	473	GLU
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	679	ASP
2	J	680	LEU
2	J	684	THR
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	140	MET
1	K	160	LEU
1	K	225	LEU
1	K	248	ILE

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Mol	Chain	Res	Type
1	K	260	LEU
1	K	297	ARG
1	K	304	LEU
1	K	316	ASN
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	574	ASP
2	L	577	LYS
2	L	579	PHE
2	L	581	SER
2	L	594	ARG
2	L	603	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	75	ASN
1	A	155	GLN
1	A	168	ASN
1	A	236	ASN
1	A	301	GLN
1	A	744	ASN
1	A	746	ASN
2	B	335	GLN
2	B	367	HIS
2	B	487	ASN
2	B	658	GLN
2	B	664	ASN
2	B	687	HIS
2	B	692	ASN
2	C	529	ASN
1	D	26	ASN
1	D	40	GLN
1	D	72	GLN
1	D	121	ASN
1	D	131	ASN

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Mol	Chain	Res	Type
1	D	148	GLN
1	D	155	GLN
1	D	236	ASN
1	D	282	ASN
1	D	284	GLN
1	D	316	ASN
2	E	331	GLN
2	E	334	GLN
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	602	GLN
2	F	610	GLN
1	G	40	GLN
1	G	75	ASN
1	G	155	GLN
1	G	168	ASN
1	G	236	ASN
1	G	301	GLN
1	G	744	ASN
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	658	GLN
2	I	664	ASN
2	I	687	HIS
2	I	692	ASN
2	J	331	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	26	ASN

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Mol	Chain	Res	Type
1	K	40	GLN
1	K	72	GLN
1	K	121	ASN
1	K	131	ASN
1	K	148	GLN
1	K	155	GLN
1	K	198	GLN
1	K	236	ASN
1	K	282	ASN
1	K	284	GLN
1	K	316	ASN
2	L	602	GLN
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 oligosaccharides 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	K	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	315:LYS	C	316:ASN	N	1.19
1	K	315:LYS	C	316:ASN	N	1.19
1	D	316:ASN	C	317:PHE	N	1.17
1	K	316:ASN	C	317:PHE	N	1.17

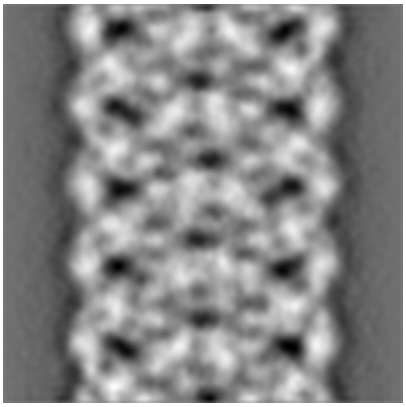
6 Map visualisation (i)

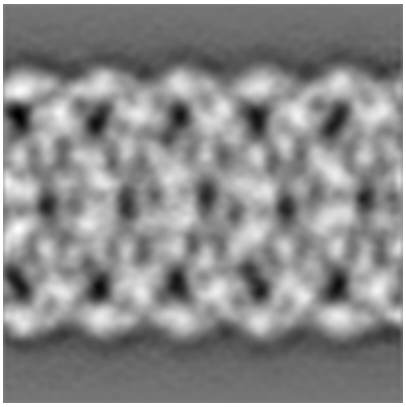
This section contains visualisations of the EMDB entry EMD-2701. These allow visual inspection of the internal detail of the map and identification of artifacts.

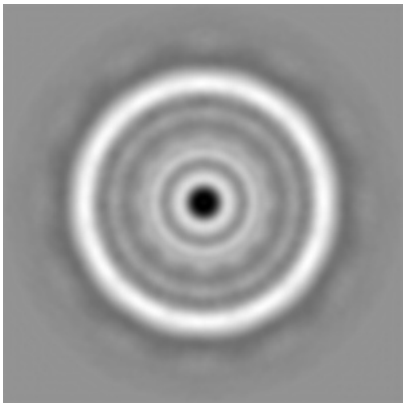
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

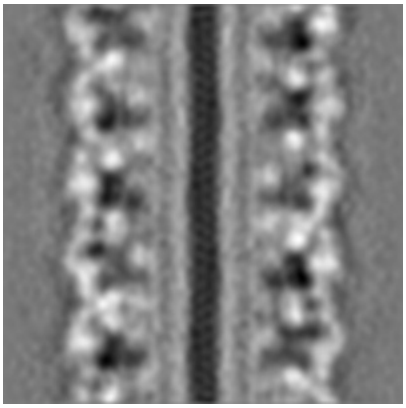

Y

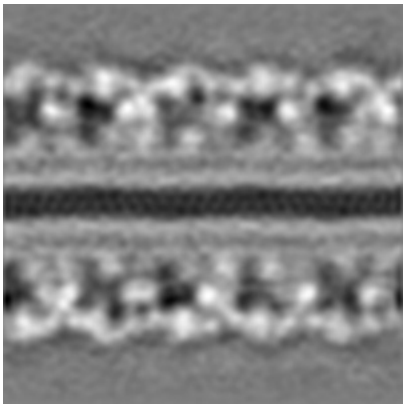

Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 100

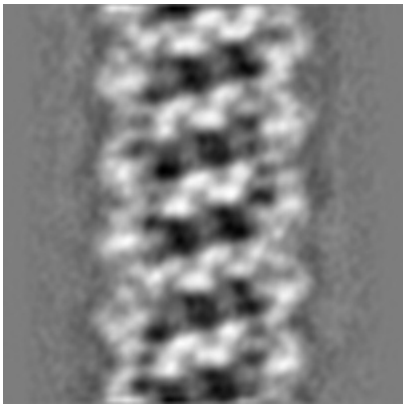

Y Index: 100

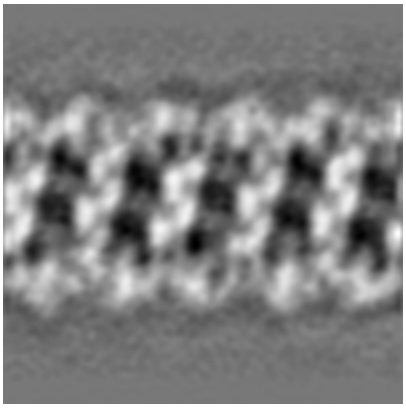
Z Index: 100

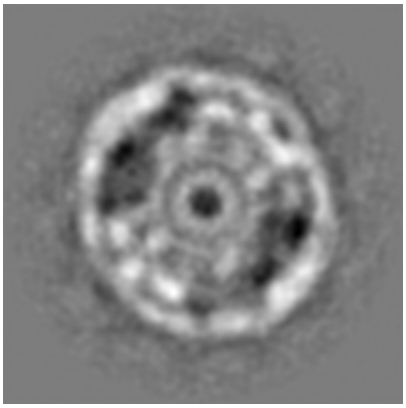
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 145

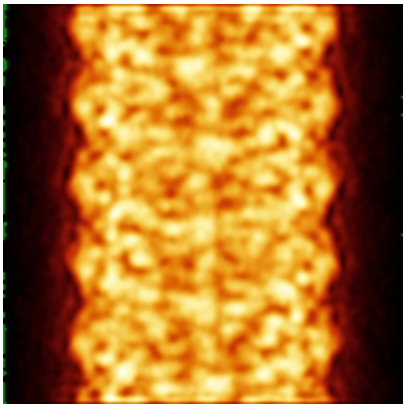

Y Index: 55

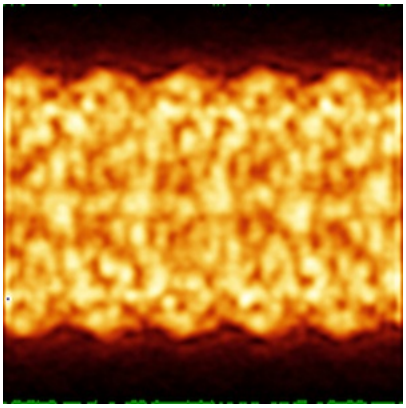

Z Index: 197

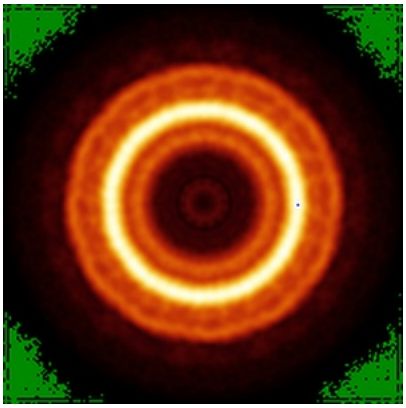
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

This section was not generated.

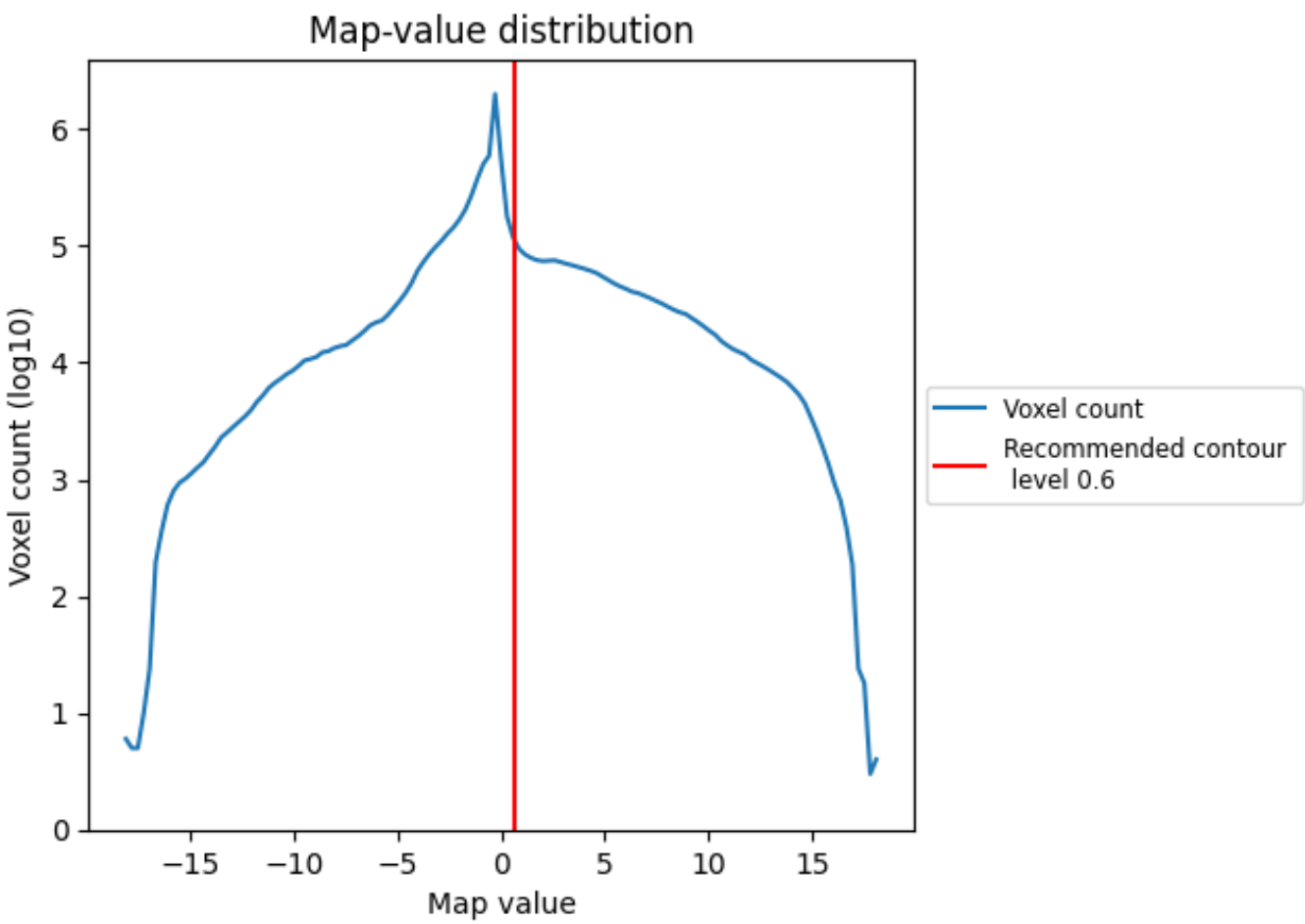
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

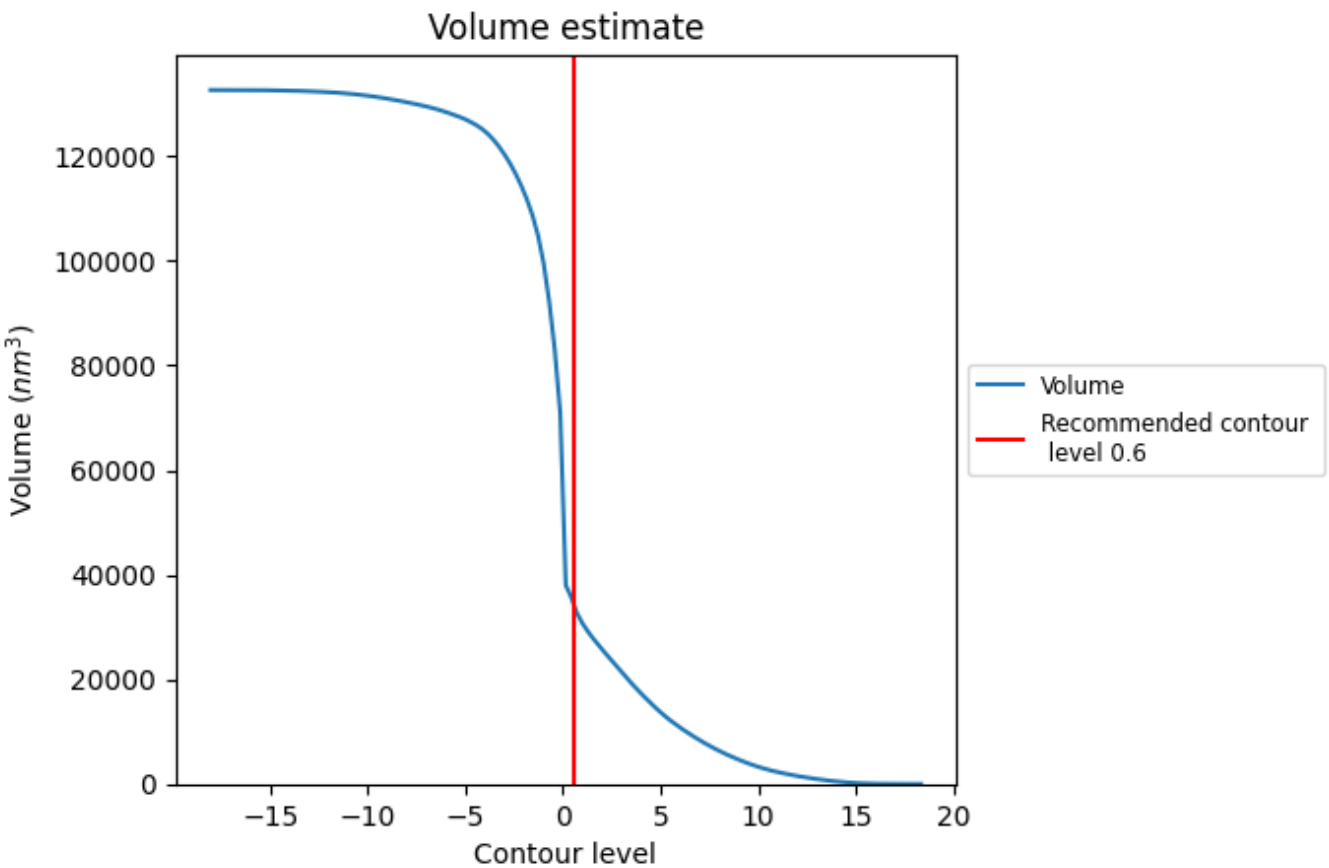
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

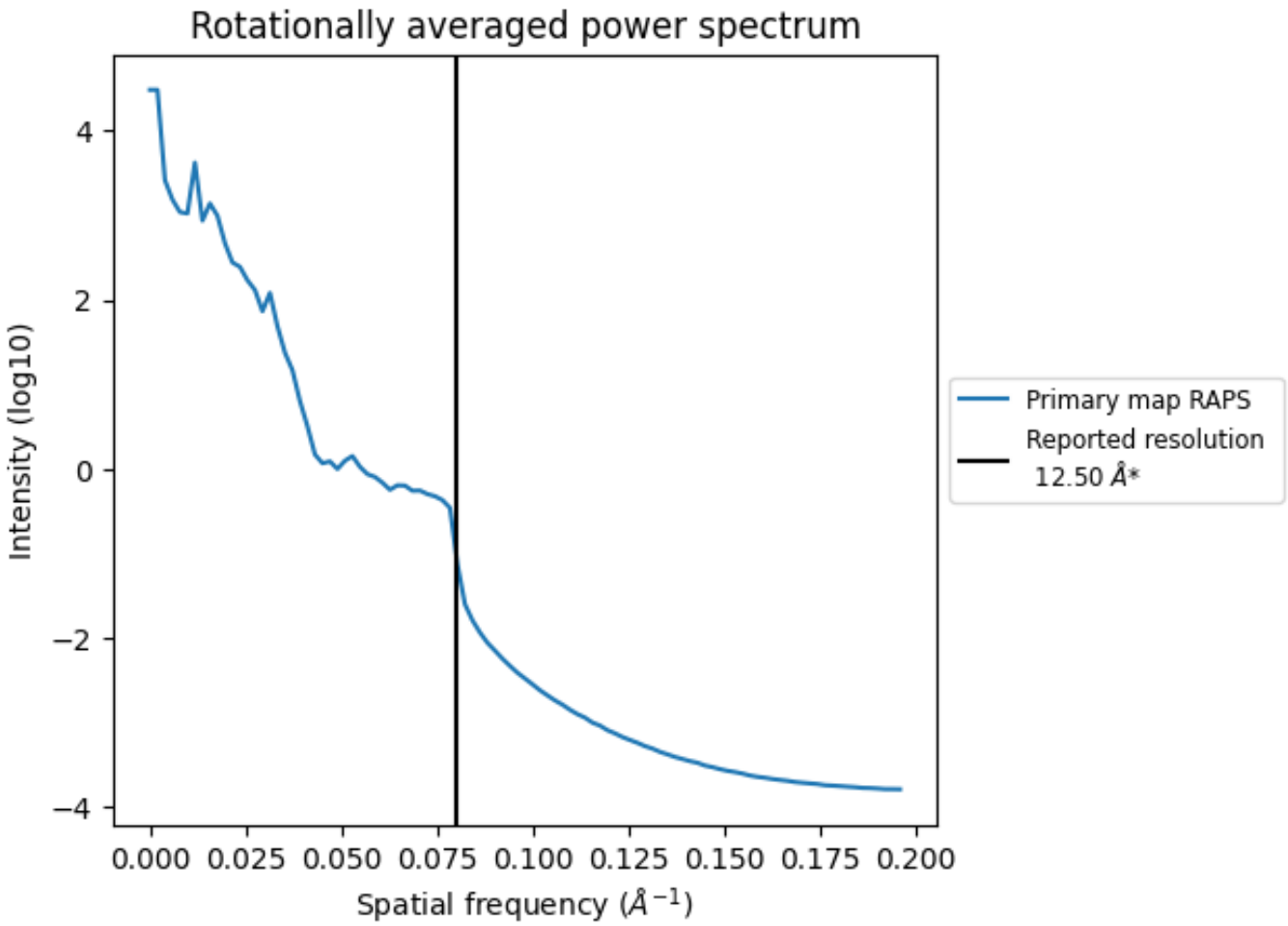
7.2 Volume estimate (i)



The volume at the recommended contour level is 33840 nm^3; this corresponds to an approximate mass of 30569 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.080 Å^{-1}

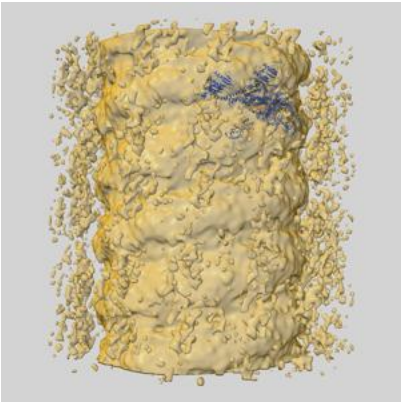
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

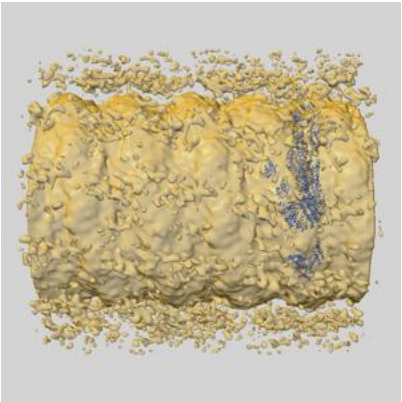
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2701 and PDB model 4UUD. Per-residue inclusion information can be found in section 3 on page 6.

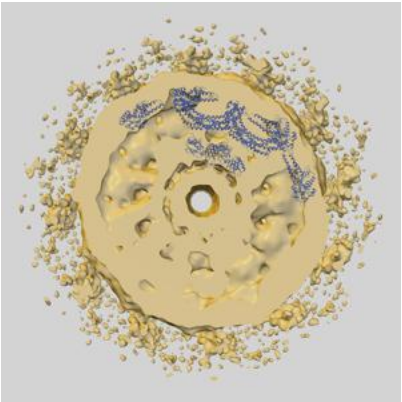
9.1 Map-model overlay (i)



X



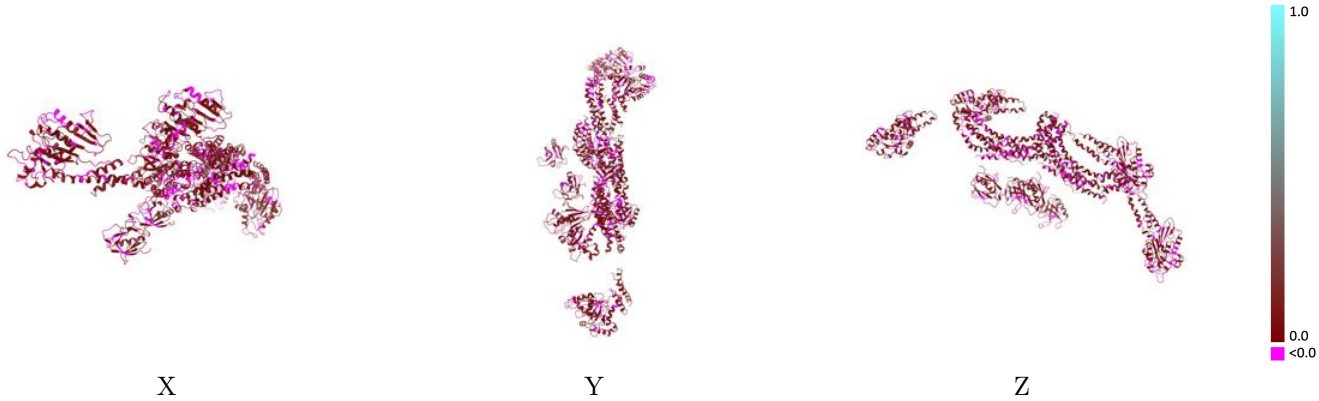
Y



Z

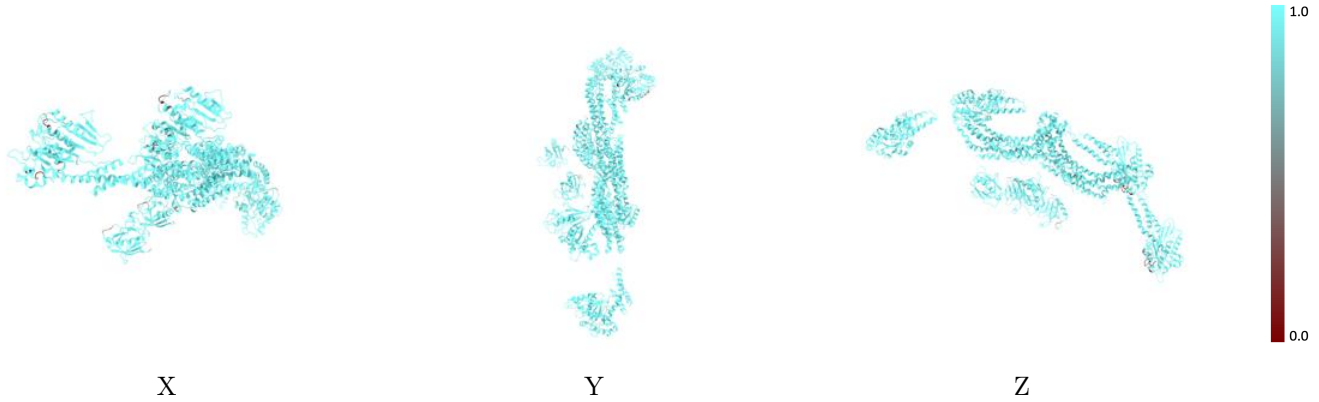
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



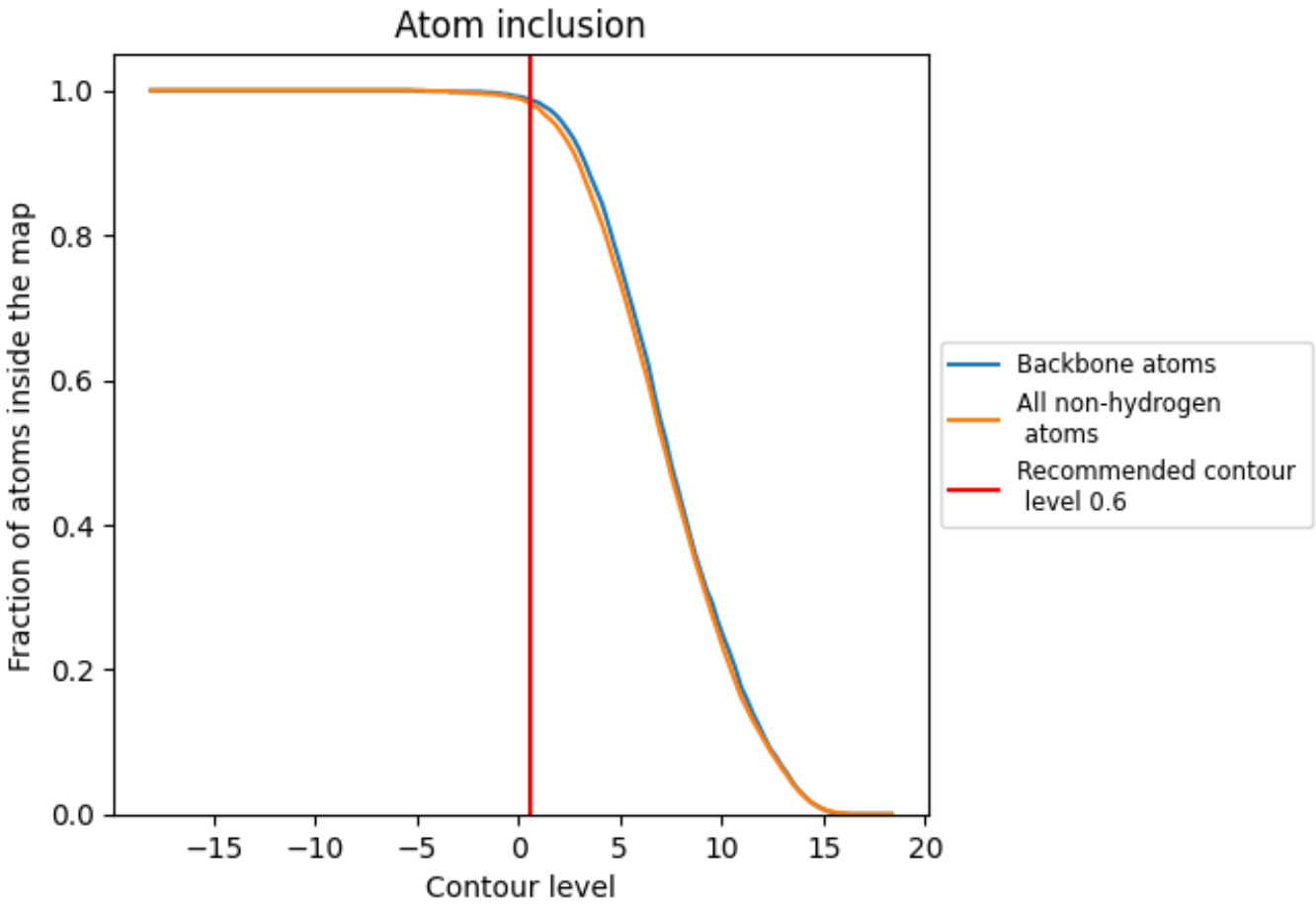
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9820	0.0550
A	0.9940	0.0640
B	0.9930	0.0490
C	0.9840	0.0640
D	0.9550	0.0480
E	0.9970	0.0530
F	0.9740	0.0520
G	0.9940	0.0660
H	0.9830	0.0660
I	0.9930	0.0480
J	0.9970	0.0540
K	0.9550	0.0480
L	0.9740	0.0530