



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:18 PM UTC

PDB ID : 5TJT / pdb_00005tjt
EMDB ID : EMD-8419
Title : T5 bacteriophage major capsid protein - one PB8 hexon
Authors : Conway, J.; Huet, A.
Deposited on : 2016-10-05
Resolution : 9.00 Å(reported)

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

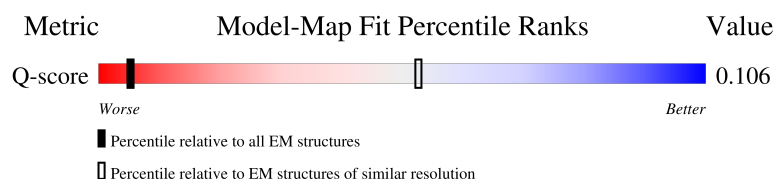
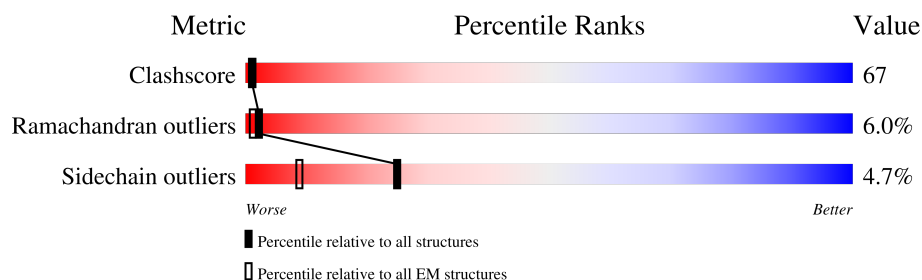
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	257 (8.50 - 9.50)

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 $\leq 5\%$. 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	299	 5% 36% 42% 17% ..
1	B	299	 6% 30% 46% 21% ..
1	C	299	 6% 30% 47% 18% ..
1	D	299	 5% 33% 48% 15% ..

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Mol	Chain	Length	Quality of chain
1	E	299	7% 34% 46% 15% • •
1	F	299	5% 35% 47% 12% • •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 27426 atoms, of which 13800 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.

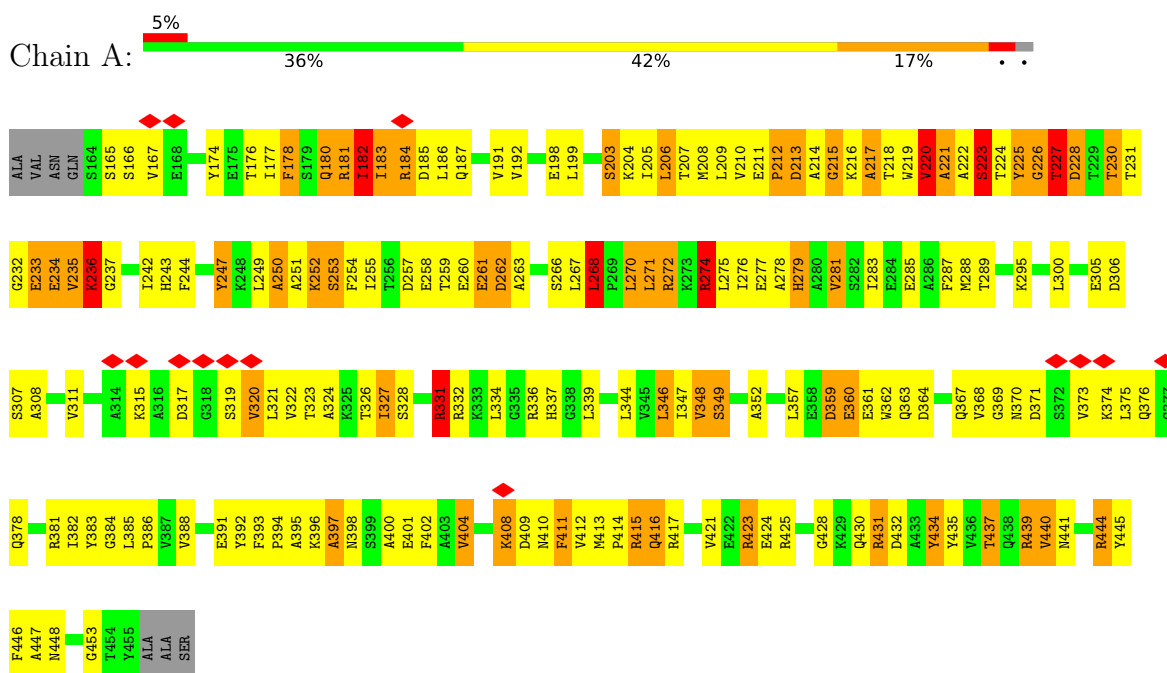
- Molecule 1 is a protein called Major capsid protein.

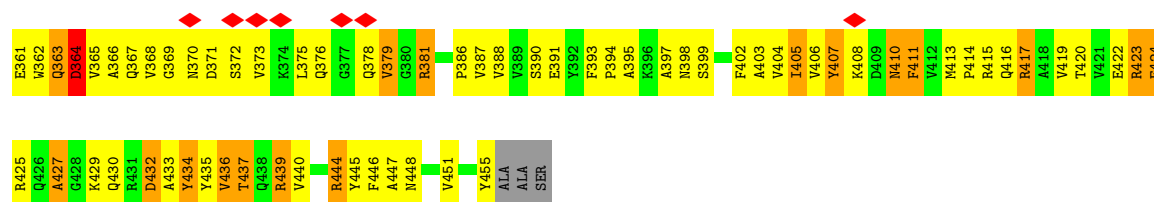
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	292	Total 4571	C 1440	H 2300	N 382	O 444	S 5	0	0
1	B	292	Total 4571	C 1440	H 2300	N 382	O 444	S 5	0	0
1	C	292	Total 4571	C 1440	H 2300	N 382	O 444	S 5	0	0
1	D	292	Total 4571	C 1440	H 2300	N 382	O 444	S 5	0	0
1	E	292	Total 4571	C 1440	H 2300	N 382	O 444	S 5	0	0
1	F	292	Total 4571	C 1440	H 2300	N 382	O 444	S 5	0	0

3 Residue-property plots

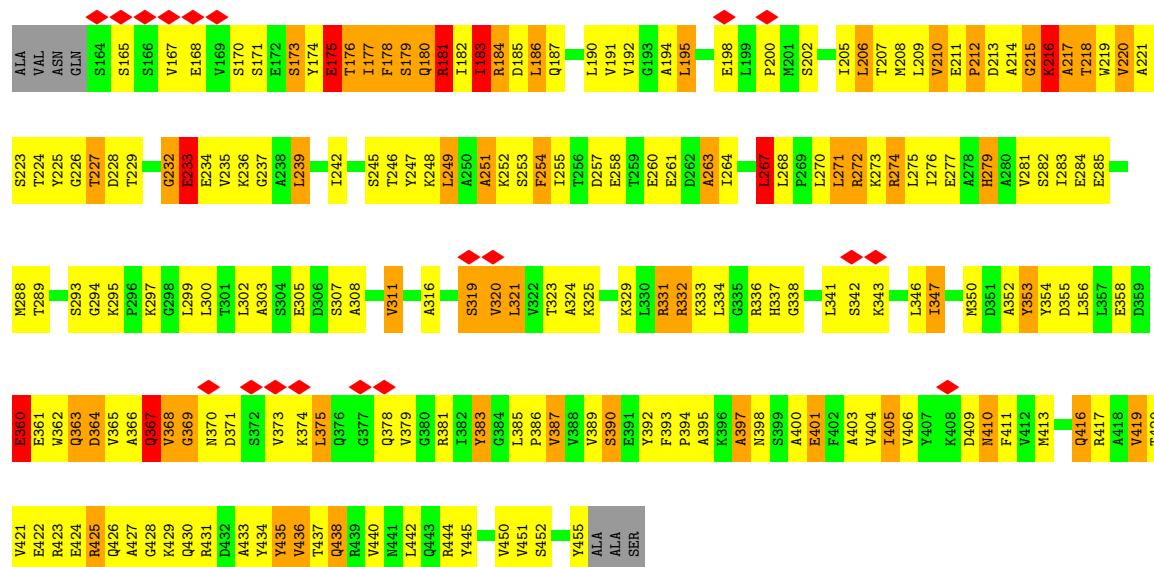
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Major capsid protein

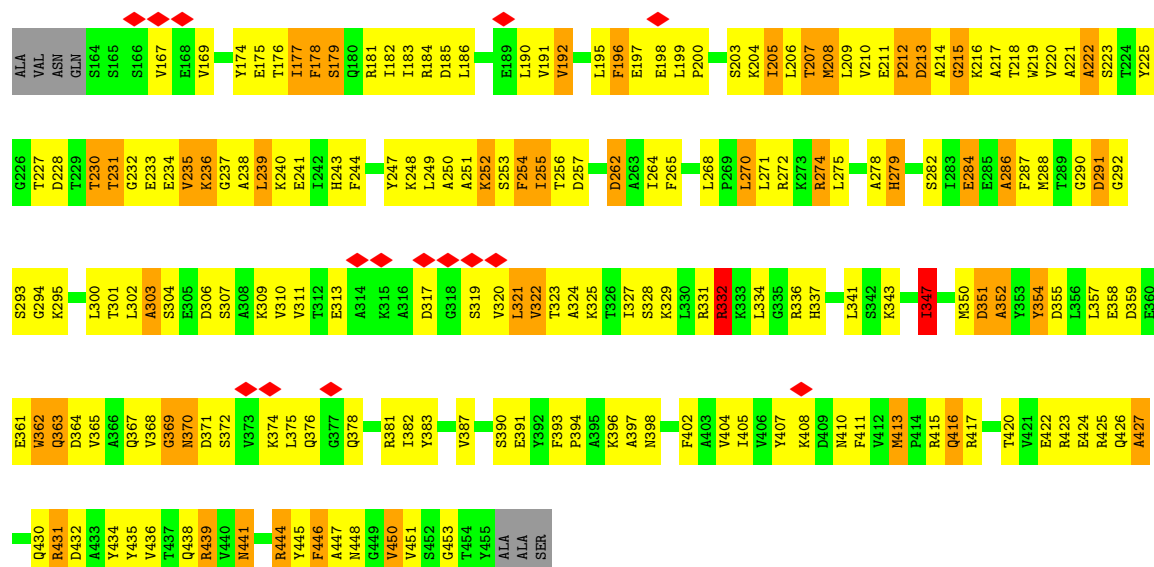




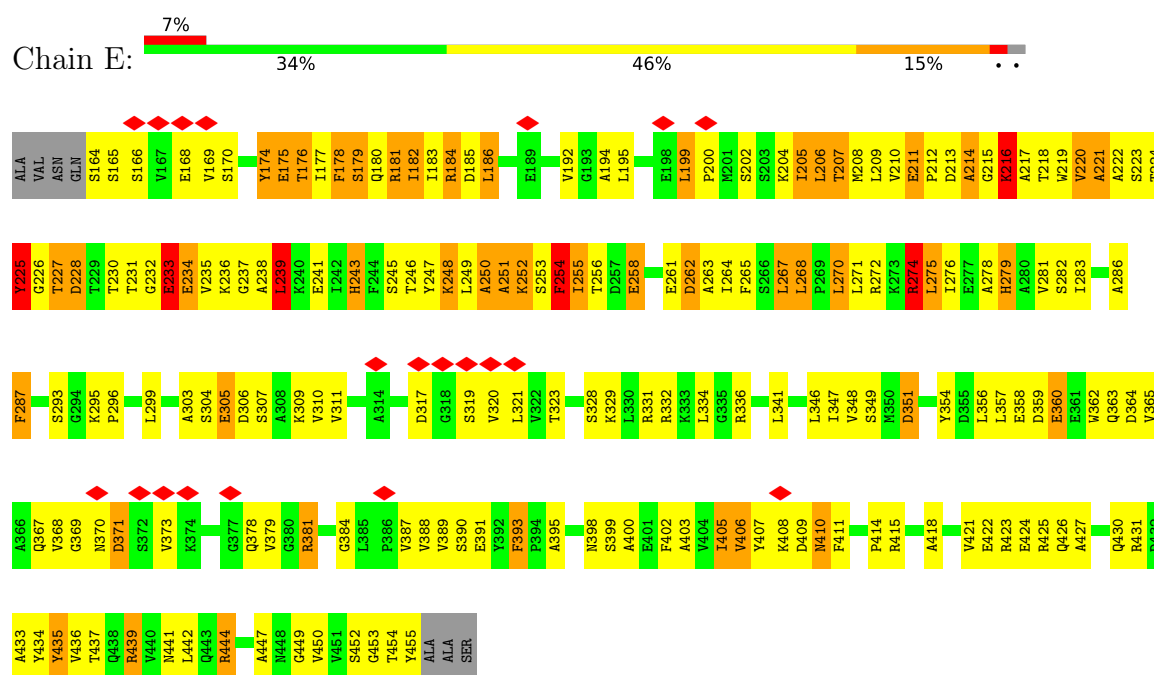
• Molecule 1: Major capsid protein



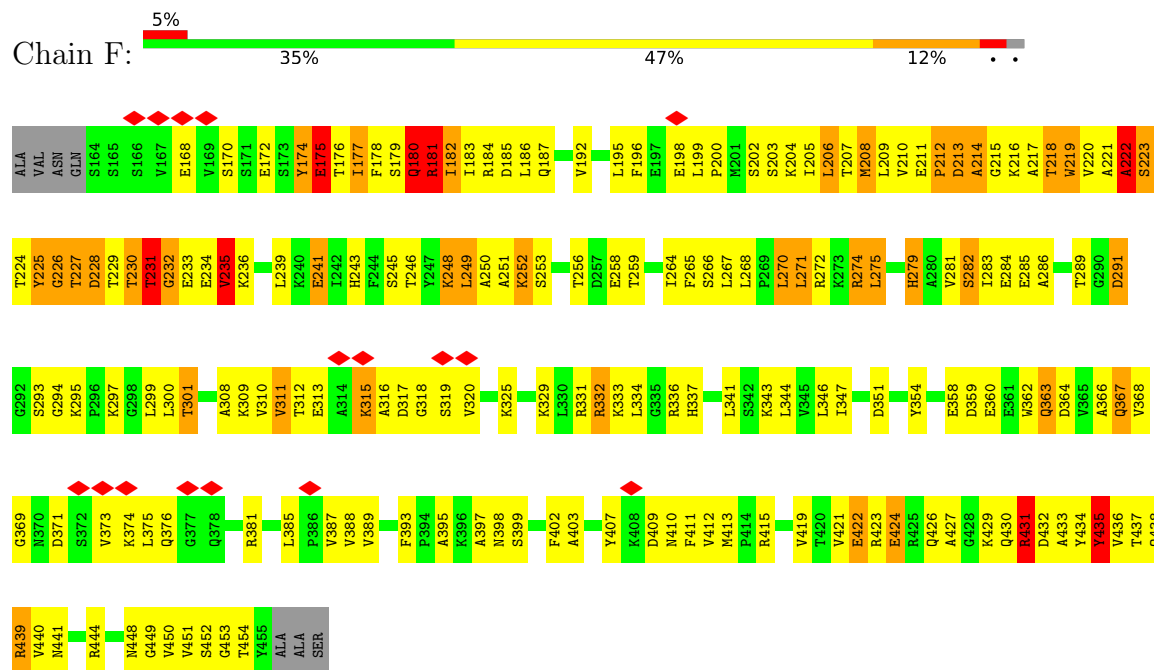
• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



• Molecule 1: Major capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1856	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	32.443	Depositor
Minimum map value	-10.389	Depositor
Average map value	-0.050	Depositor
Map value standard deviation	2.577	Depositor
Recommended contour level	10	Depositor
Map size (Å)	1372.74, 1372.74, 1372.74	wwPDB
Map dimensions	501, 501, 501	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.74, 2.74, 2.74	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.20	80/2306 (3.5%)	2.39	141/3116 (4.5%)
1	B	2.32	104/2306 (4.5%)	2.42	158/3116 (5.1%)
1	C	2.24	92/2306 (4.0%)	2.47	174/3116 (5.6%)
1	D	2.30	88/2306 (3.8%)	2.40	117/3116 (3.8%)
1	E	2.28	87/2306 (3.8%)	2.37	136/3116 (4.4%)
1	F	2.21	80/2306 (3.5%)	2.41	141/3116 (4.5%)
All	All	2.26	531/13836 (3.8%)	2.41	867/18696 (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	0	10
1	B	0	10
1	C	0	7
1	D	0	7
1	E	0	14
1	F	0	6
All	All	0	54

All (531) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	LEU	CA-C	-11.40	1.38	1.52
1	D	204	LYS	C-N	11.38	1.44	1.33
1	D	408	LYS	N-CA	-11.21	1.37	1.47
1	A	453	GLY	N-CA	-10.98	1.34	1.45
1	F	297	LYS	C-N	10.20	1.40	1.33
1	E	176	THR	CA-C	-9.54	1.41	1.52
1	D	310	VAL	N-CA	-9.42	1.34	1.46
1	D	337	HIS	ND1-CE1	9.25	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	381	ARG	N-CA	-9.08	1.34	1.46
1	A	337	HIS	CB-CG	9.00	1.62	1.50
1	B	311	VAL	CA-C	-8.99	1.42	1.53
1	D	169	VAL	CA-C	-8.96	1.41	1.52
1	D	265	PHE	CA-C	8.95	1.64	1.52
1	C	428	GLY	CA-C	8.84	1.60	1.52
1	B	403	ALA	CA-C	-8.82	1.42	1.52
1	A	181	ARG	NE-CZ	8.76	1.42	1.33
1	A	395	ALA	CA-CB	8.68	1.64	1.53
1	A	431	ARG	CD-NE	8.67	1.58	1.46
1	C	184	ARG	CZ-NH2	8.54	1.44	1.33
1	E	182	ILE	C-N	8.51	1.41	1.33
1	A	347	ILE	CA-C	-8.49	1.42	1.52
1	E	267	LEU	N-CA	-8.42	1.36	1.46
1	C	397	ALA	CA-C	-8.40	1.41	1.52
1	E	405	ILE	N-CA	-8.38	1.35	1.46
1	D	381	ARG	NE-CZ	8.37	1.42	1.33
1	B	444	ARG	CA-CB	8.33	1.64	1.52
1	D	332	ARG	CD-NE	8.26	1.57	1.46
1	E	317	ASP	CA-C	-8.02	1.42	1.52
1	E	281	VAL	CA-CB	-8.00	1.45	1.54
1	B	372	SER	N-CA	-7.96	1.36	1.46
1	E	293	SER	CA-CB	7.94	1.63	1.53
1	B	373	VAL	N-CA	-7.92	1.36	1.46
1	D	181	ARG	NE-CZ	7.91	1.41	1.33
1	B	430	GLN	CA-C	-7.83	1.43	1.52
1	B	243	HIS	ND1-CE1	7.78	1.40	1.32
1	F	214	ALA	CA-C	-7.76	1.45	1.53
1	C	427	ALA	C-N	7.76	1.41	1.34
1	E	410	ASN	CA-C	-7.71	1.47	1.52
1	B	330	LEU	N-CA	-7.70	1.36	1.46
1	D	272	ARG	NE-CZ	7.70	1.41	1.33
1	E	442	LEU	C-N	7.68	1.44	1.33
1	E	221	ALA	C-N	7.66	1.41	1.32
1	A	236	LYS	CA-C	-7.66	1.43	1.52
1	F	219	TRP	C-N	7.61	1.42	1.33
1	F	184	ARG	CD-NE	7.60	1.56	1.46
1	A	230	THR	C-N	7.58	1.43	1.33
1	A	391	GLU	CA-C	-7.56	1.43	1.52
1	E	359	ASP	C-N	7.54	1.43	1.33
1	F	267	LEU	C-N	7.52	1.43	1.33
1	F	332	ARG	NE-CZ	7.49	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	396	LYS	CA-C	-7.48	1.42	1.52
1	A	423	ARG	CA-C	7.44	1.61	1.52
1	B	332	ARG	CD-NE	7.44	1.56	1.46
1	B	378	GLN	N-CA	-7.41	1.36	1.46
1	C	397	ALA	N-CA	-7.40	1.36	1.46
1	D	208	MET	CA-C	-7.39	1.44	1.53
1	A	388	VAL	C-N	7.31	1.42	1.33
1	C	242	ILE	CA-CB	-7.30	1.42	1.55
1	B	444	ARG	CA-C	-7.29	1.45	1.53
1	F	407	TYR	CA-C	-7.29	1.44	1.52
1	C	168	GLU	C-N	7.28	1.43	1.33
1	D	415	ARG	NE-CZ	7.28	1.41	1.33
1	B	177	ILE	C-N	7.27	1.43	1.33
1	B	407	TYR	CA-CB	7.24	1.64	1.53
1	D	252	LYS	CA-C	-7.22	1.43	1.52
1	C	257	ASP	C-N	7.21	1.43	1.33
1	F	331	ARG	N-CA	-7.20	1.37	1.46
1	F	331	ARG	NE-CZ	7.20	1.41	1.33
1	C	374	LYS	CA-C	-7.18	1.43	1.52
1	A	260	GLU	CA-CB	7.17	1.65	1.53
1	C	417	ARG	C-N	7.17	1.43	1.33
1	F	341	LEU	N-CA	-7.15	1.37	1.46
1	C	174	TYR	CA-C	-7.12	1.42	1.53
1	B	285	GLU	CA-C	-7.08	1.43	1.52
1	F	337	HIS	CA-C	-7.08	1.43	1.52
1	C	247	TYR	C-N	7.07	1.43	1.33
1	B	280	ALA	C-N	7.05	1.42	1.33
1	E	243	HIS	CG-CD2	7.05	1.43	1.35
1	E	199	LEU	CA-C	7.05	1.62	1.52
1	F	310	VAL	CA-C	-7.04	1.43	1.52
1	A	446	PHE	CA-C	-7.04	1.44	1.52
1	B	255	ILE	CA-C	7.03	1.60	1.52
1	B	207	THR	CA-C	-7.01	1.44	1.52
1	D	427	ALA	CA-C	-7.00	1.43	1.52
1	D	311	VAL	N-CA	-6.97	1.37	1.46
1	A	227	THR	CA-C	-6.96	1.44	1.52
1	F	423	ARG	CA-C	-6.95	1.43	1.52
1	A	272	ARG	CZ-NH1	6.95	1.42	1.32
1	B	204	LYS	N-CA	-6.89	1.37	1.46
1	B	200	PRO	N-CA	-6.88	1.39	1.47
1	D	317	ASP	CA-C	-6.87	1.43	1.52
1	A	319	SER	CA-C	-6.85	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	313	GLU	C-N	6.84	1.41	1.33
1	B	256	THR	N-CA	-6.84	1.36	1.45
1	A	274	ARG	NE-CZ	6.83	1.40	1.33
1	F	222	ALA	CA-C	-6.83	1.43	1.52
1	D	450	VAL	C-N	6.81	1.42	1.33
1	D	453	GLY	CA-C	-6.80	1.44	1.51
1	E	379	VAL	CA-CB	-6.78	1.45	1.54
1	D	331	ARG	CZ-NH1	6.77	1.42	1.32
1	D	337	HIS	CG-ND1	6.75	1.45	1.38
1	D	236	LYS	C-N	6.75	1.43	1.33
1	B	424	GLU	N-CA	-6.73	1.36	1.45
1	D	354	TYR	CA-C	-6.70	1.43	1.52
1	D	375	LEU	N-CA	-6.69	1.38	1.46
1	D	422	GLU	CA-C	-6.68	1.44	1.52
1	E	399	SER	C-N	6.68	1.43	1.33
1	B	243	HIS	CB-CG	6.68	1.59	1.50
1	B	399	SER	C-N	6.67	1.42	1.33
1	E	205	ILE	CA-C	6.67	1.59	1.52
1	A	357	LEU	CA-CB	6.66	1.63	1.53
1	F	318	GLY	C-N	6.66	1.43	1.33
1	E	250	ALA	C-N	6.64	1.41	1.33
1	A	413	MET	CA-CB	6.63	1.63	1.53
1	D	444	ARG	NE-CZ	6.63	1.40	1.33
1	C	251	ALA	CA-C	-6.62	1.44	1.52
1	F	285	GLU	CA-C	-6.62	1.44	1.52
1	D	425	ARG	CD-NE	6.62	1.55	1.46
1	F	444	ARG	NE-CZ	6.61	1.40	1.33
1	E	228	ASP	N-CA	-6.60	1.39	1.46
1	C	264	ILE	CA-C	-6.59	1.44	1.52
1	C	272	ARG	NE-CZ	6.59	1.40	1.33
1	B	307	SER	C-N	6.58	1.42	1.33
1	D	181	ARG	CD-NE	6.57	1.55	1.46
1	F	271	LEU	C-N	6.55	1.42	1.33
1	C	239	LEU	CB-CG	6.55	1.66	1.53
1	A	288	MET	C-O	-6.54	1.16	1.24
1	D	331	ARG	CD-NE	6.54	1.55	1.46
1	E	411	PHE	CA-C	-6.54	1.44	1.52
1	C	274	ARG	C-N	6.53	1.42	1.33
1	D	439	ARG	NE-CZ	6.52	1.40	1.33
1	E	265	PHE	N-CA	-6.52	1.38	1.46
1	C	413	MET	N-CA	-6.51	1.38	1.45
1	A	260	GLU	CA-C	-6.51	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	422	GLU	CA-C	-6.50	1.44	1.52
1	C	177	ILE	CA-C	-6.50	1.44	1.52
1	B	186	LEU	N-CA	-6.50	1.37	1.46
1	C	333	LYS	CA-CB	6.50	1.63	1.53
1	E	243	HIS	ND1-CE1	6.50	1.39	1.32
1	C	224	THR	N-CA	6.48	1.53	1.46
1	E	221	ALA	CA-C	6.48	1.61	1.52
1	C	422	GLU	CA-C	-6.47	1.44	1.52
1	F	351	ASP	CA-CB	6.46	1.63	1.53
1	F	403	ALA	CA-C	-6.44	1.44	1.52
1	C	336	ARG	NE-CZ	6.43	1.40	1.33
1	B	436	VAL	CA-CB	-6.42	1.46	1.54
1	B	274	ARG	NE-CZ	6.42	1.40	1.33
1	B	249	LEU	CA-C	-6.41	1.45	1.52
1	C	341	LEU	CA-C	6.40	1.60	1.52
1	C	233	GLU	CA-CB	6.40	1.61	1.53
1	E	371	ASP	CA-C	-6.39	1.44	1.52
1	C	277	GLU	CA-C	-6.39	1.44	1.52
1	B	358	GLU	CA-C	-6.39	1.44	1.52
1	B	322	VAL	CA-C	-6.38	1.45	1.52
1	A	400	ALA	N-CA	-6.37	1.38	1.46
1	C	181	ARG	CZ-NH1	6.35	1.41	1.32
1	F	235	VAL	CA-C	-6.35	1.44	1.52
1	B	243	HIS	CA-CB	6.35	1.63	1.53
1	B	223	SER	CA-C	-6.34	1.44	1.53
1	D	446	PHE	CA-C	-6.34	1.44	1.52
1	F	301	THR	N-CA	-6.33	1.38	1.46
1	E	279	HIS	CA-CB	6.32	1.63	1.53
1	D	254	PHE	CA-CB	6.31	1.62	1.53
1	F	354	TYR	C-N	6.30	1.41	1.33
1	B	387	VAL	N-CA	-6.30	1.39	1.46
1	D	347	ILE	N-CA	-6.30	1.38	1.46
1	F	366	ALA	CA-C	-6.29	1.44	1.52
1	F	311	VAL	CA-CB	-6.27	1.46	1.54
1	A	446	PHE	N-CA	-6.27	1.38	1.45
1	F	228	ASP	CA-CB	6.27	1.64	1.53
1	B	381	ARG	NE-CZ	6.25	1.40	1.33
1	B	321	LEU	C-N	6.24	1.41	1.33
1	D	434	TYR	C-N	6.23	1.42	1.33
1	E	180	GLN	CA-CB	6.23	1.61	1.53
1	B	425	ARG	CZ-NH2	6.23	1.41	1.33
1	F	399	SER	C-N	6.23	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	222	ALA	CA-C	-6.22	1.44	1.52
1	F	274	ARG	NE-CZ	6.22	1.39	1.33
1	A	243	HIS	ND1-CE1	6.22	1.38	1.32
1	D	381	ARG	CD-NE	6.22	1.54	1.46
1	D	404	VAL	CA-C	-6.21	1.44	1.52
1	C	227	THR	CA-C	-6.21	1.45	1.52
1	C	329	LYS	CA-C	-6.20	1.44	1.52
1	D	369	GLY	CA-C	-6.18	1.43	1.51
1	E	453	GLY	N-CA	-6.18	1.39	1.45
1	F	174	TYR	N-CA	6.17	1.54	1.46
1	C	332	ARG	NE-CZ	6.17	1.39	1.33
1	D	179	SER	CA-C	-6.17	1.45	1.52
1	C	331	ARG	CD-NE	6.15	1.54	1.46
1	A	392	TYR	CA-CB	6.14	1.63	1.53
1	A	348	VAL	CA-C	6.13	1.60	1.52
1	B	332	ARG	CZ-NH1	6.13	1.41	1.32
1	B	347	ILE	CA-C	-6.12	1.45	1.52
1	E	387	VAL	N-CA	-6.12	1.39	1.46
1	A	448	ASN	CA-CB	6.12	1.61	1.53
1	F	434	TYR	C-N	6.12	1.41	1.33
1	B	255	ILE	N-CA	-6.12	1.38	1.46
1	C	442	LEU	CA-C	-6.12	1.45	1.52
1	B	231	THR	CA-CB	-6.11	1.43	1.53
1	E	181	ARG	NE-CZ	6.11	1.39	1.33
1	E	431	ARG	CD-NE	6.11	1.54	1.46
1	B	423	ARG	NE-CZ	6.11	1.39	1.33
1	A	439	ARG	NE-CZ	6.09	1.39	1.33
1	D	286	ALA	CA-CB	6.09	1.62	1.53
1	C	289	THR	CA-C	-6.08	1.45	1.52
1	B	331	ARG	CA-CB	6.08	1.62	1.53
1	E	388	VAL	CA-CB	6.07	1.60	1.53
1	F	436	VAL	CA-C	-6.04	1.45	1.52
1	B	209	LEU	CA-C	-6.03	1.45	1.52
1	D	405	ILE	CA-CB	-6.03	1.46	1.54
1	B	268	LEU	CA-CB	6.01	1.61	1.53
1	F	452	SER	CA-CB	6.01	1.62	1.53
1	C	191	VAL	CA-C	-6.01	1.46	1.52
1	C	260	GLU	CA-C	-6.01	1.45	1.52
1	C	420	THR	C-N	5.99	1.41	1.33
1	D	365	VAL	CA-C	-5.98	1.43	1.52
1	A	205	ILE	N-CA	-5.98	1.38	1.46
1	F	231	THR	C-N	5.97	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	272	ARG	NE-CZ	5.96	1.39	1.33
1	D	365	VAL	C-N	5.96	1.42	1.34
1	F	315	LYS	N-CA	-5.95	1.40	1.46
1	E	207	THR	C-N	5.94	1.41	1.33
1	E	214	ALA	CA-C	-5.93	1.45	1.52
1	F	219	TRP	NE1-CE2	5.93	1.44	1.37
1	E	409	ASP	N-CA	-5.93	1.41	1.46
1	B	334	LEU	N-CA	5.93	1.53	1.46
1	B	415	ARG	NE-CZ	5.92	1.39	1.33
1	B	398	ASN	C-N	5.91	1.41	1.33
1	E	388	VAL	CA-C	-5.91	1.46	1.52
1	B	255	ILE	CA-CB	-5.90	1.46	1.54
1	B	407	TYR	C-N	5.90	1.42	1.33
1	C	401	GLU	N-CA	-5.89	1.38	1.45
1	B	331	ARG	NE-CZ	5.88	1.39	1.33
1	D	390	SER	N-CA	-5.88	1.38	1.45
1	E	164	SER	C-N	5.88	1.41	1.33
1	B	201	MET	C-N	5.88	1.42	1.33
1	C	331	ARG	NE-CZ	5.87	1.39	1.33
1	F	181	ARG	NE-CZ	5.87	1.39	1.33
1	D	439	ARG	CD-NE	5.87	1.54	1.46
1	B	194	ALA	CA-CB	5.86	1.59	1.53
1	C	427	ALA	CA-C	-5.86	1.47	1.52
1	A	445	TYR	CA-C	-5.85	1.45	1.52
1	C	195	LEU	CA-CB	5.85	1.63	1.53
1	A	386	PRO	N-CA	5.85	1.54	1.47
1	F	385	LEU	N-CA	-5.85	1.36	1.46
1	F	450	VAL	CA-C	5.84	1.59	1.52
1	E	168	GLU	C-N	5.83	1.41	1.33
1	C	419	VAL	CA-CB	-5.83	1.48	1.54
1	B	214	ALA	C-N	5.83	1.42	1.33
1	E	252	LYS	C-N	5.82	1.40	1.33
1	C	320	VAL	CA-C	-5.82	1.45	1.52
1	F	286	ALA	CA-CB	5.82	1.62	1.53
1	C	299	LEU	CA-C	5.82	1.60	1.52
1	B	444	ARG	CD-NE	5.82	1.54	1.46
1	A	382	ILE	CA-C	-5.81	1.45	1.52
1	D	436	VAL	C-N	5.80	1.41	1.33
1	C	279	HIS	CA-C	-5.80	1.45	1.52
1	C	311	VAL	CA-C	5.79	1.60	1.52
1	C	303	ALA	N-CA	-5.78	1.38	1.46
1	D	264	ILE	C-O	-5.78	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	GLN	N-CA	-5.76	1.39	1.46
1	B	402	PHE	N-CA	-5.75	1.38	1.45
1	A	414	PRO	N-CD	-5.75	1.39	1.47
1	A	307	SER	CA-C	5.75	1.57	1.52
1	D	334	LEU	C-N	5.74	1.42	1.33
1	E	279	HIS	CE1-NE2	5.74	1.38	1.32
1	B	340	LYS	CA-C	-5.74	1.44	1.53
1	C	425	ARG	CD-NE	5.73	1.54	1.46
1	C	226	GLY	N-CA	5.73	1.52	1.44
1	D	451	VAL	C-N	5.73	1.41	1.33
1	B	425	ARG	NE-CZ	5.72	1.39	1.33
1	D	303	ALA	CA-C	5.72	1.60	1.52
1	E	363	GLN	C-N	5.72	1.41	1.33
1	C	403	ALA	CA-C	5.72	1.59	1.52
1	F	325	LYS	N-CA	-5.71	1.39	1.46
1	F	453	GLY	CA-C	-5.71	1.46	1.51
1	F	192	VAL	N-CA	-5.71	1.39	1.46
1	D	327	ILE	N-CA	-5.71	1.39	1.46
1	B	202	SER	C-N	5.70	1.41	1.33
1	E	182	ILE	N-CA	-5.70	1.39	1.46
1	E	275	LEU	N-CA	-5.70	1.39	1.46
1	B	375	LEU	CA-C	-5.70	1.45	1.52
1	F	438	GLN	N-CA	-5.69	1.38	1.45
1	C	186	LEU	CA-CB	5.68	1.63	1.53
1	C	307	SER	C-O	-5.68	1.18	1.24
1	C	325	LYS	CA-C	-5.67	1.45	1.52
1	C	429	LYS	N-CA	-5.67	1.38	1.45
1	B	316	ALA	C-N	5.66	1.41	1.33
1	B	356	LEU	C-N	5.66	1.41	1.33
1	B	364	ASP	C-N	5.66	1.40	1.33
1	E	270	LEU	C-N	5.66	1.41	1.33
1	A	417	ARG	CA-C	-5.66	1.45	1.52
1	F	432	ASP	C-N	5.65	1.41	1.33
1	C	445	TYR	N-CA	-5.64	1.39	1.46
1	A	279	HIS	ND1-CE1	5.64	1.38	1.32
1	B	429	LYS	C-N	5.63	1.40	1.33
1	A	396	LYS	C-O	5.63	1.30	1.24
1	C	386	PRO	N-CD	-5.63	1.39	1.47
1	D	417	ARG	CZ-NH1	5.63	1.40	1.32
1	E	331	ARG	CA-CB	5.62	1.62	1.53
1	F	415	ARG	CD-NE	5.62	1.54	1.46
1	E	409	ASP	CA-C	-5.62	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	ILE	CA-C	5.62	1.59	1.52
1	D	431	ARG	NE-CZ	5.62	1.39	1.33
1	E	354	TYR	C-N	5.61	1.41	1.33
1	B	225	TYR	CE1-CZ	5.61	1.51	1.38
1	C	246	THR	C-N	5.61	1.41	1.33
1	D	238	ALA	N-CA	-5.60	1.39	1.46
1	C	417	ARG	CZ-NH1	5.59	1.40	1.32
1	C	390	SER	N-CA	-5.59	1.38	1.45
1	A	381	ARG	CZ-NH1	5.58	1.40	1.32
1	A	166	SER	C-N	5.58	1.41	1.33
1	E	246	THR	C-N	5.58	1.41	1.33
1	A	447	ALA	CA-C	-5.58	1.45	1.52
1	A	315	LYS	CA-CB	5.57	1.62	1.53
1	C	187	GLN	C-N	5.56	1.41	1.33
1	F	199	LEU	C-N	5.56	1.41	1.33
1	A	437	THR	C-N	5.56	1.41	1.33
1	B	344	LEU	C-N	5.55	1.40	1.33
1	B	419	VAL	CA-C	5.55	1.59	1.52
1	C	285	GLU	N-CA	-5.55	1.39	1.46
1	C	347	ILE	CA-C	-5.54	1.46	1.52
1	A	250	ALA	N-CA	-5.54	1.39	1.46
1	D	174	TYR	CA-C	-5.54	1.46	1.52
1	E	454	THR	C-N	5.54	1.41	1.33
1	E	166	SER	CA-C	-5.53	1.46	1.52
1	F	186	LEU	N-CA	-5.53	1.39	1.46
1	D	295	LYS	N-CA	-5.53	1.38	1.46
1	B	272	ARG	CD-NE	5.52	1.53	1.46
1	B	279	HIS	CA-CB	5.52	1.61	1.53
1	A	247	TYR	C-N	5.52	1.40	1.33
1	F	388	VAL	CA-C	-5.52	1.47	1.53
1	B	247	TYR	N-CA	-5.51	1.38	1.45
1	F	226	GLY	C-N	5.51	1.40	1.33
1	E	358	GLU	C-N	5.51	1.41	1.33
1	B	236	LYS	CA-C	-5.51	1.45	1.52
1	C	283	ILE	CB-CG1	5.51	1.64	1.53
1	D	425	ARG	NE-CZ	5.51	1.39	1.33
1	C	404	VAL	C-O	-5.50	1.18	1.24
1	E	389	VAL	CA-CB	-5.50	1.47	1.53
1	C	336	ARG	CD-NE	5.50	1.53	1.46
1	F	433	ALA	CA-C	-5.49	1.46	1.52
1	A	324	ALA	C-O	5.48	1.30	1.24
1	A	234	GLU	CA-C	-5.48	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	ARG	CD-NE	5.48	1.53	1.46
1	F	232	GLY	C-N	5.47	1.41	1.33
1	E	415	ARG	CD-NE	5.46	1.53	1.46
1	A	183	ILE	CB-CG1	5.46	1.64	1.53
1	D	417	ARG	CA-C	-5.46	1.46	1.52
1	E	184	ARG	CD-NE	5.46	1.53	1.46
1	F	249	LEU	C-N	5.46	1.40	1.33
1	A	404	VAL	CA-CB	-5.46	1.47	1.54
1	B	222	ALA	C-N	5.45	1.41	1.33
1	A	423	ARG	CZ-NH1	5.45	1.40	1.32
1	B	381	ARG	CD-NE	5.45	1.53	1.46
1	E	272	ARG	C-O	-5.42	1.17	1.24
1	B	228	ASP	N-CA	-5.42	1.39	1.46
1	D	407	TYR	N-CA	-5.42	1.39	1.46
1	E	406	VAL	C-N	5.41	1.41	1.33
1	E	425	ARG	CD-NE	5.41	1.53	1.46
1	E	185	ASP	C-N	5.41	1.41	1.33
1	E	225	TYR	CA-C	-5.41	1.46	1.52
1	E	365	VAL	CA-CB	-5.41	1.47	1.54
1	E	426	GLN	N-CA	-5.40	1.39	1.46
1	A	184	ARG	CZ-NH2	5.40	1.40	1.33
1	D	213	ASP	C-N	5.40	1.40	1.33
1	E	247	TYR	CA-C	-5.40	1.46	1.52
1	B	414	PRO	N-CA	-5.40	1.40	1.47
1	F	206	LEU	CA-C	-5.39	1.46	1.52
1	C	194	ALA	C-N	5.39	1.41	1.33
1	A	408	LYS	N-CA	-5.39	1.39	1.46
1	A	349	SER	CA-C	5.39	1.59	1.52
1	C	217	ALA	N-CA	5.39	1.53	1.46
1	D	288	MET	C-N	5.39	1.40	1.33
1	C	282	SER	CA-C	-5.38	1.45	1.52
1	D	417	ARG	NE-CZ	5.38	1.39	1.33
1	D	301	THR	CA-C	-5.38	1.45	1.52
1	B	190	LEU	C-N	-5.37	1.28	1.33
1	A	261	GLU	CA-CB	5.36	1.59	1.53
1	D	291	ASP	CA-C	-5.36	1.45	1.52
1	E	395	ALA	C-O	5.36	1.30	1.24
1	A	267	LEU	N-CA	-5.36	1.40	1.46
1	D	441	ASN	N-CA	-5.36	1.38	1.46
1	F	334	LEU	CA-CB	5.35	1.61	1.53
1	F	175	GLU	C-N	5.35	1.40	1.33
1	B	320	VAL	CA-C	-5.35	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	VAL	C-N	5.33	1.40	1.33
1	B	360	GLU	C-N	5.33	1.41	1.33
1	C	383	TYR	CA-CB	5.33	1.61	1.53
1	B	363	GLN	C-N	5.33	1.41	1.33
1	E	348	VAL	N-CA	-5.32	1.40	1.46
1	B	440	VAL	CA-C	5.32	1.59	1.52
1	A	400	ALA	CA-C	-5.32	1.46	1.52
1	B	287	PHE	CA-CB	5.32	1.61	1.53
1	C	254	PHE	C-N	5.31	1.40	1.33
1	C	190	LEU	CA-CB	5.30	1.60	1.53
1	F	410	ASN	N-CA	-5.30	1.39	1.46
1	F	411	PHE	C-N	5.29	1.41	1.33
1	C	400	ALA	CA-C	-5.29	1.46	1.52
1	A	217	ALA	CA-C	-5.29	1.45	1.52
1	A	393	PHE	C-N	5.29	1.40	1.33
1	D	309	LYS	C-N	5.29	1.40	1.33
1	E	444	ARG	NE-CZ	5.29	1.38	1.33
1	F	289	THR	N-CA	5.29	1.52	1.46
1	E	184	ARG	CZ-NH2	5.29	1.40	1.33
1	F	248	LYS	C-N	5.28	1.41	1.33
1	C	352	ALA	CA-C	5.27	1.59	1.52
1	D	410	ASN	N-CA	-5.27	1.39	1.46
1	F	454	THR	CA-C	-5.27	1.46	1.52
1	E	367	GLN	CA-C	-5.26	1.45	1.52
1	A	274	ARG	CD-NE	5.26	1.53	1.46
1	A	295	LYS	CA-CB	5.26	1.61	1.53
1	A	311	VAL	CA-C	5.26	1.60	1.53
1	E	364	ASP	C-N	5.25	1.40	1.33
1	E	423	ARG	CZ-NH1	5.25	1.40	1.32
1	D	441	ASN	C-O	-5.24	1.19	1.24
1	A	235	VAL	C-N	5.24	1.39	1.33
1	A	440	VAL	CA-CB	-5.24	1.47	1.55
1	A	322	VAL	N-CA	5.23	1.52	1.46
1	D	207	THR	CB-OG1	-5.23	1.35	1.43
1	F	423	ARG	C-N	5.23	1.40	1.33
1	B	445	TYR	CB-CG	-5.23	1.40	1.51
1	E	170	SER	CA-C	-5.22	1.45	1.52
1	A	198	GLU	CA-C	-5.22	1.46	1.53
1	F	452	SER	C-N	5.22	1.40	1.33
1	B	432	ASP	CA-CB	5.22	1.62	1.53
1	C	194	ALA	N-CA	-5.22	1.40	1.46
1	E	256	THR	CA-C	-5.21	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	423	ARG	CD-NE	5.21	1.53	1.46
1	F	203	SER	N-CA	-5.21	1.39	1.46
1	F	184	ARG	CZ-NH1	5.20	1.40	1.32
1	D	236	LYS	CA-C	-5.20	1.46	1.52
1	C	190	LEU	CA-C	-5.20	1.46	1.52
1	C	308	ALA	C-O	-5.20	1.17	1.24
1	E	186	LEU	CA-C	-5.20	1.45	1.52
1	D	207	THR	CA-C	-5.19	1.48	1.53
1	C	167	VAL	CA-CB	-5.19	1.47	1.54
1	D	416	GLN	CA-CB	5.19	1.62	1.53
1	A	357	LEU	CA-C	-5.18	1.46	1.52
1	B	173	SER	CA-CB	5.18	1.62	1.53
1	E	362	TRP	N-CA	-5.18	1.39	1.46
1	C	200	PRO	N-CA	5.18	1.53	1.47
1	D	292	GLY	CA-C	-5.17	1.44	1.51
1	E	264	ILE	C-O	-5.17	1.18	1.24
1	B	178	PHE	CA-C	5.17	1.58	1.52
1	D	196	PHE	C-N	5.17	1.40	1.33
1	D	407	TYR	CA-C	-5.17	1.46	1.52
1	D	268	LEU	CB-CG	5.16	1.63	1.53
1	A	187	GLN	CA-C	-5.16	1.46	1.53
1	F	176	THR	C-N	5.16	1.40	1.33
1	B	187	GLN	N-CA	-5.14	1.40	1.46
1	C	423	ARG	NE-CZ	5.14	1.38	1.33
1	F	329	LYS	C-N	5.14	1.41	1.33
1	F	375	LEU	C-N	5.14	1.40	1.33
1	E	165	SER	CA-C	-5.14	1.46	1.52
1	D	423	ARG	CZ-NH1	5.14	1.40	1.32
1	E	304	SER	N-CA	-5.14	1.39	1.45
1	F	294	GLY	C-O	-5.13	1.17	1.24
1	A	266	SER	N-CA	-5.13	1.39	1.46
1	B	341	LEU	CA-C	-5.13	1.46	1.52
1	D	361	GLU	C-N	5.13	1.40	1.33
1	D	279	HIS	C-N	5.12	1.40	1.33
1	B	226	GLY	C-N	5.12	1.40	1.33
1	E	332	ARG	CA-C	-5.12	1.45	1.52
1	F	272	ARG	C-O	-5.12	1.18	1.24
1	B	376	GLN	CA-C	-5.12	1.46	1.52
1	A	274	ARG	CZ-NH1	5.11	1.40	1.32
1	F	358	GLU	CA-C	-5.11	1.46	1.52
1	C	246	THR	CA-C	5.11	1.59	1.52
1	B	299	LEU	N-CA	-5.11	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	257	ASP	N-CA	-5.11	1.40	1.46
1	C	444	ARG	NE-CZ	5.10	1.38	1.33
1	A	306	ASP	CA-CB	5.10	1.61	1.53
1	C	431	ARG	NE-CZ	5.10	1.38	1.33
1	F	213	ASP	CA-CB	5.10	1.62	1.53
1	D	288	MET	N-CA	-5.10	1.40	1.46
1	F	351	ASP	N-CA	-5.10	1.40	1.46
1	B	166	SER	N-CA	5.09	1.52	1.45
1	B	181	ARG	CA-CB	5.09	1.62	1.53
1	E	349	SER	CA-C	-5.09	1.46	1.52
1	B	425	ARG	C-N	5.09	1.40	1.33
1	E	307	SER	CA-C	5.08	1.59	1.53
1	B	370	ASN	N-CA	-5.08	1.39	1.46
1	A	252	LYS	N-CA	-5.08	1.39	1.45
1	B	407	TYR	CE1-CZ	5.08	1.50	1.38
1	F	371	ASP	CA-C	-5.08	1.46	1.52
1	B	308	ALA	CA-C	-5.08	1.46	1.52
1	C	410	ASN	C-O	-5.08	1.17	1.24
1	E	439	ARG	C-N	5.08	1.40	1.33
1	E	311	VAL	C-O	-5.07	1.18	1.24
1	F	412	VAL	N-CA	-5.07	1.40	1.46
1	A	257	ASP	CA-CB	5.07	1.61	1.53
1	A	251	ALA	C-N	5.07	1.40	1.33
1	C	423	ARG	CA-C	-5.06	1.46	1.52
1	C	271	LEU	C-N	5.06	1.40	1.33
1	E	418	ALA	C-N	5.06	1.40	1.33
1	A	395	ALA	CA-C	-5.06	1.46	1.53
1	C	378	GLN	CA-CB	5.06	1.61	1.53
1	E	363	GLN	C-O	5.06	1.30	1.24
1	E	447	ALA	CA-C	-5.06	1.46	1.52
1	A	375	LEU	N-CA	5.06	1.52	1.46
1	B	223	SER	N-CA	5.05	1.53	1.46
1	D	370	ASN	CA-C	-5.05	1.46	1.52
1	A	327	ILE	CA-C	-5.05	1.46	1.52
1	D	254	PHE	N-CA	-5.05	1.39	1.46
1	E	262	ASP	N-CA	5.05	1.52	1.46
1	F	210	VAL	C-N	-5.05	1.28	1.33
1	F	435	TYR	C-N	5.04	1.40	1.33
1	C	210	VAL	CA-CB	-5.04	1.47	1.54
1	D	423	ARG	N-CA	-5.04	1.39	1.46
1	A	421	VAL	N-CA	5.04	1.52	1.46
1	E	216	LYS	C-O	-5.04	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	360	GLU	CA-CB	5.04	1.60	1.53
1	E	220	VAL	CA-C	-5.04	1.46	1.52
1	C	176	THR	CA-C	-5.03	1.46	1.52
1	D	441	ASN	CA-CB	5.03	1.60	1.53
1	F	272	ARG	CZ-NH2	5.03	1.40	1.33
1	C	395	ALA	CA-C	5.03	1.59	1.52
1	A	300	LEU	CA-CB	5.02	1.61	1.53
1	C	165	SER	CA-C	-5.02	1.46	1.52
1	B	181	ARG	CZ-NH2	5.02	1.40	1.33
1	C	232	GLY	C-N	5.02	1.40	1.33
1	D	302	LEU	C-O	-5.02	1.17	1.24
1	D	185	ASP	CA-CB	5.02	1.59	1.53
1	D	402	PHE	CA-C	-5.02	1.46	1.52
1	C	421	VAL	CA-CB	-5.02	1.48	1.54
1	F	289	THR	CA-C	-5.01	1.46	1.52
1	F	300	LEU	C-N	5.01	1.40	1.33
1	C	451	VAL	N-CA	5.01	1.52	1.46
1	B	437	THR	CA-C	5.01	1.58	1.52
1	D	307	SER	N-CA	-5.00	1.40	1.46

All (867) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	PHE	CA-CB-CG	-12.49	101.31	113.80
1	E	347	ILE	CA-C-N	11.03	136.08	120.53
1	E	347	ILE	C-N-CA	11.03	136.08	120.53
1	F	448	ASN	CA-CB-CG	-10.49	102.11	112.60
1	D	350	MET	CA-C-N	10.47	134.32	120.28
1	D	350	MET	C-N-CA	10.47	134.32	120.28
1	C	424	GLU	N-CA-C	-10.19	93.92	109.41
1	F	453	GLY	O-C-N	10.13	130.97	123.27
1	B	381	ARG	NE-CZ-NH2	9.78	128.00	119.20
1	F	181	ARG	NE-CZ-NH2	9.69	127.92	119.20
1	E	370	ASN	N-CA-C	-9.64	91.55	108.13
1	D	359	ASP	CA-C-N	9.48	134.71	120.31
1	D	359	ASP	C-N-CA	9.48	134.71	120.31
1	F	268	LEU	CA-C-N	9.40	129.62	119.28
1	F	268	LEU	C-N-CA	9.40	129.62	119.28
1	A	371	ASP	CA-CB-CG	9.27	121.87	112.60
1	D	255	ILE	CA-C-O	-9.23	112.49	121.63
1	D	430	GLN	CA-C-N	9.10	138.08	121.70
1	D	430	GLN	C-N-CA	9.10	138.08	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	373	VAL	CB-CA-C	-9.09	98.08	112.16
1	C	346	LEU	CA-C-N	9.05	133.68	122.37
1	C	346	LEU	C-N-CA	9.05	133.68	122.37
1	C	398	ASN	N-CA-C	-8.99	99.67	111.71
1	C	444	ARG	NE-CZ-NH1	-8.88	112.62	121.50
1	D	351	ASP	CA-CB-CG	-8.87	103.73	112.60
1	C	334	LEU	O-C-N	-8.84	112.97	122.07
1	C	185	ASP	N-CA-C	-8.81	95.41	109.59
1	A	393	PHE	CA-C-N	8.79	128.73	119.85
1	A	393	PHE	C-N-CA	8.79	128.73	119.85
1	F	430	GLN	CA-C-N	8.72	137.39	121.70
1	F	430	GLN	C-N-CA	8.72	137.39	121.70
1	E	408	LYS	O-C-N	8.69	130.80	121.85
1	C	247	TYR	N-CA-C	-8.65	96.25	109.41
1	E	393	PHE	CB-CA-C	-8.53	97.23	110.02
1	C	370	ASN	CA-C-N	8.51	137.80	121.54
1	C	370	ASN	C-N-CA	8.51	137.80	121.54
1	B	308	ALA	N-CA-C	-8.48	101.98	111.14
1	B	370	ASN	CA-C-N	8.48	132.75	120.71
1	B	370	ASN	C-N-CA	8.48	132.75	120.71
1	C	369	GLY	N-CA-C	-8.42	103.08	115.63
1	B	313	GLU	CA-C-N	8.39	132.36	120.28
1	B	313	GLU	C-N-CA	8.39	132.36	120.28
1	C	228	ASP	CA-C-O	8.35	128.29	118.69
1	C	176	THR	O-C-N	-8.31	113.69	123.41
1	A	228	ASP	N-CA-C	-8.22	103.03	113.72
1	F	346	LEU	CA-C-N	8.21	132.31	120.91
1	F	346	LEU	C-N-CA	8.21	132.31	120.91
1	B	341	LEU	N-CA-C	-8.19	94.92	108.76
1	B	279	HIS	ND1-CE1-NE2	8.19	116.58	108.40
1	B	229	THR	N-CA-C	-8.18	103.32	113.38
1	F	398	ASN	N-CA-C	-8.12	103.35	113.18
1	C	375	LEU	CA-C-N	8.09	131.11	120.28
1	C	375	LEU	C-N-CA	8.09	131.11	120.28
1	C	428	GLY	N-CA-C	-8.07	104.95	113.58
1	D	186	LEU	CA-C-N	8.03	135.66	122.73
1	D	186	LEU	C-N-CA	8.03	135.66	122.73
1	B	447	ALA	N-CA-C	-8.00	103.52	113.28
1	C	324	ALA	CA-C-N	8.00	131.00	120.28
1	C	324	ALA	C-N-CA	8.00	131.00	120.28
1	B	333	LYS	CA-C-N	7.98	130.81	120.44
1	B	333	LYS	C-N-CA	7.98	130.81	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	423	ARG	NE-CZ-NH1	-7.97	113.53	121.50
1	D	393	PHE	CA-C-N	7.96	129.79	119.84
1	D	393	PHE	C-N-CA	7.96	129.79	119.84
1	E	387	VAL	N-CA-CB	7.93	119.17	110.53
1	F	174	TYR	CA-C-N	7.93	136.69	121.54
1	F	174	TYR	C-N-CA	7.93	136.69	121.54
1	D	239	LEU	CA-C-N	7.92	135.96	121.70
1	D	239	LEU	C-N-CA	7.92	135.96	121.70
1	D	336	ARG	N-CA-C	-7.90	103.43	113.23
1	F	376	GLN	CA-C-O	-7.90	112.18	120.55
1	A	412	VAL	N-CA-C	-7.89	96.97	109.20
1	A	281	VAL	CB-CA-C	-7.87	101.51	112.14
1	F	308	ALA	N-CA-C	-7.80	104.93	114.75
1	B	370	ASN	CA-CB-CG	7.77	120.37	112.60
1	B	398	ASN	N-CA-C	-7.75	103.40	113.17
1	A	300	LEU	CA-C-N	7.74	130.65	120.28
1	A	300	LEU	C-N-CA	7.74	130.65	120.28
1	A	346	LEU	CA-C-N	7.73	132.67	122.93
1	A	346	LEU	C-N-CA	7.73	132.67	122.93
1	E	441	ASN	CA-CB-CG	7.71	120.31	112.60
1	E	230	THR	N-CA-C	-7.69	101.37	108.75
1	C	257	ASP	CA-CB-CG	-7.66	104.94	112.60
1	F	265	PHE	CA-CB-CG	-7.66	106.14	113.80
1	A	381	ARG	NE-CZ-NH2	7.65	126.09	119.20
1	D	205	ILE	N-CA-C	-7.64	96.90	107.75
1	A	441	ASN	CA-CB-CG	7.63	120.23	112.60
1	E	179	SER	N-CA-CB	7.62	121.29	110.24
1	C	337	HIS	CE1-NE2-CD2	-7.61	101.39	109.00
1	E	407	TYR	N-CA-C	-7.59	101.12	110.61
1	B	416	GLN	OE1-CD-NE2	7.56	130.16	122.60
1	F	451	VAL	O-C-N	-7.54	114.92	123.07
1	A	279	HIS	CA-CB-CG	7.54	121.34	113.80
1	B	196	PHE	CA-CB-CG	-7.54	106.26	113.80
1	B	239	LEU	N-CA-C	-7.53	97.86	109.52
1	E	367	GLN	CA-C-N	7.50	135.48	121.97
1	E	367	GLN	C-N-CA	7.50	135.48	121.97
1	A	424	GLU	N-CA-C	-7.50	97.96	109.14
1	F	180	GLN	CA-C-N	7.49	135.85	121.54
1	F	180	GLN	C-N-CA	7.49	135.85	121.54
1	D	167	VAL	CA-C-N	7.49	135.46	123.93
1	D	167	VAL	C-N-CA	7.49	135.46	123.93
1	E	435	TYR	CA-CB-CG	-7.48	100.44	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	GLU	N-CA-C	-7.48	103.13	111.28
1	C	427	ALA	N-CA-C	-7.47	102.75	113.21
1	C	444	ARG	CD-NE-CZ	-7.46	113.96	124.40
1	C	268	LEU	O-C-N	-7.45	113.47	120.55
1	A	421	VAL	N-CA-C	-7.45	97.71	108.36
1	B	376	GLN	N-CA-C	7.44	119.39	111.28
1	D	365	VAL	O-C-N	7.43	128.92	122.16
1	F	373	VAL	CA-C-N	7.42	130.09	120.44
1	F	373	VAL	C-N-CA	7.42	130.09	120.44
1	F	343	LYS	N-CA-CB	7.37	122.81	111.46
1	A	324	ALA	CA-C-N	7.36	130.15	120.28
1	A	324	ALA	C-N-CA	7.36	130.15	120.28
1	D	235	VAL	N-CA-C	-7.35	98.64	108.35
1	E	233	GLU	N-CA-C	7.35	121.04	110.24
1	A	262	ASP	N-CA-CB	7.34	122.90	110.49
1	F	229	THR	N-CA-C	-7.32	103.97	113.12
1	B	188	LYS	N-CA-C	-7.31	97.82	109.59
1	F	308	ALA	CB-CA-C	-7.29	99.75	109.16
1	A	281	VAL	N-CA-CB	7.23	120.38	110.54
1	B	257	ASP	CA-CB-CG	-7.23	105.37	112.60
1	E	424	GLU	CB-CG-CD	-7.22	100.33	112.60
1	D	306	ASP	N-CA-C	7.21	119.22	111.36
1	C	239	LEU	N-CA-C	-7.21	97.37	108.76
1	B	306	ASP	CA-C-O	-7.18	112.94	120.55
1	F	409	ASP	CA-CB-CG	-7.18	105.42	112.60
1	A	223	SER	N-CA-CB	7.18	122.62	110.49
1	C	411	PHE	CA-CB-CG	7.17	120.97	113.80
1	F	199	LEU	O-C-N	-7.15	113.42	121.36
1	A	242	ILE	CA-C-O	-7.15	112.90	120.76
1	E	174	TYR	CA-C-N	7.14	135.18	121.54
1	E	174	TYR	C-N-CA	7.14	135.18	121.54
1	D	177	ILE	CA-C-O	-7.14	113.93	121.93
1	E	275	LEU	N-CA-C	7.14	118.71	111.07
1	B	285	GLU	O-C-N	-7.13	114.73	122.07
1	F	387	VAL	N-CA-C	-7.11	98.34	108.58
1	E	329	LYS	CA-C-N	7.10	129.80	120.28
1	E	329	LYS	C-N-CA	7.10	129.80	120.28
1	E	406	VAL	CA-C-O	-7.10	114.25	122.13
1	E	341	LEU	N-CA-C	-7.09	98.24	109.23
1	F	354	TYR	N-CA-C	-7.09	104.64	113.28
1	E	436	VAL	N-CA-C	-7.08	97.92	108.46
1	B	272	ARG	NE-CZ-NH1	-7.07	114.43	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	388	VAL	N-CA-CB	7.06	120.52	111.83
1	F	266	SER	CA-C-N	7.06	129.62	120.44
1	F	266	SER	C-N-CA	7.06	129.62	120.44
1	D	199	LEU	CA-C-N	7.05	126.81	119.76
1	D	199	LEU	C-N-CA	7.05	126.81	119.76
1	F	181	ARG	NE-CZ-NH1	-7.04	114.46	121.50
1	D	423	ARG	NE-CZ-NH2	7.02	125.52	119.20
1	A	183	ILE	N-CA-CB	7.02	121.77	111.52
1	C	431	ARG	N-CA-CB	7.01	122.41	110.50
1	B	430	GLN	CA-C-N	7.01	134.31	121.70
1	B	430	GLN	C-N-CA	7.01	134.31	121.70
1	E	398	ASN	CA-C-N	7.01	131.94	120.94
1	E	398	ASN	C-N-CA	7.01	131.94	120.94
1	A	244	PHE	N-CA-CB	7.00	121.83	110.42
1	A	270	LEU	CA-C-N	7.00	129.66	120.28
1	A	270	LEU	C-N-CA	7.00	129.66	120.28
1	C	274	ARG	NE-CZ-NH1	-6.99	114.51	121.50
1	B	325	LYS	CA-C-N	6.99	129.64	120.28
1	B	325	LYS	C-N-CA	6.99	129.64	120.28
1	C	258	GLU	N-CA-C	6.98	119.78	111.33
1	F	275	LEU	CA-C-O	6.96	127.93	120.55
1	E	243	HIS	CE1-NE2-CD2	-6.96	102.04	109.00
1	A	243	HIS	CA-CB-CG	6.96	120.76	113.80
1	B	234	GLU	CA-C-N	6.96	134.49	121.97
1	B	234	GLU	C-N-CA	6.96	134.49	121.97
1	A	220	VAL	N-CA-C	-6.95	97.53	108.86
1	F	412	VAL	N-CA-C	-6.94	98.16	108.85
1	E	373	VAL	CA-C-N	6.94	129.58	120.28
1	E	373	VAL	C-N-CA	6.94	129.58	120.28
1	C	430	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	A	307	SER	O-C-N	6.92	128.29	121.85
1	E	402	PHE	CA-CB-CG	6.91	120.71	113.80
1	A	411	PHE	N-CA-CB	6.91	122.16	110.49
1	F	374	LYS	N-CA-C	6.91	118.46	111.07
1	A	326	THR	O-C-N	6.90	129.27	122.09
1	B	323	THR	N-CA-C	6.88	118.43	111.07
1	B	381	ARG	N-CA-C	-6.88	98.61	109.07
1	C	354	TYR	CA-C-N	6.86	129.48	120.28
1	C	354	TYR	C-N-CA	6.86	129.48	120.28
1	D	240	LYS	CA-C-N	6.85	130.44	120.71
1	D	240	LYS	C-N-CA	6.85	130.44	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	228	ASP	CA-C-N	6.82	129.31	120.44
1	E	228	ASP	C-N-CA	6.82	129.31	120.44
1	F	279	HIS	CE1-NE2-CD2	-6.82	102.18	109.00
1	D	378	GLN	OE1-CD-NE2	6.81	129.41	122.60
1	A	394	PRO	CA-C-N	6.81	132.31	122.85
1	A	394	PRO	C-N-CA	6.81	132.31	122.85
1	B	370	ASN	N-CA-C	-6.81	96.30	110.80
1	D	293	SER	CA-C-O	-6.80	113.96	121.58
1	B	189	GLU	CB-CG-CD	-6.80	101.04	112.60
1	A	180	GLN	N-CA-C	-6.80	98.20	108.46
1	D	422	GLU	N-CA-C	-6.79	98.86	109.72
1	F	281	VAL	N-CA-C	6.79	116.94	110.42
1	E	381	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	B	311	VAL	CA-C-N	6.77	131.40	121.31
1	B	311	VAL	C-N-CA	6.77	131.40	121.31
1	C	362	TRP	N-CA-CB	6.77	121.93	110.49
1	B	358	GLU	CB-CG-CD	-6.76	101.10	112.60
1	E	304	SER	CA-C-N	6.75	132.16	120.68
1	E	304	SER	C-N-CA	6.75	132.16	120.68
1	B	363	GLN	N-CA-C	-6.75	104.18	112.88
1	D	444	ARG	NE-CZ-NH1	-6.74	114.76	121.50
1	D	382	ILE	N-CA-C	-6.73	98.58	108.54
1	F	344	LEU	N-CA-C	-6.72	97.63	109.06
1	D	398	ASN	N-CA-C	-6.72	104.83	113.16
1	E	360	GLU	N-CA-C	-6.72	104.66	112.92
1	B	190	LEU	CA-C-N	6.71	129.62	122.11
1	B	190	LEU	C-N-CA	6.71	129.62	122.11
1	C	325	LYS	CA-C-N	6.71	129.27	120.28
1	C	325	LYS	C-N-CA	6.71	129.27	120.28
1	F	359	ASP	CA-C-N	6.70	129.93	120.28
1	F	359	ASP	C-N-CA	6.70	129.93	120.28
1	E	299	LEU	N-CA-C	-6.70	106.06	114.56
1	C	295	LYS	CA-C-O	-6.69	114.89	120.71
1	E	403	ALA	N-CA-CB	6.69	121.28	110.77
1	B	210	VAL	CA-C-N	6.68	131.00	122.64
1	B	210	VAL	C-N-CA	6.68	131.00	122.64
1	C	236	LYS	CA-C-N	6.68	128.38	122.43
1	C	236	LYS	C-N-CA	6.68	128.38	122.43
1	B	203	SER	CA-C-N	6.67	129.76	120.29
1	B	203	SER	C-N-CA	6.67	129.76	120.29
1	D	391	GLU	N-CA-C	-6.67	103.08	113.02
1	D	402	PHE	CA-CB-CG	-6.67	107.13	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	270	LEU	CA-C-N	6.67	129.22	120.28
1	D	270	LEU	C-N-CA	6.67	129.22	120.28
1	D	453	GLY	O-C-N	6.66	129.95	123.76
1	F	411	PHE	N-CA-CB	6.65	119.75	110.17
1	D	192	VAL	N-CA-CB	6.65	122.20	111.23
1	C	422	GLU	N-CA-C	-6.64	98.07	108.90
1	A	359	ASP	N-CA-C	-6.63	99.51	108.86
1	F	241	GLU	CB-CG-CD	-6.63	101.33	112.60
1	E	178	PHE	N-CA-C	-6.62	99.68	109.81
1	F	449	GLY	O-C-N	6.62	129.82	122.27
1	D	264	ILE	N-CA-C	-6.61	98.96	108.48
1	C	274	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	D	225	TYR	O-C-N	6.61	128.88	122.07
1	B	311	VAL	N-CA-C	-6.60	100.77	108.82
1	A	258	GLU	N-CA-C	6.58	118.45	111.28
1	B	388	VAL	O-C-N	6.58	129.66	122.36
1	C	176	THR	N-CA-C	-6.58	97.51	108.75
1	C	361	GLU	N-CA-C	-6.58	104.19	111.82
1	F	333	LYS	CA-C-N	6.56	128.97	120.44
1	F	333	LYS	C-N-CA	6.56	128.97	120.44
1	C	413	MET	O-C-N	-6.56	115.03	121.19
1	A	410	ASN	CA-C-N	6.54	134.03	121.54
1	A	410	ASN	C-N-CA	6.54	134.03	121.54
1	C	343	LYS	N-CA-C	-6.53	98.79	108.79
1	D	424	GLU	N-CA-C	-6.53	99.72	108.74
1	E	346	LEU	CA-C-N	6.53	129.99	120.91
1	E	346	LEU	C-N-CA	6.53	129.99	120.91
1	C	267	LEU	CA-C-O	6.53	127.67	120.82
1	D	243	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	C	375	LEU	CB-CA-C	-6.52	99.97	110.79
1	A	274	ARG	N-CA-C	6.51	118.38	111.28
1	D	438	GLN	CA-C-O	-6.50	114.24	121.51
1	B	354	TYR	CA-C-N	6.49	129.28	120.38
1	B	354	TYR	C-N-CA	6.49	129.28	120.38
1	D	243	HIS	CE1-NE2-CD2	-6.49	102.51	109.00
1	C	416	GLN	CA-C-O	-6.49	110.81	119.11
1	C	331	ARG	NE-CZ-NH2	6.48	125.03	119.20
1	D	341	LEU	N-CA-C	-6.48	99.19	109.23
1	A	374	LYS	N-CA-CB	6.47	119.40	110.01
1	C	374	LYS	N-CA-C	6.47	118.34	111.28
1	A	206	LEU	N-CA-CB	6.46	120.92	110.77
1	C	337	HIS	CG-CD2-NE2	6.46	113.66	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	337	HIS	ND1-CE1-NE2	6.45	114.85	108.40
1	D	198	GLU	N-CA-CB	6.45	121.35	110.46
1	D	225	TYR	CA-C-O	-6.44	114.05	120.82
1	D	374	LYS	CA-C-O	-6.44	114.05	120.82
1	A	285	GLU	CB-CG-CD	-6.44	101.65	112.60
1	E	356	LEU	N-CA-C	-6.43	104.46	113.20
1	C	410	ASN	OD1-CG-ND2	6.42	129.02	122.60
1	E	295	LYS	CA-C-N	6.42	127.87	119.84
1	E	295	LYS	C-N-CA	6.42	127.87	119.84
1	B	230	THR	N-CA-C	-6.42	99.81	108.86
1	A	321	LEU	CB-CA-C	6.42	120.15	109.89
1	C	338	GLY	N-CA-C	-6.41	106.29	114.37
1	B	337	HIS	CE1-NE2-CD2	-6.41	102.59	109.00
1	F	316	ALA	O-C-N	6.41	129.42	122.05
1	C	228	ASP	N-CA-C	-6.40	105.10	114.39
1	B	174	TYR	N-CA-C	-6.40	101.05	110.52
1	B	444	ARG	NE-CZ-NH1	-6.40	115.10	121.50
1	E	334	LEU	CA-C-O	-6.39	113.77	120.55
1	F	214	ALA	CA-C-O	6.38	126.53	120.09
1	B	243	HIS	CA-CB-CG	6.38	120.18	113.80
1	F	180	GLN	CA-C-O	-6.38	114.41	121.23
1	E	421	VAL	N-CA-C	-6.37	99.25	108.17
1	D	243	HIS	ND1-CE1-NE2	6.37	114.77	108.40
1	C	423	ARG	NE-CZ-NH2	6.36	124.93	119.20
1	B	312	THR	CA-CB-OG1	6.36	119.14	109.60
1	D	372	SER	N-CA-C	-6.36	99.38	109.23
1	B	425	ARG	N-CA-C	-6.33	106.52	114.56
1	F	351	ASP	CA-C-O	-6.33	113.84	120.55
1	B	303	ALA	CA-C-O	6.33	125.76	118.55
1	E	234	GLU	N-CA-CB	6.32	121.01	110.59
1	E	334	LEU	N-CA-CB	6.30	119.39	110.12
1	C	368	VAL	N-CA-C	-6.29	104.37	110.72
1	D	313	GLU	CB-CG-CD	-6.29	101.92	112.60
1	D	343	LYS	N-CA-CB	6.28	121.30	111.56
1	C	206	LEU	CA-C-N	6.27	129.73	120.95
1	C	206	LEU	C-N-CA	6.27	129.73	120.95
1	F	259	THR	CA-C-N	6.27	129.85	120.31
1	F	259	THR	C-N-CA	6.27	129.85	120.31
1	F	435	TYR	CB-CG-CD1	6.27	130.21	120.80
1	E	388	VAL	CA-C-N	6.27	130.58	121.18
1	E	388	VAL	C-N-CA	6.27	130.58	121.18
1	B	199	LEU	O-C-N	-6.26	115.59	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	LEU	CA-C-N	6.26	133.50	121.54
1	B	356	LEU	C-N-CA	6.26	133.50	121.54
1	C	305	GLU	CA-C-N	6.26	128.96	120.44
1	C	305	GLU	C-N-CA	6.26	128.96	120.44
1	D	203	SER	O-C-N	6.26	130.36	123.22
1	A	336	ARG	NE-CZ-NH2	6.26	124.83	119.20
1	E	194	ALA	N-CA-C	-6.25	97.08	108.02
1	D	382	ILE	N-CA-CB	6.23	117.93	110.95
1	C	423	ARG	CA-C-O	6.22	127.22	120.32
1	B	295	LYS	CA-C-N	6.21	127.61	119.84
1	B	295	LYS	C-N-CA	6.21	127.61	119.84
1	A	305	GLU	CA-C-N	6.21	128.89	120.38
1	A	305	GLU	C-N-CA	6.21	128.89	120.38
1	A	373	VAL	CA-C-N	6.21	128.51	120.44
1	A	373	VAL	C-N-CA	6.21	128.51	120.44
1	C	444	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	E	384	GLY	N-CA-C	-6.20	106.77	115.32
1	B	256	THR	CA-CB-OG1	6.20	118.90	109.60
1	B	211	GLU	N-CA-C	-6.19	95.35	108.73
1	B	423	ARG	NE-CZ-NH2	-6.19	113.63	119.20
1	B	386	PRO	N-CA-CB	6.18	108.84	103.27
1	F	281	VAL	CA-C-N	6.18	129.71	120.31
1	F	281	VAL	C-N-CA	6.18	129.71	120.31
1	B	424	GLU	O-C-N	-6.18	114.47	122.94
1	C	428	GLY	O-C-N	6.18	127.65	122.71
1	C	300	LEU	N-CA-C	-6.18	105.43	114.39
1	B	259	THR	CA-CB-OG1	-6.17	100.34	109.60
1	B	287	PHE	CA-C-N	6.17	129.06	120.29
1	B	287	PHE	C-N-CA	6.17	129.06	120.29
1	F	285	GLU	N-CA-C	6.17	118.01	111.28
1	B	331	ARG	NE-CZ-NH2	6.17	124.75	119.20
1	E	255	ILE	N-CA-C	-6.17	99.37	107.88
1	C	332	ARG	CD-NE-CZ	-6.16	115.77	124.40
1	F	367	GLN	N-CA-CB	6.16	120.90	110.49
1	A	332	ARG	CB-CA-C	-6.16	100.57	110.79
1	F	258	GLU	N-CA-C	6.16	118.78	111.33
1	D	257	ASP	CA-C-N	6.15	128.81	120.38
1	D	257	ASP	C-N-CA	6.15	128.81	120.38
1	E	370	ASN	CB-CA-C	6.15	119.22	110.24
1	C	237	GLY	CA-C-O	-6.15	115.50	122.33
1	D	274	ARG	CA-C-N	6.15	128.52	120.28
1	D	274	ARG	C-N-CA	6.15	128.52	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	LEU	N-CA-CB	6.14	122.12	111.13
1	F	202	SER	CA-C-O	6.14	125.53	119.08
1	A	384	GLY	CA-C-O	6.14	127.21	119.72
1	C	379	VAL	CA-CB-CG2	6.13	120.82	110.40
1	D	426	GLN	CB-CG-CD	-6.13	102.19	112.60
1	B	410	ASN	CA-C-O	-6.12	114.19	121.60
1	E	425	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	D	358	GLU	CA-C-N	6.12	132.20	122.59
1	D	358	GLU	C-N-CA	6.12	132.20	122.59
1	C	385	LEU	CB-CA-C	6.12	116.69	109.47
1	C	321	LEU	N-CA-C	-6.11	100.54	110.20
1	D	352	ALA	CA-C-O	-6.11	113.19	120.10
1	C	336	ARG	CA-C-N	6.11	129.07	120.28
1	C	336	ARG	C-N-CA	6.11	129.07	120.28
1	B	293	SER	N-CA-C	-6.10	97.80	110.80
1	A	397	ALA	N-CA-C	-6.08	97.85	110.80
1	B	296	PRO	N-CA-CB	6.08	109.63	103.25
1	E	409	ASP	CA-C-O	6.06	125.45	119.08
1	F	187	GLN	N-CA-C	-6.06	103.08	111.81
1	B	247	TYR	CA-C-N	6.05	131.07	122.72
1	B	247	TYR	C-N-CA	6.05	131.07	122.72
1	D	294	GLY	N-CA-C	-6.05	105.17	115.08
1	C	393	PHE	CA-C-N	6.04	127.40	119.84
1	C	393	PHE	C-N-CA	6.04	127.40	119.84
1	B	371	ASP	N-CA-C	-6.04	101.47	110.23
1	C	319	SER	N-CA-CB	6.04	120.69	110.49
1	A	300	LEU	N-CA-C	-6.03	105.00	112.90
1	D	284	GLU	N-CA-C	6.03	117.85	111.28
1	F	252	LYS	CA-C-O	-6.03	114.59	121.58
1	B	224	THR	CA-C-N	6.02	131.62	122.95
1	B	224	THR	C-N-CA	6.02	131.62	122.95
1	A	226	GLY	N-CA-C	-6.02	98.92	113.18
1	B	330	LEU	N-CA-C	6.01	117.91	111.36
1	A	444	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	B	446	PHE	N-CA-C	-6.00	99.95	109.07
1	F	279	HIS	ND1-CE1-NE2	6.00	114.39	108.40
1	E	310	VAL	N-CA-C	-5.99	99.12	107.80
1	E	405	ILE	CA-C-N	5.99	129.80	120.34
1	E	405	ILE	C-N-CA	5.99	129.80	120.34
1	D	290	GLY	CA-C-N	5.98	128.79	120.29
1	D	290	GLY	C-N-CA	5.98	128.79	120.29
1	E	234	GLU	CB-CA-C	-5.97	101.52	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	376	GLN	O-C-N	5.96	128.44	122.12
1	F	200	PRO	N-CA-CB	-5.96	97.79	103.34
1	F	312	THR	CA-CB-OG1	5.96	118.54	109.60
1	E	230	THR	CA-CB-OG1	5.96	118.54	109.60
1	E	391	GLU	N-CA-C	-5.96	104.20	112.30
1	C	347	ILE	CA-C-O	-5.95	113.69	120.65
1	E	245	SER	CA-C-N	5.95	130.89	122.09
1	E	245	SER	C-N-CA	5.95	130.89	122.09
1	C	218	THR	CA-C-N	5.95	130.93	122.72
1	C	218	THR	C-N-CA	5.95	130.93	122.72
1	F	393	PHE	CA-C-N	5.93	125.95	119.90
1	F	393	PHE	C-N-CA	5.93	125.95	119.90
1	F	421	VAL	N-CA-C	-5.93	99.80	108.11
1	B	265	PHE	N-CA-CB	-5.93	101.93	110.65
1	A	178	PHE	CA-C-N	5.92	129.53	120.82
1	A	178	PHE	C-N-CA	5.92	129.53	120.82
1	B	186	LEU	N-CA-CB	5.92	120.50	110.49
1	C	177	ILE	N-CA-C	-5.91	99.12	107.75
1	A	283	ILE	O-C-N	5.91	127.60	121.87
1	C	341	LEU	N-CA-C	-5.90	99.03	109.06
1	F	429	LYS	N-CA-C	-5.90	100.60	108.74
1	F	225	TYR	O-C-N	5.89	128.36	122.12
1	F	284	GLU	CA-C-O	-5.88	114.18	120.42
1	B	166	SER	N-CA-C	-5.88	100.20	108.96
1	A	349	SER	N-CA-C	5.87	117.68	111.28
1	C	423	ARG	NE-CZ-NH1	-5.87	115.63	121.50
1	C	342	SER	CA-C-O	-5.86	112.13	120.51
1	E	449	GLY	CA-C-N	5.86	132.52	121.97
1	E	449	GLY	C-N-CA	5.86	132.52	121.97
1	D	176	THR	N-CA-C	-5.85	99.80	108.99
1	A	317	ASP	N-CA-CB	5.85	119.02	109.95
1	C	422	GLU	O-C-N	-5.85	116.34	123.30
1	B	393	PHE	CB-CA-C	-5.84	100.28	109.52
1	E	175	GLU	CB-CG-CD	-5.84	102.66	112.60
1	C	273	LYS	N-CA-C	5.84	117.32	111.07
1	F	431	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	B	258	GLU	N-CA-C	5.84	119.22	111.75
1	B	316	ALA	N-CA-C	-5.83	104.39	112.03
1	D	423	ARG	CA-C-O	5.83	127.72	120.54
1	B	242	ILE	N-CA-CB	5.83	120.92	111.36
1	B	194	ALA	N-CA-C	-5.82	96.95	107.60
1	C	365	VAL	CA-C-O	5.82	128.05	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	357	LEU	CA-C-N	-5.82	114.45	122.30
1	D	357	LEU	C-N-CA	-5.82	114.45	122.30
1	E	430	GLN	CA-C-N	5.82	132.17	121.70
1	E	430	GLN	C-N-CA	5.82	132.17	121.70
1	B	185	ASP	CA-C-N	5.81	132.64	121.54
1	B	185	ASP	C-N-CA	5.81	132.64	121.54
1	E	227	THR	N-CA-CB	5.81	120.36	110.71
1	E	261	GLU	CB-CG-CD	-5.81	102.72	112.60
1	F	441	ASN	CA-C-N	-5.80	114.81	122.99
1	F	441	ASN	C-N-CA	-5.80	114.81	122.99
1	C	288	MET	CG-SD-CE	-5.80	88.14	100.90
1	F	209	LEU	N-CA-C	5.79	118.17	108.96
1	D	197	GLU	N-CA-C	-5.79	101.72	110.28
1	C	360	GLU	CA-C-N	5.79	129.10	120.31
1	C	360	GLU	C-N-CA	5.79	129.10	120.31
1	F	223	SER	N-CA-CB	5.79	120.27	110.49
1	B	367	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	D	328	SER	CA-C-O	-5.78	114.43	120.55
1	A	381	ARG	NE-CZ-NH1	-5.77	115.73	121.50
1	C	229	THR	CA-C-O	5.77	126.64	120.24
1	B	278	ALA	CA-C-N	5.77	128.01	120.28
1	B	278	ALA	C-N-CA	5.77	128.01	120.28
1	B	176	THR	N-CA-C	-5.76	98.70	108.26
1	C	261	GLU	O-C-N	5.76	129.78	123.04
1	E	414	PRO	N-CA-C	-5.75	100.62	112.47
1	C	395	ALA	CA-C-O	-5.75	114.42	121.78
1	A	332	ARG	NE-CZ-NH1	-5.75	115.75	121.50
1	A	203	SER	CA-C-N	5.74	128.55	120.28
1	A	203	SER	C-N-CA	5.74	128.55	120.28
1	C	417	ARG	CB-CA-C	5.74	119.56	109.80
1	B	284	GLU	N-CA-C	5.74	117.54	111.28
1	A	396	LYS	N-CA-C	5.74	117.21	111.07
1	E	205	ILE	N-CA-C	-5.74	100.03	108.23
1	D	304	SER	CA-CB-OG	5.73	122.57	111.10
1	A	281	VAL	O-C-N	-5.73	116.31	121.87
1	A	327	ILE	N-CA-CB	5.73	118.33	110.54
1	E	411	PHE	CA-C-N	5.73	132.29	122.67
1	E	411	PHE	C-N-CA	5.73	132.29	122.67
1	F	299	LEU	N-CA-C	-5.72	105.12	111.36
1	E	251	ALA	CA-C-O	-5.72	115.15	121.33
1	B	300	LEU	CA-C-O	5.71	126.54	119.97
1	B	367	GLN	CG-CD-NE2	5.71	124.97	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	HIS	CA-C-N	5.70	127.91	120.28
1	B	279	HIS	C-N-CA	5.70	127.91	120.28
1	A	385	LEU	O-C-N	-5.69	116.33	121.39
1	B	343	LYS	N-CA-C	-5.69	100.29	108.60
1	C	393	PHE	O-C-N	5.69	127.16	121.30
1	B	187	GLN	CA-C-O	5.69	125.31	119.97
1	D	228	ASP	CB-CA-C	-5.68	101.53	110.85
1	F	309	LYS	N-CA-CB	5.68	120.55	111.91
1	F	389	VAL	CB-CA-C	-5.68	103.71	111.33
1	A	225	TYR	CB-CA-C	-5.68	100.58	110.17
1	E	237	GLY	N-CA-C	-5.68	101.77	112.10
1	D	387	VAL	N-CA-CB	-5.68	104.53	110.72
1	A	311	VAL	N-CA-C	-5.67	100.90	108.96
1	B	221	ALA	CB-CA-C	-5.67	100.02	109.55
1	B	391	GLU	N-CA-C	-5.67	103.86	112.99
1	B	331	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	C	331	ARG	O-C-N	5.67	128.12	122.12
1	A	431	ARG	N-CA-CB	5.66	120.06	110.49
1	E	305	GLU	CA-C-N	5.66	127.87	120.28
1	E	305	GLU	C-N-CA	5.66	127.87	120.28
1	B	279	HIS	CE1-NE2-CD2	-5.66	103.34	109.00
1	C	268	LEU	N-CA-C	5.66	120.60	113.25
1	C	350	MET	CA-C-N	5.66	127.86	120.28
1	C	350	MET	C-N-CA	5.66	127.86	120.28
1	F	309	LYS	O-C-N	5.66	129.37	122.58
1	D	363	GLN	CB-CG-CD	-5.65	102.99	112.60
1	E	328	SER	CA-C-N	5.65	127.86	120.28
1	E	328	SER	C-N-CA	5.65	127.86	120.28
1	D	288	MET	N-CA-CB	5.65	118.27	110.07
1	E	206	LEU	CA-C-O	5.65	127.38	120.60
1	F	230	THR	CA-C-N	5.65	132.34	121.54
1	F	230	THR	C-N-CA	5.65	132.34	121.54
1	C	393	PHE	CA-C-O	-5.65	114.30	120.17
1	C	321	LEU	N-CA-CB	5.64	118.58	110.06
1	D	365	VAL	N-CA-C	-5.64	107.48	112.90
1	D	445	TYR	N-CA-C	-5.64	107.04	114.04
1	E	287	PHE	N-CA-CB	5.64	118.51	110.16
1	F	367	GLN	CA-C-N	5.64	132.13	121.97
1	F	367	GLN	C-N-CA	5.64	132.13	121.97
1	F	317	ASP	N-CA-C	-5.64	99.23	108.76
1	A	331	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	B	288	MET	CA-C-O	-5.64	114.44	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	PHE	CB-CG-CD1	-5.64	111.12	120.70
1	F	299	LEU	CB-CA-C	-5.64	101.27	110.85
1	D	413	MET	O-C-N	-5.63	115.89	121.19
1	C	416	GLN	CB-CG-CD	5.63	122.18	112.60
1	A	319	SER	N-CA-CB	5.63	120.00	110.49
1	D	420	THR	N-CA-C	-5.62	100.75	109.24
1	A	415	ARG	CA-C-O	-5.62	114.44	120.46
1	B	232	GLY	CA-C-N	5.62	132.27	121.54
1	B	232	GLY	C-N-CA	5.62	132.27	121.54
1	C	198	GLU	O-C-N	-5.62	115.71	123.01
1	A	308	ALA	CA-C-N	5.61	130.93	122.68
1	A	308	ALA	C-N-CA	5.61	130.93	122.68
1	A	337	HIS	CE1-NE2-CD2	-5.61	103.39	109.00
1	B	417	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	B	410	ASN	N-CA-C	5.61	117.77	109.69
1	E	262	ASP	N-CA-CB	5.61	119.97	110.49
1	E	407	TYR	CA-C-N	5.61	129.84	120.70
1	E	407	TYR	C-N-CA	5.61	129.84	120.70
1	C	272	ARG	N-CA-CB	5.61	118.36	110.12
1	B	390	SER	CA-C-N	5.60	129.59	120.23
1	B	390	SER	C-N-CA	5.60	129.59	120.23
1	B	222	ALA	CA-C-N	5.60	130.81	122.74
1	B	222	ALA	C-N-CA	5.60	130.81	122.74
1	D	364	ASP	N-CA-CB	5.60	119.96	110.49
1	E	431	ARG	N-CA-CB	5.60	120.02	110.50
1	E	348	VAL	CA-CB-CG2	5.60	119.92	110.40
1	A	224	THR	CA-C-O	5.60	127.31	121.38
1	E	452	SER	N-CA-C	-5.60	101.63	109.69
1	D	448	ASN	CA-CB-CG	-5.59	107.00	112.60
1	A	295	LYS	O-C-N	5.59	125.73	121.65
1	F	431	ARG	N-CA-CB	5.59	120.01	110.50
1	E	334	LEU	CB-CA-C	-5.58	101.52	110.79
1	A	402	PHE	N-CA-C	-5.58	100.68	109.50
1	A	373	VAL	CG1-CB-CG2	-5.58	98.53	110.80
1	E	202	SER	CA-C-N	5.57	129.69	120.94
1	E	202	SER	C-N-CA	5.57	129.69	120.94
1	F	451	VAL	CA-C-O	5.57	126.50	120.43
1	C	183	ILE	N-CA-C	-5.57	100.57	109.20
1	C	404	VAL	O-C-N	5.57	128.97	123.18
1	E	176	THR	N-CA-C	-5.57	99.01	108.26
1	F	291	ASP	N-CA-C	-5.56	106.49	113.28
1	F	248	LYS	CA-C-O	5.56	126.71	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	LYS	CA-C-O	5.56	126.60	120.71
1	C	387	VAL	CA-C-N	-5.55	116.48	122.59
1	C	387	VAL	C-N-CA	-5.55	116.48	122.59
1	C	284	GLU	CA-C-N	5.55	128.03	120.54
1	C	284	GLU	C-N-CA	5.55	128.03	120.54
1	F	440	VAL	CA-C-O	-5.55	115.89	121.49
1	C	363	GLN	OE1-CD-NE2	5.54	128.14	122.60
1	B	319	SER	N-CA-CB	5.54	119.84	110.49
1	F	393	PHE	N-CA-CB	5.54	118.77	110.02
1	C	385	LEU	N-CA-C	-5.53	101.01	109.64
1	A	205	ILE	CA-C-N	5.53	130.57	122.77
1	A	205	ILE	C-N-CA	5.53	130.57	122.77
1	C	367	GLN	CA-C-O	5.53	128.42	120.51
1	F	332	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	D	432	ASP	O-C-N	-5.52	116.85	123.31
1	C	450	VAL	N-CA-C	-5.52	100.53	108.42
1	F	374	LYS	CA-C-N	5.52	128.13	120.29
1	F	374	LYS	C-N-CA	5.52	128.13	120.29
1	B	405	ILE	N-CA-CB	5.52	120.34	111.23
1	D	336	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	F	395	ALA	CA-C-N	5.51	127.94	120.44
1	F	395	ALA	C-N-CA	5.51	127.94	120.44
1	A	395	ALA	CA-C-N	5.51	127.61	120.44
1	A	395	ALA	C-N-CA	5.51	127.61	120.44
1	C	397	ALA	N-CA-C	-5.51	99.06	110.80
1	E	393	PHE	CA-CB-CG	-5.51	108.29	113.80
1	D	284	GLU	O-C-N	5.50	127.95	122.12
1	E	239	LEU	O-C-N	-5.50	116.04	122.96
1	B	322	VAL	CA-CB-CG1	-5.49	101.07	110.40
1	D	304	SER	CA-C-N	5.48	129.37	120.60
1	D	304	SER	C-N-CA	5.48	129.37	120.60
1	D	378	GLN	N-CA-C	-5.48	104.15	112.04
1	A	424	GLU	N-CA-CB	5.47	120.49	111.62
1	C	334	LEU	N-CA-CB	5.47	117.94	110.01
1	C	260	GLU	CA-C-N	5.47	129.32	121.50
1	C	260	GLU	C-N-CA	5.47	129.32	121.50
1	E	281	VAL	N-CA-C	5.47	115.67	110.42
1	E	425	ARG	CD-NE-CZ	-5.47	116.75	124.40
1	F	311	VAL	O-C-N	-5.46	115.74	122.57
1	D	374	LYS	CA-C-N	5.46	127.87	120.44
1	D	374	LYS	C-N-CA	5.46	127.87	120.44
1	E	453	GLY	N-CA-C	-5.46	101.31	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	275	LEU	N-CA-C	5.46	117.23	111.28
1	B	230	THR	CA-CB-OG1	5.46	117.78	109.60
1	F	219	TRP	CB-CA-C	-5.45	99.51	109.54
1	A	278	ALA	N-CA-C	5.45	117.22	111.28
1	F	403	ALA	N-CA-CB	5.45	120.22	110.80
1	C	389	VAL	CB-CA-C	-5.44	103.20	111.69
1	F	174	TYR	N-CA-CB	5.44	118.64	109.94
1	A	274	ARG	CA-C-N	5.43	127.56	120.28
1	A	274	ARG	C-N-CA	5.43	127.56	120.28
1	E	224	THR	N-CA-C	-5.43	101.25	108.74
1	B	448	ASN	N-CA-C	-5.42	105.98	112.59
1	C	323	THR	N-CA-C	5.42	116.87	111.07
1	C	245	SER	CA-C-N	5.41	128.92	120.75
1	C	245	SER	C-N-CA	5.41	128.92	120.75
1	F	245	SER	CA-C-O	-5.41	114.97	120.71
1	A	259	THR	CA-C-N	5.41	128.53	120.31
1	A	259	THR	C-N-CA	5.41	128.53	120.31
1	E	423	ARG	CA-C-N	5.41	131.02	122.36
1	E	423	ARG	C-N-CA	5.41	131.02	122.36
1	C	281	VAL	N-CA-CB	5.41	116.88	110.55
1	C	178	PHE	CA-C-N	5.40	131.86	121.54
1	C	178	PHE	C-N-CA	5.40	131.86	121.54
1	A	320	VAL	CA-C-O	5.40	127.53	120.78
1	A	206	LEU	CB-CA-C	-5.39	101.52	110.14
1	A	376	GLN	CB-CA-C	-5.39	101.85	110.79
1	F	413	MET	CB-CA-C	-5.38	104.84	110.17
1	A	276	ILE	CA-C-N	5.38	127.94	120.29
1	A	276	ILE	C-N-CA	5.38	127.94	120.29
1	F	424	GLU	CA-CB-CG	5.38	124.86	114.10
1	A	221	ALA	N-CA-CB	5.38	118.28	110.26
1	B	230	THR	N-CA-CB	5.38	120.29	111.31
1	C	220	VAL	N-CA-C	-5.38	100.91	108.27
1	D	176	THR	O-C-N	-5.37	117.26	123.33
1	D	300	LEU	CA-C-N	5.37	127.48	120.28
1	D	300	LEU	C-N-CA	5.37	127.48	120.28
1	E	276	ILE	CA-C-N	5.37	127.42	120.44
1	E	276	ILE	C-N-CA	5.37	127.42	120.44
1	C	258	GLU	CA-C-O	5.37	126.43	120.63
1	B	166	SER	N-CA-CB	5.37	120.04	111.56
1	F	402	PHE	N-CA-C	-5.37	101.13	109.24
1	B	291	ASP	O-C-N	-5.36	116.51	122.09
1	B	350	MET	CA-C-N	5.36	127.47	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	MET	C-N-CA	5.36	127.47	120.28
1	D	327	ILE	N-CA-CB	5.36	117.83	110.54
1	D	362	TRP	N-CA-CB	5.36	119.55	110.49
1	A	243	HIS	CG-CD2-NE2	5.36	112.56	107.20
1	A	425	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	B	391	GLU	CB-CG-CD	-5.35	103.50	112.60
1	F	218	THR	CA-C-N	5.35	129.34	120.94
1	F	218	THR	C-N-CA	5.35	129.34	120.94
1	A	425	ARG	N-CA-C	-5.34	107.78	114.56
1	E	364	ASP	N-CA-CB	5.33	119.51	110.49
1	C	267	LEU	N-CA-C	5.33	116.78	111.07
1	A	396	LYS	O-C-N	5.33	127.56	122.07
1	B	254	PHE	N-CA-C	-5.33	100.62	108.99
1	B	371	ASP	N-CA-CB	5.33	117.87	109.83
1	C	294	GLY	CA-C-O	5.33	125.03	119.06
1	A	287	PHE	CB-CA-C	-5.32	101.80	110.85
1	C	324	ALA	CB-CA-C	-5.32	101.96	110.79
1	D	417	ARG	N-CA-C	-5.31	98.92	108.48
1	F	362	TRP	CA-CB-CG	5.31	123.69	113.60
1	B	237	GLY	CA-C-O	-5.31	116.12	121.64
1	B	262	ASP	N-CA-CB	5.31	119.46	110.49
1	F	219	TRP	N-CA-CB	5.31	117.81	110.17
1	C	215	GLY	O-C-N	-5.30	117.59	123.05
1	F	389	VAL	N-CA-CB	5.30	116.71	110.82
1	B	381	ARG	NE-CZ-NH1	-5.30	116.20	121.50
1	A	398	ASN	CA-C-O	5.29	125.47	119.18
1	D	426	GLN	CA-CB-CG	5.29	124.68	114.10
1	A	233	GLU	N-CA-CB	-5.29	102.56	110.17
1	F	218	THR	N-CA-CB	5.29	119.59	111.24
1	E	279	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
1	A	416	GLN	CB-CG-CD	5.27	121.56	112.60
1	B	218	THR	N-CA-C	-5.27	100.73	108.79
1	F	198	GLU	CA-C-O	-5.27	114.87	120.40
1	A	268	LEU	N-CA-C	5.26	120.77	113.45
1	E	296	PRO	CA-C-N	5.26	128.82	121.24
1	E	296	PRO	C-N-CA	5.26	128.82	121.24
1	E	306	ASP	CA-C-O	-5.26	114.98	120.55
1	F	218	THR	CA-C-O	-5.26	115.69	121.31
1	C	369	GLY	CA-C-N	5.25	131.57	121.54
1	C	369	GLY	C-N-CA	5.25	131.57	121.54
1	F	388	VAL	CA-C-O	5.25	127.19	121.04
1	A	182	ILE	CB-CA-C	-5.25	104.03	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	181	ARG	N-CA-CB	5.25	119.36	110.49
1	D	213	ASP	CA-C-O	-5.25	115.12	120.89
1	A	272	ARG	N-CA-CB	5.24	117.83	110.12
1	A	441	ASN	O-C-N	-5.24	116.35	122.96
1	B	337	HIS	CA-CB-CG	-5.24	108.56	113.80
1	A	167	VAL	CA-C-N	5.24	132.00	123.93
1	A	167	VAL	C-N-CA	5.24	132.00	123.93
1	A	322	VAL	CA-C-O	-5.24	116.33	121.67
1	D	324	ALA	CA-C-N	5.24	127.30	120.28
1	D	324	ALA	C-N-CA	5.24	127.30	120.28
1	D	241	GLU	CA-C-O	5.23	126.95	121.19
1	C	175	GLU	N-CA-C	5.23	121.94	110.80
1	C	263	ALA	CA-C-N	5.23	130.00	123.14
1	C	263	ALA	C-N-CA	5.23	130.00	123.14
1	C	405	ILE	CA-C-N	5.23	128.10	120.98
1	C	405	ILE	C-N-CA	5.23	128.10	120.98
1	C	272	ARG	O-C-N	-5.23	116.58	122.12
1	C	428	GLY	CA-C-N	5.23	130.73	122.36
1	C	428	GLY	C-N-CA	5.23	130.73	122.36
1	F	315	LYS	N-CA-C	-5.23	104.64	112.54
1	E	418	ALA	N-CA-C	-5.23	103.13	110.50
1	D	200	PRO	N-CA-CB	5.23	108.20	103.34
1	E	331	ARG	CB-CA-C	-5.23	102.11	110.79
1	F	336	ARG	N-CA-CB	-5.23	102.89	110.47
1	B	366	ALA	N-CA-C	5.22	119.71	113.23
1	C	173	SER	CA-C-O	5.22	125.81	119.38
1	E	351	ASP	CA-CB-CG	-5.22	107.38	112.60
1	E	441	ASN	N-CA-C	5.22	115.43	108.38
1	F	413	MET	CA-C-O	-5.22	114.97	119.36
1	D	351	ASP	CA-C-O	-5.22	115.02	120.55
1	E	390	SER	N-CA-C	-5.22	101.36	109.24
1	F	393	PHE	CA-C-O	-5.22	114.61	120.25
1	C	409	ASP	CA-CB-CG	-5.22	107.38	112.60
1	F	285	GLU	CA-C-N	5.22	127.70	120.29
1	F	285	GLU	C-N-CA	5.22	127.70	120.29
1	D	453	GLY	N-CA-C	-5.21	103.15	110.91
1	C	343	LYS	N-CA-CB	5.21	119.63	111.56
1	C	438	GLN	O-C-N	-5.21	117.44	123.33
1	C	302	LEU	N-CA-CB	5.21	118.02	110.26
1	E	224	THR	CA-CB-OG1	5.21	117.41	109.60
1	E	268	LEU	O-C-N	-5.21	115.55	120.70
1	F	419	VAL	CA-CB-CG1	5.20	119.25	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	422	GLU	N-CA-C	-5.20	101.39	109.72
1	B	276	ILE	CA-C-N	5.20	127.20	120.44
1	B	276	ILE	C-N-CA	5.20	127.20	120.44
1	C	257	ASP	CA-C-N	5.20	127.50	120.38
1	C	257	ASP	C-N-CA	5.20	127.50	120.38
1	D	323	THR	O-C-N	-5.20	116.61	122.12
1	E	231	THR	N-CA-C	5.20	117.03	110.33
1	D	368	VAL	CA-C-N	5.19	131.59	121.41
1	D	368	VAL	C-N-CA	5.19	131.59	121.41
1	E	422	GLU	O-C-N	-5.19	116.44	123.19
1	A	411	PHE	CB-CA-C	-5.19	100.08	110.42
1	D	244	PHE	CB-CG-CD1	5.19	129.53	120.70
1	D	410	ASN	CA-C-N	5.19	130.96	122.81
1	D	410	ASN	C-N-CA	5.19	130.96	122.81
1	D	230	THR	CA-CB-OG1	5.19	117.38	109.60
1	B	201	MET	CA-C-O	-5.18	115.91	121.45
1	E	283	ILE	N-CA-C	5.18	115.39	110.42
1	A	439	ARG	CB-CG-CD	5.18	123.21	111.30
1	F	402	PHE	CA-C-N	-5.17	114.77	122.74
1	F	402	PHE	C-N-CA	-5.17	114.77	122.74
1	E	303	ALA	N-CA-C	-5.17	105.02	113.19
1	E	439	ARG	CA-C-N	-5.17	115.74	122.51
1	E	439	ARG	C-N-CA	-5.17	115.74	122.51
1	F	432	ASP	CA-CB-CG	-5.17	107.43	112.60
1	C	285	GLU	CB-CG-CD	-5.17	103.81	112.60
1	B	451	VAL	CA-CB-CG2	-5.17	101.62	110.40
1	B	337	HIS	CG-CD2-NE2	5.16	112.36	107.20
1	C	426	GLN	O-C-N	-5.16	117.19	123.13
1	C	426	GLN	CB-CG-CD	-5.16	103.82	112.60
1	A	337	HIS	CG-CD2-NE2	5.16	112.36	107.20
1	A	434	TYR	CB-CG-CD2	-5.16	113.06	120.80
1	C	174	TYR	CA-C-N	5.16	131.39	121.54
1	C	174	TYR	C-N-CA	5.16	131.39	121.54
1	F	214	ALA	CA-C-N	5.15	128.91	121.44
1	F	214	ALA	C-N-CA	5.15	128.91	121.44
1	C	293	SER	CA-C-O	-5.15	115.19	120.54
1	C	374	LYS	CB-CA-C	-5.15	102.24	110.79
1	B	427	ALA	CA-C-N	5.14	131.49	121.41
1	B	427	ALA	C-N-CA	5.14	131.49	121.41
1	C	171	SER	CA-C-N	5.14	127.68	120.28
1	C	171	SER	C-N-CA	5.14	127.68	120.28
1	E	323	THR	CA-C-N	5.14	127.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	323	THR	C-N-CA	5.14	127.17	120.28
1	E	166	SER	N-CA-C	-5.14	102.59	110.14
1	A	328	SER	CA-C-N	5.13	127.16	120.28
1	A	328	SER	C-N-CA	5.13	127.16	120.28
1	A	383	TYR	CA-C-N	5.13	130.06	120.87
1	A	383	TYR	C-N-CA	5.13	130.06	120.87
1	F	175	GLU	N-CA-CB	5.13	119.16	110.49
1	A	323	THR	N-CA-C	5.12	116.55	111.07
1	B	378	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	F	381	ARG	O-C-N	5.12	129.67	123.01
1	A	253	SER	CA-C-N	5.12	130.38	123.11
1	A	253	SER	C-N-CA	5.12	130.38	123.11
1	C	347	ILE	CA-C-N	5.12	127.75	120.53
1	C	347	ILE	C-N-CA	5.12	127.75	120.53
1	E	255	ILE	O-C-N	-5.12	118.51	122.97
1	A	199	LEU	CB-CA-C	5.12	115.69	109.85
1	F	224	THR	N-CA-C	-5.12	101.12	108.60
1	F	282	SER	CA-C-N	5.12	127.01	120.56
1	F	282	SER	C-N-CA	5.12	127.01	120.56
1	A	339	LEU	N-CA-CB	5.12	118.75	110.41
1	C	398	ASN	O-C-N	-5.12	115.86	122.21
1	A	295	LYS	N-CA-C	-5.12	102.32	108.25
1	B	330	LEU	CA-C-N	5.12	127.13	120.28
1	B	330	LEU	C-N-CA	5.12	127.13	120.28
1	C	285	GLU	CA-C-O	-5.11	115.43	120.90
1	E	329	LYS	N-CA-C	5.11	116.85	111.28
1	B	395	ALA	CB-CA-C	-5.11	99.59	109.76
1	C	192	VAL	N-CA-CB	5.11	119.66	111.23
1	C	271	LEU	CA-C-N	5.11	127.12	120.28
1	C	271	LEU	C-N-CA	5.11	127.12	120.28
1	B	191	VAL	CA-C-N	5.10	131.15	121.97
1	B	191	VAL	C-N-CA	5.10	131.15	121.97
1	E	450	VAL	CG1-CB-CG2	5.10	122.02	110.80
1	C	297	LYS	O-C-N	-5.10	116.84	122.86
1	C	180	GLN	CA-C-O	-5.10	115.28	120.89
1	A	409	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	277	GLU	N-CA-CB	5.09	117.70	110.16
1	D	196	PHE	CA-CB-CG	-5.09	108.71	113.80
1	C	277	GLU	CA-C-N	5.09	127.10	120.28
1	C	277	GLU	C-N-CA	5.09	127.10	120.28
1	F	177	ILE	N-CA-C	-5.09	99.93	107.51
1	F	319	SER	O-C-N	5.08	129.84	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	ILE	CA-C-N	5.08	127.35	120.44
1	C	276	ILE	C-N-CA	5.08	127.35	120.44
1	A	289	THR	CA-C-O	5.08	127.07	120.11
1	F	185	ASP	N-CA-C	-5.08	101.87	109.95
1	A	268	LEU	CA-C-O	-5.08	113.66	118.33
1	B	206	LEU	CA-C-O	-5.08	114.86	120.30
1	B	257	ASP	CA-C-N	5.08	127.80	120.38
1	B	257	ASP	C-N-CA	5.08	127.80	120.38
1	C	249	LEU	N-CA-C	-5.08	101.48	109.50
1	F	264	ILE	N-CA-C	-5.08	101.00	108.11
1	E	454	THR	N-CA-C	-5.08	100.14	108.41
1	A	165	SER	O-C-N	5.07	129.07	122.89
1	B	340	LYS	CA-C-O	5.06	128.19	121.46
1	A	281	VAL	CA-C-O	5.06	126.21	120.95
1	F	337	HIS	CE1-NE2-CD2	-5.06	103.94	109.00
1	A	271	LEU	CA-C-N	5.05	127.05	120.28
1	A	271	LEU	C-N-CA	5.05	127.05	120.28
1	F	270	LEU	CB-CA-C	-5.05	102.31	110.79
1	E	248	LYS	N-CA-C	-5.05	100.68	108.90
1	E	258	GLU	N-CA-C	5.05	121.55	110.80
1	D	310	VAL	N-CA-C	-5.04	100.39	107.75
1	A	428	GLY	N-CA-C	-5.04	107.89	113.79
1	C	329	LYS	CA-C-N	5.04	127.45	120.29
1	C	329	LYS	C-N-CA	5.04	127.45	120.29
1	E	356	LEU	CA-C-N	5.04	131.17	121.54
1	E	356	LEU	C-N-CA	5.04	131.17	121.54
1	B	220	VAL	O-C-N	5.04	127.38	122.69
1	A	378	GLN	CA-C-N	5.03	127.57	120.42
1	A	378	GLN	C-N-CA	5.03	127.57	120.42
1	A	271	LEU	CA-C-O	-5.03	115.22	120.55
1	C	452	SER	N-CA-C	-5.03	102.45	109.69
1	E	425	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	F	232	GLY	CA-C-O	-5.03	117.25	122.28
1	A	401	GLU	N-CA-CB	5.02	117.33	109.85
1	E	405	ILE	N-CA-C	-5.02	98.89	109.34
1	E	168	GLU	CA-C-O	5.02	127.69	120.51
1	E	410	ASN	CB-CA-C	-5.02	105.43	114.52
1	C	333	LYS	CA-C-N	5.02	126.96	120.44
1	C	333	LYS	C-N-CA	5.02	126.96	120.44
1	B	387	VAL	N-CA-CB	5.01	116.56	110.95
1	B	425	ARG	NE-CZ-NH1	-5.01	116.49	121.50
1	A	432	ASP	N-CA-CB	5.01	119.47	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	VAL	CA-CB-CG2	5.01	118.92	110.40
1	F	293	SER	CA-C-N	5.01	131.11	122.05
1	F	293	SER	C-N-CA	5.01	131.11	122.05
1	C	260	GLU	CB-CA-C	-5.01	102.34	110.85
1	D	231	THR	CA-C-N	5.00	127.57	121.06
1	D	231	THR	C-N-CA	5.00	127.57	121.06
1	A	336	ARG	N-CA-CB	-5.00	102.08	110.39
1	C	358	GLU	CA-C-O	5.00	126.76	121.16

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	225	TYR	Sidechain
1	A	247	TYR	Sidechain
1	A	261	GLU	Peptide
1	A	272	ARG	Sidechain
1	A	274	ARG	Sidechain
1	A	331	ARG	Sidechain
1	A	415	ARG	Sidechain
1	A	423	ARG	Sidechain
1	A	430	GLN	Peptide
1	A	444	ARG	Sidechain
1	B	196	PHE	Sidechain
1	B	247	TYR	Sidechain
1	B	407	TYR	Sidechain
1	B	411	PHE	Sidechain
1	B	417	ARG	Sidechain
1	B	423	ARG	Sidechain
1	B	434	TYR	Sidechain
1	B	439	ARG	Sidechain
1	B	444	ARG	Sidechain
1	B	455	TYR	Sidechain
1	C	272	ARG	Sidechain
1	C	353	TYR	Sidechain
1	C	381	ARG	Sidechain
1	C	392	TYR	Sidechain
1	C	425	ARG	Sidechain
1	C	435	TYR	Sidechain
1	C	455	TYR	Sidechain
1	D	178	PHE	Sidechain
1	D	196	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	D	215	GLY	Peptide
1	D	247	TYR	Sidechain
1	D	332	ARG	Sidechain
1	D	354	TYR	Sidechain
1	D	411	PHE	Sidechain
1	E	174	TYR	Sidechain
1	E	211	GLU	Peptide
1	E	225	TYR	Sidechain
1	E	236	LYS	Peptide
1	E	238	ALA	Peptide
1	E	239	LEU	Peptide
1	E	243	HIS	Sidechain
1	E	254	PHE	Peptide
1	E	274	ARG	Sidechain
1	E	287	PHE	Sidechain
1	E	336	ARG	Sidechain
1	E	381	ARG	Sidechain
1	E	393	PHE	Peptide
1	E	435	TYR	Sidechain
1	F	174	TYR	Sidechain
1	F	196	PHE	Sidechain
1	F	225	TYR	Sidechain
1	F	239	LEU	Peptide
1	F	435	TYR	Sidechain
1	F	439	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2271	2300	2281	563	0
1	B	2271	2300	2282	603	0
1	C	2271	2300	2279	626	0
1	D	2271	2300	2291	664	0
1	E	2271	2300	2287	627	0
1	F	2271	2300	2289	561	0
All	All	13626	13800	13709	1842	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 67.

All (1842) 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)
1:D:216:LYS:CG	1:E:278:ALA:HB2	1.21	1.67
1:A:178:PHE:CD2	1:F:207:THR:CG2	1.74	1.64
1:C:217:ALA:CB	1:D:279:HIS:HB2	1.16	1.64
1:D:207:THR:H	1:E:177:ILE:CB	1.02	1.62
1:C:235:VAL:CG2	1:D:271:LEU:HD11	1.23	1.61
1:A:235:VAL:HG23	1:B:271:LEU:CD2	1.20	1.59
1:D:216:LYS:HG3	1:E:278:ALA:CB	1.17	1.59
1:C:216:LYS:HE3	1:D:278:ALA:CB	1.33	1.58
1:B:220:VAL:CG2	1:C:437:THR:HG22	1.23	1.58
1:C:220:VAL:HB	1:D:250:ALA:CB	1.30	1.57
1:C:221:ALA:HA	1:D:248:LYS:CB	1.24	1.57
1:E:211:GLU:CG	1:F:182:ILE:HD12	1.30	1.56
1:A:362:TRP:HH2	1:B:362:TRP:CD1	1.24	1.55
1:A:178:PHE:CD2	1:F:207:THR:HG22	1.30	1.55
1:A:215:GLY:CA	1:B:271:LEU:HD12	1.27	1.54
1:E:211:GLU:HG2	1:F:182:ILE:CD1	1.24	1.54
1:E:213:ASP:HA	1:F:274:ARG:CD	1.11	1.54
1:E:213:ASP:CG	1:F:274:ARG:HD3	1.29	1.53
1:C:217:ALA:HB3	1:D:279:HIS:CB	1.37	1.53
1:E:214:ALA:CB	1:F:271:LEU:HA	1.09	1.53
1:A:178:PHE:CE2	1:F:207:THR:HG21	1.42	1.52
1:A:275:LEU:CD2	1:F:216:LYS:N	1.70	1.52
1:D:211:GLU:C	1:E:182:ILE:HG12	1.13	1.52
1:B:217:ALA:H	1:C:275:LEU:CD2	1.17	1.52
1:A:220:VAL:CG2	1:B:252:LYS:HG2	1.40	1.51
1:A:250:ALA:H	1:F:219:TRP:CB	1.04	1.51
1:D:211:GLU:C	1:E:182:ILE:CG1	1.83	1.50
1:E:241:GLU:CG	1:F:179:SER:HB3	1.36	1.50
1:A:271:LEU:CD1	1:F:236:LYS:H	1.18	1.50
1:D:217:ALA:H	1:E:278:ALA:CB	1.24	1.49
1:E:213:ASP:C	1:F:274:ARG:HG3	1.22	1.49
1:D:217:ALA:N	1:E:278:ALA:HB3	1.17	1.48
1:E:232:GLY:C	1:F:252:LYS:HB2	1.36	1.48
1:C:219:TRP:CZ2	1:D:282:SER:O	1.67	1.48
1:E:210:VAL:CA	1:F:182:ILE:HA	1.38	1.47
1:D:235:VAL:HG21	1:E:255:ILE:CG1	1.44	1.47
1:E:232:GLY:CA	1:F:252:LYS:HB2	1.45	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:VAL:CB	1:D:250:ALA:HB3	1.41	1.47
1:D:212:PRO:CA	1:E:182:ILE:HD13	1.42	1.47
1:E:214:ALA:H	1:F:274:ARG:CB	1.28	1.47
1:E:220:VAL:HG11	1:F:435:TYR:CE1	1.50	1.47
1:E:217:ALA:CB	1:F:279:HIS:HB2	1.38	1.46
1:C:213:ASP:CA	1:D:274:ARG:HD3	1.20	1.46
1:A:271:LEU:CD1	1:F:236:LYS:N	1.72	1.45
1:E:234:GLU:N	1:F:253:SER:CA	1.72	1.45
1:E:232:GLY:C	1:F:252:LYS:CB	1.89	1.45
1:A:215:GLY:N	1:B:271:LEU:CD1	1.80	1.44
1:B:212:PRO:CB	1:C:183:ILE:O	1.63	1.44
1:A:220:VAL:HG23	1:B:251:ALA:C	1.36	1.44
1:B:220:VAL:HG21	1:C:437:THR:CG2	1.46	1.44
1:D:233:GLU:OE1	1:E:433:ALA:CA	1.65	1.44
1:A:220:VAL:HG22	1:B:252:LYS:CG	1.43	1.43
1:D:233:GLU:OE1	1:E:433:ALA:CB	1.64	1.43
1:E:214:ALA:N	1:F:274:ARG:HG3	1.24	1.43
1:A:215:GLY:CA	1:B:271:LEU:CD1	1.95	1.42
1:E:210:VAL:HA	1:F:182:ILE:CA	1.46	1.42
1:E:233:GLU:N	1:F:252:LYS:CB	1.81	1.42
1:C:214:ALA:CB	1:D:271:LEU:HA	1.46	1.42
1:E:241:GLU:HG3	1:F:179:SER:CB	1.47	1.42
1:C:331:ARG:CZ	1:D:376:GLN:NE2	1.83	1.42
1:A:233:GLU:HG2	1:B:434:TYR:N	1.10	1.41
1:A:361:GLU:HG2	1:B:363:GLN:CD	1.43	1.41
1:C:216:LYS:N	1:D:275:LEU:HA	1.26	1.41
1:D:217:ALA:N	1:E:278:ALA:CB	1.79	1.41
1:D:211:GLU:CA	1:E:182:ILE:HG12	1.20	1.41
1:A:331:ARG:NH1	1:B:355:ASP:HB3	1.29	1.40
1:E:214:ALA:N	1:F:274:ARG:CG	1.85	1.39
1:C:233:GLU:OE1	1:D:252:LYS:CB	1.71	1.39
1:B:210:VAL:HG12	1:C:182:ILE:CA	1.53	1.38
1:D:235:VAL:CA	1:E:271:LEU:HD11	1.51	1.38
1:C:221:ALA:CA	1:D:248:LYS:HB2	1.53	1.38
1:E:213:ASP:OD1	1:F:274:ARG:CD	1.66	1.38
1:A:331:ARG:HH12	1:B:355:ASP:CB	1.36	1.37
1:E:213:ASP:CA	1:F:274:ARG:CD	2.00	1.37
1:E:214:ALA:CB	1:F:271:LEU:CA	2.00	1.37
1:A:362:TRP:CH2	1:B:362:TRP:CD1	2.11	1.36
1:A:235:VAL:CG2	1:B:271:LEU:HD22	1.54	1.36
1:D:214:ALA:H	1:E:274:ARG:CG	1.37	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ILE:N	1:F:211:GLU:O	1.58	1.35
1:D:237:GLY:HA2	1:E:267:LEU:CD1	1.57	1.35
1:C:220:VAL:CG2	1:D:250:ALA:O	1.73	1.34
1:D:207:THR:OG1	1:E:177:ILE:N	1.60	1.34
1:A:176:THR:HA	1:F:205:ILE:CG2	1.55	1.34
1:D:233:GLU:CD	1:E:434:TYR:N	1.86	1.34
1:B:233:GLU:OE1	1:C:433:ALA:CB	1.72	1.34
1:A:235:VAL:CG2	1:B:271:LEU:CD2	2.04	1.34
1:A:217:ALA:CA	1:B:275:LEU:HB3	1.45	1.34
1:C:235:VAL:HG23	1:D:271:LEU:CD1	1.56	1.34
1:A:217:ALA:CB	1:B:275:LEU:HB3	1.56	1.33
1:B:213:ASP:O	1:C:274:ARG:NH2	1.59	1.33
1:C:218:THR:HG22	1:D:251:ALA:CB	1.55	1.33
1:D:216:LYS:O	1:E:275:LEU:HA	1.27	1.33
1:A:216:LYS:H	1:B:275:LEU:CD2	1.41	1.33
1:A:219:TRP:CD1	1:B:279:HIS:HE1	1.47	1.33
1:E:228:ASP:HB3	1:F:252:LYS:NZ	1.39	1.33
1:A:221:ALA:O	1:B:439:ARG:NH1	1.57	1.33
1:C:216:LYS:CE	1:D:278:ALA:CB	2.05	1.33
1:C:227:THR:OG1	1:D:435:TYR:CZ	1.78	1.33
1:B:220:VAL:CG2	1:C:437:THR:CG2	2.01	1.32
1:D:235:VAL:HG21	1:E:255:ILE:CB	1.58	1.32
1:E:220:VAL:HG23	1:F:250:ALA:C	1.49	1.32
1:A:362:TRP:C	1:F:360:GLU:OE1	1.72	1.32
1:B:217:ALA:N	1:C:275:LEU:CD2	1.91	1.32
1:A:220:VAL:CG2	1:B:252:LYS:CG	2.00	1.32
1:D:212:PRO:CB	1:E:183:ILE:O	1.78	1.32
1:C:218:THR:CG2	1:D:251:ALA:HB2	1.59	1.31
1:C:216:LYS:CA	1:D:278:ALA:HB3	1.60	1.31
1:D:235:VAL:CG2	1:E:255:ILE:HD12	1.59	1.31
1:E:213:ASP:CA	1:F:274:ARG:HD2	1.55	1.31
1:B:217:ALA:CB	1:C:436:VAL:HG21	1.59	1.31
1:E:234:GLU:N	1:F:253:SER:CB	1.93	1.31
1:A:250:ALA:H	1:F:219:TRP:CG	1.47	1.30
1:E:217:ALA:HB1	1:F:279:HIS:CB	1.60	1.30
1:A:210:VAL:CG1	1:B:182:ILE:HA	1.60	1.30
1:A:217:ALA:HB3	1:B:275:LEU:C	1.53	1.30
1:B:217:ALA:HB1	1:C:436:VAL:CG2	1.62	1.30
1:C:220:VAL:N	1:D:250:ALA:N	1.79	1.30
1:D:237:GLY:CA	1:E:267:LEU:HD11	1.62	1.29
1:A:271:LEU:HD12	1:F:215:GLY:N	1.45	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:LYS:C	1:E:275:LEU:HA	1.57	1.29
1:A:178:PHE:C	1:F:208:MET:CA	1.92	1.29
1:C:211:GLU:OE2	1:D:270:LEU:HD23	1.18	1.29
1:C:233:GLU:OE1	1:D:252:LYS:HB2	1.27	1.29
1:E:211:GLU:HG3	1:F:182:ILE:CB	1.61	1.29
1:E:232:GLY:C	1:F:252:LYS:CA	1.93	1.29
1:A:352:ALA:HB1	1:F:332:ARG:NE	1.47	1.29
1:D:235:VAL:CG2	1:E:255:ILE:HB	1.61	1.29
1:A:271:LEU:HD12	1:F:214:ALA:C	1.58	1.28
1:C:221:ALA:CA	1:D:248:LYS:CB	2.07	1.28
1:D:212:PRO:HB3	1:E:183:ILE:O	1.28	1.28
1:B:210:VAL:CG1	1:C:182:ILE:HA	1.62	1.28
1:D:212:PRO:HA	1:E:182:ILE:CD1	1.63	1.28
1:D:235:VAL:HA	1:E:271:LEU:CD1	1.60	1.28
1:B:233:GLU:OE2	1:C:435:TYR:CE2	1.86	1.28
1:B:212:PRO:CG	1:C:183:ILE:O	1.80	1.28
1:D:235:VAL:HG11	1:E:255:ILE:CA	1.64	1.28
1:C:213:ASP:CA	1:D:274:ARG:CD	1.79	1.27
1:D:235:VAL:HG21	1:E:255:ILE:CD1	1.62	1.27
1:D:214:ALA:N	1:E:274:ARG:HG3	1.48	1.27
1:D:207:THR:N	1:E:177:ILE:HB	0.94	1.27
1:A:212:PRO:O	1:B:184:ARG:HG2	1.17	1.26
1:D:212:PRO:CA	1:E:182:ILE:CD1	2.12	1.26
1:A:214:ALA:O	1:B:274:ARG:HB2	1.11	1.26
1:A:216:LYS:N	1:B:275:LEU:HD23	1.47	1.26
1:A:361:GLU:CG	1:B:363:GLN:OE1	1.83	1.26
1:D:235:VAL:CG1	1:E:255:ILE:HA	1.63	1.26
1:D:208:MET:HA	1:E:178:PHE:O	1.35	1.26
1:A:279:HIS:HE1	1:F:219:TRP:CD1	1.53	1.26
1:C:209:LEU:O	1:D:179:SER:CB	1.82	1.25
1:E:213:ASP:HA	1:F:274:ARG:CG	1.65	1.25
1:A:210:VAL:HA	1:B:181:ARG:O	1.37	1.25
1:A:178:PHE:O	1:F:208:MET:HA	1.37	1.24
1:A:182:ILE:CA	1:F:211:GLU:O	1.85	1.24
1:A:215:GLY:H	1:B:271:LEU:CD1	1.45	1.24
1:E:214:ALA:N	1:F:274:ARG:CB	1.97	1.24
1:A:178:PHE:CG	1:F:207:THR:HG22	1.71	1.24
1:D:233:GLU:OE2	1:E:434:TYR:N	1.67	1.24
1:A:275:LEU:HD11	1:F:234:GLU:O	1.37	1.24
1:A:275:LEU:HD22	1:F:217:ALA:N	1.53	1.23
1:C:235:VAL:CG2	1:D:271:LEU:CD1	2.10	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:THR:HB	1:C:252:LYS:CD	1.52	1.23
1:D:211:GLU:C	1:E:182:ILE:CD1	2.11	1.23
1:A:217:ALA:H	1:B:275:LEU:CD2	1.51	1.23
1:E:217:ALA:HB3	1:F:279:HIS:N	1.52	1.23
1:C:208:MET:HA	1:D:179:SER:N	1.53	1.23
1:E:233:GLU:OE2	1:F:252:LYS:HE2	1.33	1.23
1:B:212:PRO:CB	1:C:183:ILE:C	2.10	1.23
1:A:214:ALA:O	1:B:274:ARG:CB	1.86	1.22
1:D:232:GLY:O	1:E:252:LYS:O	1.54	1.22
1:A:178:PHE:C	1:F:208:MET:HA	1.22	1.22
1:A:275:LEU:HD23	1:F:216:LYS:CA	1.67	1.22
1:A:233:GLU:HG3	1:B:434:TYR:O	1.38	1.22
1:E:227:THR:O	1:F:252:LYS:CD	1.88	1.22
1:A:352:ALA:HB1	1:F:332:ARG:CD	1.68	1.22
1:A:362:TRP:CH2	1:B:362:TRP:CG	2.27	1.22
1:C:216:LYS:H	1:D:275:LEU:CD1	1.53	1.22
1:E:232:GLY:C	1:F:252:LYS:N	1.97	1.21
1:C:219:TRP:HZ2	1:D:282:SER:O	0.86	1.21
1:D:215:GLY:CA	1:E:275:LEU:HD23	1.69	1.21
1:A:233:GLU:OE1	1:B:433:ALA:HB1	1.05	1.21
1:B:234:GLU:O	1:C:275:LEU:HD11	1.39	1.21
1:C:216:LYS:HE3	1:D:278:ALA:CA	1.70	1.21
1:C:216:LYS:HA	1:D:278:ALA:CB	1.70	1.21
1:E:233:GLU:N	1:F:252:LYS:HB2	1.42	1.21
1:B:210:VAL:CG1	1:C:182:ILE:CA	2.18	1.21
1:E:208:MET:C	1:F:180:GLN:H	1.47	1.21
1:E:211:GLU:CG	1:F:182:ILE:CD1	1.95	1.21
1:A:220:VAL:HG23	1:B:251:ALA:O	1.35	1.20
1:A:235:VAL:CB	1:B:271:LEU:HD21	1.70	1.20
1:A:250:ALA:N	1:F:219:TRP:HB3	1.35	1.20
1:C:214:ALA:HB3	1:D:271:LEU:HA	1.22	1.20
1:B:214:ALA:C	1:C:271:LEU:HA	1.66	1.20
1:C:213:ASP:HA	1:D:274:ARG:CD	1.05	1.20
1:D:233:GLU:OE2	1:E:434:TYR:C	1.85	1.20
1:B:227:THR:OG1	1:C:252:LYS:HE2	1.39	1.20
1:C:216:LYS:N	1:D:275:LEU:HD12	1.55	1.20
1:C:221:ALA:O	1:D:248:LYS:HG2	1.03	1.20
1:E:213:ASP:CA	1:F:274:ARG:HG3	1.70	1.20
1:A:233:GLU:CG	1:B:434:TYR:N	2.03	1.20
1:D:214:ALA:N	1:E:274:ARG:CG	1.99	1.20
1:D:232:GLY:O	1:E:252:LYS:C	1.83	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ALA:CA	1:C:275:LEU:HD22	1.71	1.19
1:C:209:LEU:O	1:D:179:SER:HB3	1.42	1.19
1:D:232:GLY:O	1:E:252:LYS:HG3	1.40	1.19
1:D:216:LYS:O	1:E:275:LEU:CA	1.89	1.19
1:A:215:GLY:N	1:B:271:LEU:HD12	0.87	1.19
1:A:254:PHE:CD1	1:F:233:GLU:OE1	1.94	1.19
1:E:232:GLY:CA	1:F:252:LYS:CB	2.13	1.19
1:A:215:GLY:O	1:B:274:ARG:HB3	1.37	1.19
1:E:232:GLY:O	1:F:252:LYS:N	1.59	1.18
1:A:271:LEU:O	1:F:214:ALA:O	1.61	1.18
1:A:275:LEU:HD23	1:F:216:LYS:N	0.87	1.18
1:B:233:GLU:OE1	1:C:433:ALA:HB1	1.05	1.18
1:C:227:THR:O	1:D:252:LYS:HD2	1.44	1.18
1:A:216:LYS:NZ	1:B:278:ALA:N	1.81	1.18
1:E:217:ALA:CB	1:F:279:HIS:CB	2.18	1.17
1:E:221:ALA:HA	1:F:248:LYS:CB	1.74	1.17
1:C:216:LYS:O	1:D:279:HIS:N	1.76	1.17
1:B:209:LEU:O	1:C:180:GLN:C	1.86	1.17
1:D:219:TRP:CZ2	1:E:286:ALA:HB2	1.79	1.17
1:C:227:THR:OG1	1:D:435:TYR:OH	1.61	1.16
1:D:216:LYS:C	1:E:278:ALA:HB3	1.70	1.16
1:D:223:SER:N	1:E:439:ARG:NH1	1.93	1.16
1:E:207:THR:OG1	1:F:177:ILE:O	1.62	1.16
1:B:232:GLY:O	1:C:253:SER:HA	1.38	1.16
1:C:216:LYS:HE3	1:D:278:ALA:HB1	1.20	1.16
1:C:221:ALA:O	1:D:248:LYS:CG	1.92	1.16
1:A:233:GLU:OE1	1:B:433:ALA:CB	1.92	1.16
1:E:205:ILE:CG2	1:F:177:ILE:HG12	1.75	1.16
1:E:227:THR:O	1:F:252:LYS:HD2	1.00	1.16
1:A:220:VAL:HG12	1:B:437:THR:CG2	1.74	1.15
1:C:215:GLY:HA3	1:D:275:LEU:N	1.60	1.15
1:D:212:PRO:CB	1:E:182:ILE:HD13	1.74	1.15
1:E:225:TYR:HA	1:F:422:GLU:OE2	1.47	1.15
1:A:215:GLY:HA2	1:B:271:LEU:CD1	1.75	1.15
1:A:231:THR:O	1:B:252:LYS:HB2	1.46	1.15
1:A:234:GLU:HB2	1:B:275:LEU:HD22	1.18	1.15
1:D:206:LEU:HA	1:E:177:ILE:CG1	1.76	1.15
1:D:235:VAL:CB	1:E:255:ILE:HB	1.76	1.15
1:A:217:ALA:CB	1:B:275:LEU:CB	2.25	1.15
1:D:233:GLU:OE1	1:E:433:ALA:HB1	1.21	1.15
1:A:226:GLY:HA3	1:B:424:GLU:OE1	1.45	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD13	1:F:236:LYS:N	1.36	1.14
1:C:220:VAL:H	1:D:250:ALA:N	1.37	1.14
1:A:184:ARG:HA	1:F:212:PRO:O	1.46	1.14
1:B:235:VAL:HG11	1:C:255:ILE:HG12	1.30	1.14
1:A:271:LEU:HA	1:F:214:ALA:CB	1.78	1.13
1:B:233:GLU:OE2	1:C:435:TYR:CD2	2.01	1.13
1:A:219:TRP:CD1	1:B:279:HIS:CE1	2.37	1.13
1:A:362:TRP:HH2	1:B:362:TRP:CG	1.64	1.13
1:E:211:GLU:HG2	1:F:182:ILE:HD13	1.26	1.13
1:D:206:LEU:C	1:E:177:ILE:HB	1.73	1.13
1:E:219:TRP:HB3	1:F:249:LEU:HA	1.27	1.13
1:B:217:ALA:N	1:C:275:LEU:HD23	1.54	1.13
1:A:434:TYR:O	1:F:233:GLU:HG3	1.45	1.13
1:B:210:VAL:HG12	1:C:182:ILE:C	1.74	1.12
1:D:235:VAL:HB	1:E:254:PHE:O	1.45	1.12
1:A:216:LYS:NZ	1:B:277:GLU:C	2.07	1.12
1:A:217:ALA:HB2	1:B:275:LEU:HB3	1.28	1.12
1:A:352:ALA:CB	1:F:332:ARG:CD	2.27	1.12
1:B:207:THR:OG1	1:C:177:ILE:HB	1.49	1.12
1:E:220:VAL:HG23	1:F:251:ALA:N	1.64	1.12
1:A:178:PHE:CG	1:F:207:THR:CG2	2.28	1.12
1:A:222:ALA:C	1:B:439:ARG:NH1	2.08	1.12
1:A:233:GLU:HG3	1:B:434:TYR:C	1.74	1.12
1:A:271:LEU:HA	1:F:214:ALA:C	1.73	1.12
1:A:362:TRP:CA	1:F:360:GLU:OE1	1.94	1.12
1:C:216:LYS:CE	1:D:278:ALA:HB1	1.71	1.12
1:C:219:TRP:CD1	1:D:249:LEU:HD13	1.84	1.12
1:C:234:GLU:HB2	1:D:275:LEU:HD11	1.15	1.12
1:A:352:ALA:CB	1:F:332:ARG:HD2	1.79	1.12
1:B:220:VAL:HG21	1:C:437:THR:HG23	1.27	1.12
1:D:236:LYS:N	1:E:271:LEU:HD12	1.65	1.12
1:A:217:ALA:CA	1:B:275:LEU:CB	2.25	1.12
1:A:222:ALA:C	1:B:439:ARG:HH12	1.55	1.11
1:E:214:ALA:H	1:F:274:ARG:HB3	1.09	1.11
1:A:178:PHE:CD2	1:F:207:THR:HG21	1.58	1.11
1:B:209:LEU:O	1:C:180:GLN:O	1.66	1.11
1:C:217:ALA:CB	1:D:279:HIS:CB	2.09	1.11
1:E:214:ALA:O	1:F:274:ARG:CB	1.98	1.11
1:D:233:GLU:OE2	1:E:434:TYR:CA	1.99	1.11
1:B:217:ALA:CB	1:C:275:LEU:HB3	1.80	1.11
1:B:220:VAL:CG1	1:C:251:ALA:O	1.98	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLU:C	1:C:275:LEU:HD21	1.75	1.11
1:C:234:GLU:HB2	1:D:275:LEU:CD1	1.80	1.11
1:D:235:VAL:HG23	1:E:271:LEU:HD13	1.20	1.11
1:A:236:LYS:H	1:B:271:LEU:HD13	1.13	1.11
1:D:208:MET:HA	1:E:178:PHE:C	1.57	1.11
1:E:205:ILE:HG22	1:F:177:ILE:HG12	1.25	1.11
1:A:214:ALA:C	1:B:271:LEU:HA	1.73	1.10
1:B:227:THR:CB	1:C:252:LYS:HD3	1.81	1.10
1:A:217:ALA:HB2	1:B:275:LEU:CB	1.79	1.10
1:A:236:LYS:H	1:B:271:LEU:CD1	1.65	1.10
1:C:209:LEU:O	1:D:179:SER:OG	1.68	1.10
1:E:220:VAL:CG1	1:F:435:TYR:HE1	1.64	1.10
1:C:219:TRP:C	1:D:250:ALA:H	1.60	1.10
1:E:214:ALA:H	1:F:274:ARG:CG	1.54	1.10
1:E:214:ALA:HB1	1:F:271:LEU:HG	1.31	1.10
1:E:228:ASP:CB	1:F:252:LYS:NZ	2.15	1.10
1:A:182:ILE:CB	1:F:211:GLU:O	2.00	1.10
1:D:214:ALA:H	1:E:274:ARG:HG2	0.95	1.10
1:E:219:TRP:C	1:F:250:ALA:O	1.94	1.10
1:A:271:LEU:HD11	1:F:236:LYS:N	1.66	1.09
1:D:215:GLY:HA3	1:E:275:LEU:HD23	1.32	1.09
1:A:219:TRP:HD1	1:B:279:HIS:CE1	1.70	1.09
1:A:250:ALA:N	1:F:219:TRP:CB	1.78	1.09
1:B:209:LEU:N	1:C:180:GLN:H	1.50	1.09
1:B:217:ALA:HA	1:C:275:LEU:HD22	1.26	1.09
1:C:210:VAL:HG13	1:D:182:ILE:HA	1.12	1.09
1:C:214:ALA:HB1	1:D:271:LEU:HA	1.25	1.09
1:D:232:GLY:HA2	1:E:252:LYS:HE2	1.23	1.09
1:C:220:VAL:CG2	1:D:250:ALA:C	2.26	1.09
1:C:235:VAL:HG23	1:D:271:LEU:CD2	1.83	1.09
1:D:232:GLY:O	1:E:252:LYS:CG	2.01	1.09
1:A:206:LEU:HA	1:B:177:ILE:CG1	1.81	1.09
1:A:361:GLU:CG	1:B:363:GLN:CD	2.23	1.09
1:B:215:GLY:N	1:C:271:LEU:HA	1.66	1.09
1:C:211:GLU:OE2	1:D:270:LEU:CD2	1.99	1.09
1:C:215:GLY:CA	1:D:275:LEU:HB2	1.82	1.09
1:B:217:ALA:HB2	1:C:275:LEU:HB3	1.29	1.09
1:C:207:THR:O	1:D:177:ILE:HG22	1.53	1.09
1:B:210:VAL:CG1	1:C:182:ILE:C	2.26	1.08
1:B:212:PRO:HG3	1:C:183:ILE:O	1.48	1.08
1:E:227:THR:C	1:F:252:LYS:HD2	1.77	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ALA:HA	1:D:248:LYS:HB3	1.21	1.08
1:D:215:GLY:N	1:E:271:LEU:HG	1.68	1.08
1:C:220:VAL:N	1:D:250:ALA:H	1.46	1.08
1:A:207:THR:CB	1:B:177:ILE:N	2.16	1.08
1:B:212:PRO:HB3	1:C:183:ILE:C	1.75	1.08
1:C:210:VAL:CG1	1:D:182:ILE:HA	1.84	1.08
1:D:211:GLU:CA	1:E:182:ILE:CG1	2.13	1.08
1:E:234:GLU:O	1:F:253:SER:HB3	1.53	1.08
1:A:233:GLU:HG2	1:B:434:TYR:CA	1.84	1.08
1:A:271:LEU:HA	1:F:214:ALA:O	1.53	1.08
1:E:213:ASP:C	1:F:274:ARG:CG	2.17	1.08
1:A:210:VAL:HG12	1:B:182:ILE:HA	1.32	1.07
1:E:234:GLU:O	1:F:253:SER:CB	2.02	1.07
1:A:233:GLU:CG	1:B:434:TYR:C	2.27	1.07
1:C:214:ALA:CB	1:D:271:LEU:CA	2.31	1.07
1:C:219:TRP:HB3	1:D:249:LEU:CD2	1.85	1.07
1:D:237:GLY:HA2	1:E:267:LEU:HD11	1.11	1.07
1:A:362:TRP:CH2	1:B:362:TRP:CB	2.37	1.07
1:C:227:THR:CB	1:D:435:TYR:CZ	2.38	1.07
1:E:206:LEU:HA	1:F:177:ILE:HG21	1.34	1.07
1:A:212:PRO:O	1:B:184:ARG:CG	2.01	1.07
1:A:254:PHE:CG	1:F:233:GLU:OE1	2.07	1.07
1:A:271:LEU:CA	1:F:214:ALA:HB3	1.84	1.07
1:A:275:LEU:CD2	1:F:217:ALA:N	2.18	1.07
1:A:279:HIS:CE1	1:F:219:TRP:CD1	2.43	1.07
1:C:216:LYS:N	1:D:275:LEU:CA	2.18	1.07
1:A:216:LYS:H	1:B:275:LEU:CG	1.66	1.07
1:B:235:VAL:CG1	1:C:255:ILE:HG12	1.84	1.07
1:C:216:LYS:CD	1:D:278:ALA:CB	2.32	1.07
1:E:213:ASP:OD1	1:F:274:ARG:HD3	0.89	1.07
1:A:176:THR:HG23	1:F:205:ILE:HG21	1.35	1.06
1:A:271:LEU:CA	1:F:214:ALA:CB	2.33	1.06
1:A:275:LEU:HA	1:F:216:LYS:CA	1.86	1.06
1:B:233:GLU:OE1	1:C:433:ALA:CA	2.02	1.06
1:D:235:VAL:CB	1:E:254:PHE:O	2.02	1.06
1:A:176:THR:HA	1:F:205:ILE:HG23	1.34	1.06
1:B:212:PRO:HB2	1:C:183:ILE:C	1.80	1.06
1:B:232:GLY:O	1:C:253:SER:CA	2.01	1.06
1:D:206:LEU:HA	1:E:177:ILE:HG13	1.34	1.06
1:B:209:LEU:H	1:C:180:GLN:N	1.53	1.05
1:B:214:ALA:HB3	1:C:270:LEU:C	1.80	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ASP:CA	1:D:274:ARG:HD2	1.74	1.05
1:D:211:GLU:O	1:E:182:ILE:HD11	1.54	1.05
1:A:212:PRO:HB2	1:B:184:ARG:HA	1.34	1.05
1:A:217:ALA:CB	1:B:275:LEU:C	2.27	1.05
1:D:207:THR:CB	1:E:177:ILE:N	2.09	1.05
1:D:232:GLY:C	1:E:252:LYS:HG3	1.56	1.05
1:E:214:ALA:HB2	1:F:271:LEU:HA	1.09	1.05
1:A:206:LEU:HA	1:B:177:ILE:HG13	1.34	1.05
1:C:216:LYS:H	1:D:275:LEU:HD12	0.92	1.05
1:D:210:VAL:HG13	1:E:182:ILE:CB	1.84	1.05
1:E:211:GLU:CG	1:F:182:ILE:HB	1.86	1.05
1:A:215:GLY:HA2	1:B:271:LEU:HD11	1.38	1.05
1:A:216:LYS:HZ1	1:B:277:GLU:C	1.64	1.05
1:C:227:THR:OG1	1:D:435:TYR:CE2	1.96	1.05
1:A:220:VAL:HG12	1:B:437:THR:HG21	1.33	1.05
1:A:271:LEU:N	1:F:214:ALA:HB3	1.71	1.05
1:D:210:VAL:CG1	1:E:182:ILE:CB	2.35	1.04
1:D:211:GLU:O	1:E:182:ILE:CD1	2.05	1.04
1:D:212:PRO:HA	1:E:182:ILE:HD11	1.37	1.04
1:D:235:VAL:CG2	1:E:255:ILE:CD1	2.27	1.04
1:E:214:ALA:HB3	1:F:271:LEU:HA	1.12	1.04
1:E:234:GLU:N	1:F:253:SER:HB3	1.71	1.04
1:B:215:GLY:N	1:C:271:LEU:HD12	1.72	1.04
1:C:219:TRP:CA	1:D:250:ALA:H	1.70	1.04
1:A:217:ALA:H	1:B:275:LEU:HD22	1.21	1.04
1:A:253:SER:H	1:F:233:GLU:HG3	1.20	1.04
1:C:217:ALA:H	1:D:275:LEU:CD1	1.71	1.04
1:C:220:VAL:HG23	1:D:250:ALA:O	0.88	1.04
1:D:215:GLY:HA3	1:E:275:LEU:CD2	1.86	1.04
1:D:217:ALA:H	1:E:278:ALA:HB1	0.92	1.04
1:A:220:VAL:CG2	1:B:251:ALA:C	2.29	1.04
1:A:234:GLU:HB2	1:B:275:LEU:CD2	1.88	1.04
1:A:361:GLU:HG2	1:B:363:GLN:CG	1.88	1.04
1:D:232:GLY:CA	1:E:252:LYS:HE2	1.82	1.04
1:B:232:GLY:HA3	1:C:254:PHE:CD1	1.92	1.03
1:C:220:VAL:HG23	1:D:250:ALA:C	1.81	1.03
1:D:216:LYS:HG3	1:E:278:ALA:HB1	1.38	1.03
1:D:233:GLU:OE1	1:E:433:ALA:HA	1.58	1.03
1:D:236:LYS:H	1:E:271:LEU:CD1	1.72	1.03
1:A:439:ARG:NH1	1:F:221:ALA:O	1.89	1.03
1:B:210:VAL:HG12	1:C:182:ILE:HA	1.08	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ALA:N	1:D:275:LEU:HD12	1.74	1.03
1:E:214:ALA:HB1	1:F:271:LEU:HA	1.37	1.03
1:B:235:VAL:CG1	1:C:255:ILE:HG21	1.87	1.03
1:C:235:VAL:HG22	1:D:271:LEU:HD11	1.08	1.03
1:E:221:ALA:HA	1:F:248:LYS:HB2	1.35	1.03
1:C:219:TRP:CB	1:D:249:LEU:HD22	1.87	1.03
1:E:217:ALA:HB3	1:F:279:HIS:CA	1.88	1.03
1:D:235:VAL:CG2	1:E:271:LEU:HD13	1.88	1.02
1:E:227:THR:OG1	1:F:435:TYR:CZ	2.13	1.02
1:C:207:THR:HB	1:D:177:ILE:O	1.58	1.02
1:C:215:GLY:HA3	1:D:275:LEU:CA	1.88	1.02
1:D:210:VAL:HG13	1:E:182:ILE:CA	1.88	1.02
1:E:220:VAL:CG2	1:F:250:ALA:C	2.26	1.02
1:A:220:VAL:CG2	1:B:251:ALA:O	2.07	1.02
1:B:212:PRO:HB3	1:C:183:ILE:N	1.74	1.02
1:B:220:VAL:HG13	1:C:436:VAL:O	1.57	1.02
1:C:232:GLY:HA2	1:D:251:ALA:HA	1.39	1.02
1:A:235:VAL:CA	1:B:271:LEU:HD21	1.90	1.02
1:B:241:GLU:OE2	1:C:178:PHE:HB3	1.57	1.02
1:E:211:GLU:HG3	1:F:182:ILE:CG1	1.89	1.02
1:A:233:GLU:CG	1:B:434:TYR:H	1.66	1.01
1:A:331:ARG:CZ	1:B:355:ASP:HB3	1.90	1.01
1:C:216:LYS:CG	1:D:278:ALA:HB1	1.90	1.01
1:D:216:LYS:CA	1:E:275:LEU:HA	1.90	1.01
1:A:217:ALA:N	1:B:275:LEU:CD2	2.22	1.01
1:A:434:TYR:H	1:F:233:GLU:HG2	1.18	1.01
1:E:222:ALA:HB3	1:F:439:ARG:NH2	1.75	1.01
1:E:225:TYR:CA	1:F:422:GLU:OE2	2.07	1.01
1:E:241:GLU:CD	1:F:179:SER:HB3	1.85	1.01
1:A:210:VAL:HG13	1:B:182:ILE:HA	1.38	1.01
1:A:220:VAL:HG13	1:B:252:LYS:HE3	1.37	1.01
1:A:362:TRP:CZ2	1:B:362:TRP:CB	2.44	1.01
1:C:220:VAL:H	1:D:249:LEU:C	1.66	1.01
1:D:211:GLU:O	1:E:182:ILE:CG1	2.08	1.01
1:A:181:ARG:N	1:F:211:GLU:OE2	1.93	1.01
1:A:182:ILE:C	1:F:211:GLU:O	2.04	1.01
1:A:182:ILE:HB	1:F:211:GLU:O	1.59	1.01
1:B:234:GLU:O	1:C:275:LEU:HD21	1.61	1.01
1:E:221:ALA:O	1:F:248:LYS:HG2	1.59	1.01
1:E:223:SER:OG	1:F:439:ARG:NH1	1.94	1.01
1:A:362:TRP:CZ2	1:B:362:TRP:CG	2.49	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:CD	1:D:278:ALA:HB1	1.91	1.01
1:E:211:GLU:CD	1:F:182:ILE:HD12	1.86	1.01
1:A:362:TRP:CH2	1:B:362:TRP:HB2	1.95	1.00
1:C:215:GLY:C	1:D:275:LEU:HA	1.86	1.00
1:A:216:LYS:HA	1:B:274:ARG:C	1.82	1.00
1:C:216:LYS:CE	1:D:278:ALA:HB2	1.86	1.00
1:C:234:GLU:O	1:D:253:SER:HB3	1.61	1.00
1:D:215:GLY:CA	1:E:275:LEU:CD2	2.39	1.00
1:E:213:ASP:CB	1:F:274:ARG:HD3	1.89	1.00
1:A:178:PHE:CZ	1:F:207:THR:HG21	1.96	1.00
1:C:331:ARG:NH1	1:D:376:GLN:NE2	2.09	1.00
1:D:235:VAL:CG2	1:E:255:ILE:CG1	2.39	1.00
1:E:205:ILE:CG2	1:F:177:ILE:CG1	2.39	1.00
1:B:235:VAL:HG12	1:C:255:ILE:HG21	1.44	1.00
1:D:221:ALA:HA	1:E:248:LYS:HB3	1.42	1.00
1:E:205:ILE:HG23	1:F:177:ILE:CG1	1.90	1.00
1:E:228:ASP:CB	1:F:252:LYS:HZ2	1.70	1.00
1:A:220:VAL:CG1	1:B:437:THR:CG2	2.40	1.00
1:A:331:ARG:HH22	1:B:355:ASP:CG	1.70	1.00
1:A:352:ALA:HB2	1:F:332:ARG:HD2	1.41	1.00
1:A:222:ALA:HB2	1:B:437:THR:HG21	1.44	0.99
1:B:220:VAL:HG22	1:C:436:VAL:O	1.61	0.99
1:C:235:VAL:HG23	1:D:271:LEU:HD21	1.42	0.99
1:A:178:PHE:CE2	1:F:207:THR:CG2	2.19	0.99
1:B:231:THR:O	1:C:252:LYS:HB2	1.62	0.99
1:A:207:THR:HB	1:B:177:ILE:N	1.49	0.99
1:B:212:PRO:HB3	1:C:183:ILE:O	1.55	0.99
1:C:214:ALA:HB1	1:D:271:LEU:CA	1.91	0.99
1:D:233:GLU:OE1	1:E:433:ALA:C	2.05	0.99
1:B:217:ALA:HB1	1:C:436:VAL:HG21	1.17	0.99
1:A:249:LEU:HB3	1:F:219:TRP:CD1	1.98	0.99
1:C:217:ALA:HB1	1:D:279:HIS:HB2	1.42	0.99
1:B:220:VAL:HG23	1:C:437:THR:HG22	0.99	0.99
1:C:233:GLU:HB3	1:D:254:PHE:N	1.78	0.99
1:C:235:VAL:HG23	1:D:271:LEU:HD11	1.00	0.99
1:E:222:ALA:CB	1:F:439:ARG:HH22	1.76	0.99
1:A:216:LYS:H	1:B:275:LEU:HD23	1.04	0.98
1:C:215:GLY:HA3	1:D:275:LEU:CB	1.92	0.98
1:E:205:ILE:O	1:F:177:ILE:HG13	1.62	0.98
1:E:220:VAL:CG2	1:F:251:ALA:N	2.25	0.98
1:A:271:LEU:HD13	1:F:236:LYS:CA	1.92	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:TRP:HB3	1:D:249:LEU:HD22	1.38	0.98
1:A:217:ALA:O	1:B:279:HIS:HB2	1.62	0.98
1:E:220:VAL:HG23	1:F:251:ALA:CA	1.92	0.98
1:D:232:GLY:C	1:E:252:LYS:CG	2.37	0.98
1:A:362:TRP:HH2	1:B:362:TRP:HD1	1.03	0.98
1:B:234:GLU:O	1:C:275:LEU:CD1	2.10	0.98
1:A:271:LEU:CD1	1:F:215:GLY:N	2.25	0.98
1:C:218:THR:O	1:D:279:HIS:CE1	2.15	0.98
1:E:207:THR:HG22	1:F:179:SER:HA	1.44	0.98
1:A:214:ALA:O	1:B:271:LEU:HA	1.62	0.98
1:E:227:THR:OG1	1:F:435:TYR:CE2	2.17	0.98
1:E:232:GLY:HA3	1:F:252:LYS:HB2	1.45	0.98
1:E:234:GLU:C	1:F:253:SER:CB	2.36	0.98
1:A:235:VAL:HA	1:B:271:LEU:HD21	1.43	0.98
1:C:223:SER:H	1:D:439:ARG:NH1	1.60	0.98
1:C:220:VAL:HB	1:D:250:ALA:CA	1.94	0.97
1:D:236:LYS:H	1:E:271:LEU:HD12	0.83	0.97
1:A:233:GLU:CG	1:B:434:TYR:O	2.12	0.97
1:B:210:VAL:CG1	1:C:183:ILE:N	2.28	0.97
1:C:233:GLU:C	1:D:253:SER:HA	1.84	0.97
1:C:331:ARG:CZ	1:D:376:GLN:HE22	1.56	0.97
1:E:220:VAL:HG23	1:F:250:ALA:O	1.65	0.97
1:A:275:LEU:CD2	1:F:217:ALA:H	1.74	0.97
1:A:361:GLU:HG2	1:B:363:GLN:OE1	1.48	0.97
1:E:233:GLU:N	1:F:252:LYS:HB3	1.79	0.97
1:A:434:TYR:O	1:F:233:GLU:CG	2.11	0.97
1:B:210:VAL:C	1:C:182:ILE:HA	1.86	0.97
1:B:220:VAL:HG13	1:C:251:ALA:O	1.65	0.97
1:A:218:THR:HG23	1:B:251:ALA:HA	1.46	0.97
1:B:215:GLY:H	1:C:271:LEU:HD12	1.20	0.97
1:D:208:MET:CA	1:E:178:PHE:C	2.29	0.96
1:E:211:GLU:HG3	1:F:182:ILE:HB	0.98	0.96
1:C:213:ASP:HA	1:D:274:ARG:HD2	1.34	0.96
1:D:215:GLY:O	1:E:274:ARG:HB2	1.62	0.96
1:A:271:LEU:HD13	1:F:236:LYS:H	0.83	0.96
1:B:232:GLY:HA2	1:C:252:LYS:HB3	1.44	0.96
1:B:207:THR:OG1	1:C:177:ILE:CB	2.12	0.96
1:C:232:GLY:HA3	1:D:252:LYS:HG3	1.43	0.96
1:D:210:VAL:CG1	1:E:182:ILE:HB	1.94	0.96
1:E:220:VAL:CG2	1:F:251:ALA:HA	1.95	0.96
1:C:208:MET:HB2	1:D:179:SER:HA	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:PRO:HB2	1:D:184:ARG:CA	1.96	0.96
1:C:216:LYS:HA	1:D:278:ALA:HB3	0.98	0.96
1:A:176:THR:HG22	1:F:207:THR:OG1	1.64	0.95
1:D:212:PRO:N	1:E:182:ILE:HD13	1.79	0.95
1:A:184:ARG:CA	1:F:212:PRO:O	2.12	0.95
1:A:218:THR:CG2	1:B:252:LYS:H	1.78	0.95
1:A:250:ALA:H	1:F:219:TRP:HB3	0.96	0.95
1:B:233:GLU:HB3	1:C:434:TYR:HB2	1.44	0.95
1:E:219:TRP:HE1	1:F:282:SER:C	1.72	0.95
1:D:223:SER:N	1:E:439:ARG:HH11	1.63	0.95
1:D:233:GLU:CD	1:E:434:TYR:H	1.57	0.95
1:C:211:GLU:HB3	1:D:182:ILE:HG12	1.46	0.95
1:C:214:ALA:HB3	1:D:271:LEU:CA	1.95	0.95
1:A:235:VAL:HG23	1:B:271:LEU:HD21	1.42	0.95
1:E:213:ASP:CA	1:F:274:ARG:CG	2.21	0.95
1:D:209:LEU:HB2	1:E:178:PHE:HB2	1.46	0.95
1:E:227:THR:OG1	1:F:435:TYR:OH	1.85	0.95
1:A:275:LEU:HD22	1:F:217:ALA:H	1.21	0.95
1:E:227:THR:CB	1:F:435:TYR:CZ	2.50	0.95
1:A:235:VAL:HG12	1:B:254:PHE:O	1.66	0.94
1:A:254:PHE:CE1	1:F:233:GLU:OE1	2.18	0.94
1:B:214:ALA:C	1:C:274:ARG:HB2	1.92	0.94
1:C:219:TRP:CD1	1:D:249:LEU:HB3	2.02	0.94
1:E:232:GLY:HA2	1:F:252:LYS:HG3	1.49	0.94
1:A:178:PHE:O	1:F:208:MET:CA	2.00	0.94
1:A:252:LYS:O	1:F:217:ALA:HA	1.66	0.94
1:D:215:GLY:O	1:E:274:ARG:CB	2.15	0.94
1:E:234:GLU:C	1:F:253:SER:HB3	1.92	0.94
1:E:205:ILE:C	1:F:177:ILE:HG13	1.92	0.94
1:B:220:VAL:CG1	1:C:436:VAL:O	2.16	0.94
1:C:233:GLU:HB3	1:D:253:SER:CA	1.97	0.94
1:E:211:GLU:CG	1:F:182:ILE:CB	2.45	0.94
1:A:176:THR:HA	1:F:205:ILE:HG22	1.48	0.94
1:A:216:LYS:CA	1:B:275:LEU:HD23	1.97	0.94
1:A:220:VAL:HG22	1:B:252:LYS:HG3	0.97	0.94
1:A:220:VAL:HG21	1:B:252:LYS:HG2	0.96	0.94
1:A:250:ALA:N	1:F:219:TRP:CD1	2.36	0.94
1:D:233:GLU:HG2	1:E:434:TYR:O	1.68	0.94
1:E:206:LEU:CA	1:F:177:ILE:HG21	1.96	0.94
1:E:219:TRP:HB3	1:F:249:LEU:CA	1.97	0.94
1:E:220:VAL:CG1	1:F:435:TYR:CE1	2.43	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:N	1:F:218:THR:H	1.48	0.94
1:A:271:LEU:HB2	1:F:214:ALA:HB1	1.50	0.94
1:B:207:THR:CB	1:C:177:ILE:CB	2.46	0.94
1:A:216:LYS:N	1:B:275:LEU:CD2	2.16	0.94
1:A:361:GLU:CB	1:B:363:GLN:OE1	2.15	0.93
1:C:215:GLY:HA3	1:D:275:LEU:HB2	1.45	0.93
1:A:217:ALA:HB3	1:B:275:LEU:O	1.67	0.93
1:B:212:PRO:C	1:C:182:ILE:CD1	1.77	0.93
1:E:207:THR:CG2	1:F:178:PHE:C	2.41	0.93
1:C:234:GLU:O	1:D:253:SER:CB	2.16	0.93
1:E:207:THR:HG21	1:F:178:PHE:C	1.92	0.93
1:E:220:VAL:CG2	1:F:251:ALA:CA	2.46	0.93
1:C:216:LYS:CA	1:D:278:ALA:CB	2.39	0.93
1:E:220:VAL:O	1:F:250:ALA:HB2	1.67	0.93
1:E:214:ALA:O	1:F:274:ARG:HB3	1.68	0.93
1:B:215:GLY:CA	1:C:275:LEU:HG	1.98	0.93
1:D:207:THR:H	1:E:177:ILE:CA	1.78	0.93
1:E:228:ASP:HB3	1:F:252:LYS:HZ3	1.10	0.93
1:C:207:THR:O	1:D:177:ILE:CG2	2.15	0.93
1:C:332:ARG:HD3	1:D:355:ASP:OD2	1.68	0.93
1:B:210:VAL:HG12	1:C:183:ILE:N	1.83	0.92
1:B:216:LYS:CA	1:C:274:ARG:O	2.14	0.92
1:E:233:GLU:OE2	1:F:252:LYS:CE	2.18	0.92
1:A:216:LYS:H	1:B:275:LEU:HG	1.34	0.92
1:A:271:LEU:CG	1:F:236:LYS:H	1.70	0.92
1:C:235:VAL:HG21	1:D:255:ILE:HD12	1.49	0.92
1:E:221:ALA:HA	1:F:248:LYS:HB3	1.47	0.92
1:D:210:VAL:HG13	1:E:182:ILE:HA	1.48	0.92
1:D:210:VAL:HG12	1:E:182:ILE:HB	1.47	0.92
1:D:235:VAL:HB	1:E:255:ILE:HB	1.50	0.92
1:E:214:ALA:O	1:F:274:ARG:HB2	1.67	0.92
1:B:220:VAL:CG2	1:C:436:VAL:O	2.17	0.92
1:A:271:LEU:CB	1:F:214:ALA:HB1	2.00	0.92
1:A:434:TYR:N	1:F:233:GLU:HG2	1.83	0.92
1:D:216:LYS:CD	1:E:278:ALA:HB2	2.00	0.92
1:E:207:THR:N	1:F:177:ILE:CG2	2.33	0.92
1:E:232:GLY:HA2	1:F:252:LYS:CB	2.00	0.92
1:B:233:GLU:HB3	1:C:434:TYR:CB	1.95	0.91
1:A:207:THR:C	1:B:177:ILE:HG22	1.94	0.91
1:B:214:ALA:C	1:C:271:LEU:CA	2.43	0.91
1:E:213:ASP:CB	1:F:274:ARG:CD	2.46	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:GLU:C	1:F:252:LYS:O	1.99	0.91
1:A:216:LYS:HZ2	1:B:278:ALA:N	1.56	0.91
1:C:216:LYS:CD	1:D:278:ALA:HB2	1.97	0.91
1:C:217:ALA:N	1:D:275:LEU:CD1	2.30	0.91
1:E:232:GLY:HA2	1:F:252:LYS:CG	1.99	0.91
1:A:182:ILE:HA	1:F:211:GLU:O	1.68	0.91
1:A:275:LEU:HA	1:F:216:LYS:HA	1.50	0.91
1:B:216:LYS:H	1:C:275:LEU:HD23	1.36	0.91
1:C:233:GLU:OE1	1:D:252:LYS:HB3	1.71	0.91
1:A:220:VAL:CB	1:B:437:THR:HG22	1.99	0.91
1:A:236:LYS:N	1:B:271:LEU:CD1	2.34	0.91
1:A:271:LEU:CA	1:F:214:ALA:O	2.17	0.90
1:A:233:GLU:CD	1:B:433:ALA:HB1	1.95	0.90
1:A:234:GLU:O	1:B:275:LEU:HD11	1.72	0.90
1:B:227:THR:CB	1:C:252:LYS:CD	2.29	0.90
1:E:214:ALA:HB1	1:F:271:LEU:CA	1.96	0.90
1:C:219:TRP:HA	1:D:250:ALA:N	1.86	0.90
1:C:235:VAL:HG23	1:D:271:LEU:CG	2.01	0.90
1:D:235:VAL:HG23	1:E:271:LEU:CD1	2.01	0.90
1:B:237:GLY:N	1:C:267:LEU:HD21	1.87	0.90
1:C:233:GLU:HB3	1:D:253:SER:HA	1.51	0.90
1:D:235:VAL:CG1	1:E:254:PHE:O	2.19	0.90
1:C:220:VAL:CB	1:D:250:ALA:C	2.45	0.90
1:A:275:LEU:CD1	1:F:234:GLU:O	2.20	0.90
1:E:220:VAL:O	1:F:250:ALA:CB	2.18	0.90
1:A:178:PHE:HA	1:F:207:THR:HG22	1.51	0.90
1:A:275:LEU:HA	1:F:216:LYS:C	1.97	0.90
1:A:182:ILE:HB	1:F:211:GLU:C	1.97	0.90
1:A:275:LEU:HD23	1:F:215:GLY:C	1.95	0.90
1:C:215:GLY:HA3	1:D:275:LEU:H	1.28	0.90
1:E:216:LYS:H	1:F:275:LEU:HD12	1.37	0.90
1:D:212:PRO:HB2	1:E:183:ILE:O	1.73	0.89
1:C:216:LYS:C	1:D:278:ALA:HB3	1.96	0.89
1:A:183:ILE:HG13	1:F:212:PRO:HB3	1.53	0.89
1:A:218:THR:HG23	1:B:251:ALA:CA	2.02	0.89
1:A:226:GLY:CA	1:B:424:GLU:OE1	2.19	0.89
1:C:215:GLY:CA	1:D:275:LEU:N	2.34	0.89
1:D:222:ALA:C	1:E:439:ARG:HH11	1.80	0.89
1:A:215:GLY:O	1:B:274:ARG:CB	2.19	0.89
1:A:233:GLU:HG2	1:B:434:TYR:H	1.06	0.89
1:C:207:THR:CG2	1:D:177:ILE:O	2.20	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PRO:C	1:C:182:ILE:HD11	1.71	0.89
1:C:223:SER:H	1:D:439:ARG:HH12	0.92	0.89
1:D:209:LEU:HB3	1:E:178:PHE:HD1	1.35	0.89
1:D:216:LYS:CG	1:E:278:ALA:CB	2.02	0.89
1:E:217:ALA:HB3	1:F:279:HIS:H	1.30	0.89
1:A:214:ALA:C	1:B:274:ARG:HB2	1.96	0.89
1:A:217:ALA:HA	1:B:275:LEU:HB3	1.55	0.89
1:B:214:ALA:CB	1:C:270:LEU:HG	2.02	0.89
1:C:208:MET:CA	1:D:179:SER:N	2.35	0.89
1:A:362:TRP:CZ2	1:B:362:TRP:HB3	2.08	0.89
1:E:214:ALA:HB3	1:F:271:LEU:CA	1.79	0.89
1:E:234:GLU:C	1:F:253:SER:HB2	1.97	0.89
1:B:210:VAL:CA	1:C:182:ILE:HA	2.02	0.88
1:C:219:TRP:CH2	1:D:286:ALA:HB2	2.07	0.88
1:D:208:MET:CA	1:E:179:SER:HA	1.90	0.88
1:E:208:MET:C	1:F:180:GLN:N	2.31	0.88
1:E:211:GLU:CG	1:F:182:ILE:CG1	2.50	0.88
1:E:211:GLU:HG3	1:F:182:ILE:CD1	2.02	0.88
1:D:212:PRO:N	1:E:182:ILE:CD1	2.33	0.88
1:A:221:ALA:O	1:B:439:ARG:CZ	2.21	0.88
1:A:279:HIS:HE1	1:F:219:TRP:HD1	1.14	0.88
1:B:235:VAL:HG12	1:C:255:ILE:CG2	2.02	0.88
1:D:214:ALA:N	1:E:274:ARG:HG2	1.76	0.88
1:D:219:TRP:CH2	1:E:286:ALA:HB2	2.08	0.88
1:A:216:LYS:HA	1:B:274:ARG:O	1.74	0.88
1:B:232:GLY:HA3	1:C:254:PHE:CE1	2.09	0.88
1:B:234:GLU:HB2	1:C:275:LEU:CD2	2.04	0.88
1:D:216:LYS:HA	1:E:274:ARG:C	1.98	0.88
1:A:176:THR:CA	1:F:205:ILE:CG2	2.47	0.88
1:C:210:VAL:CG1	1:D:183:ILE:H	1.86	0.88
1:A:178:PHE:HD2	1:F:207:THR:HG22	1.37	0.88
1:B:217:ALA:H	1:C:275:LEU:HD23	0.73	0.88
1:D:235:VAL:CG2	1:E:271:LEU:CD1	2.52	0.88
1:D:233:GLU:OE2	1:E:434:TYR:O	1.91	0.88
1:C:233:GLU:OE1	1:D:252:LYS:HD3	1.74	0.87
1:A:235:VAL:CG1	1:B:254:PHE:O	2.22	0.87
1:D:209:LEU:HB3	1:E:178:PHE:CD1	2.09	0.87
1:C:216:LYS:HE3	1:D:278:ALA:HA	1.54	0.87
1:C:234:GLU:H	1:D:253:SER:HB3	1.39	0.87
1:D:219:TRP:NE1	1:E:249:LEU:HD13	1.89	0.87
1:D:233:GLU:CD	1:E:433:ALA:C	2.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:ALA:C	1:F:274:ARG:HB2	1.99	0.87
1:B:215:GLY:N	1:C:274:ARG:HB2	1.88	0.87
1:D:212:PRO:HB3	1:E:182:ILE:HD13	1.54	0.87
1:C:208:MET:CB	1:D:179:SER:HA	2.04	0.87
1:C:215:GLY:HA2	1:D:275:LEU:HB2	1.54	0.87
1:C:223:SER:N	1:D:439:ARG:HH12	1.71	0.87
1:C:219:TRP:CA	1:D:250:ALA:N	2.38	0.87
1:E:222:ALA:HB2	1:F:437:THR:OG1	1.74	0.87
1:C:233:GLU:CB	1:D:253:SER:HA	2.05	0.87
1:A:213:ASP:C	1:B:274:ARG:HH21	1.80	0.86
1:A:217:ALA:O	1:B:275:LEU:O	1.91	0.86
1:A:235:VAL:CG2	1:B:271:LEU:HD21	1.84	0.86
1:B:216:LYS:HA	1:C:274:ARG:O	1.48	0.86
1:E:220:VAL:HG23	1:F:251:ALA:HA	1.53	0.86
1:B:207:THR:HB	1:C:177:ILE:HG22	1.57	0.86
1:E:227:THR:HB	1:F:435:TYR:CZ	2.10	0.86
1:A:271:LEU:C	1:F:214:ALA:O	2.17	0.86
1:C:208:MET:HA	1:D:178:PHE:C	2.01	0.86
1:E:214:ALA:HB3	1:F:271:LEU:C	2.01	0.86
1:C:233:GLU:N	1:D:252:LYS:HB2	1.88	0.86
1:D:216:LYS:CB	1:E:278:ALA:HB2	2.05	0.86
1:D:235:VAL:CA	1:E:271:LEU:CD1	2.35	0.86
1:A:214:ALA:O	1:B:274:ARG:CG	2.18	0.86
1:B:236:LYS:O	1:C:274:ARG:NH1	2.08	0.86
1:C:215:GLY:CA	1:D:275:LEU:CB	2.51	0.86
1:C:215:GLY:CA	1:D:275:LEU:CA	2.53	0.86
1:C:217:ALA:H	1:D:275:LEU:HD12	1.32	0.86
1:D:216:LYS:HA	1:E:274:ARG:O	1.76	0.86
1:A:271:LEU:HA	1:F:214:ALA:HB3	1.49	0.86
1:B:217:ALA:HB1	1:C:436:VAL:HG23	1.56	0.86
1:B:227:THR:HB	1:C:252:LYS:HD3	0.86	0.86
1:C:227:THR:HB	1:D:435:TYR:CZ	2.11	0.86
1:E:233:GLU:H	1:F:252:LYS:CB	1.87	0.86
1:A:221:ALA:C	1:B:439:ARG:NH1	2.34	0.85
1:D:235:VAL:HG12	1:E:254:PHE:O	1.76	0.85
1:B:213:ASP:O	1:C:274:ARG:CZ	2.12	0.85
1:D:209:LEU:CB	1:E:178:PHE:HB2	2.05	0.85
1:E:207:THR:N	1:F:177:ILE:HG21	1.91	0.85
1:E:214:ALA:CA	1:F:274:ARG:HB2	2.05	0.85
1:C:216:LYS:HE3	1:D:278:ALA:HB2	1.48	0.85
1:E:228:ASP:HB3	1:F:252:LYS:HZ2	1.28	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:VAL:HG12	1:C:251:ALA:O	1.75	0.85
1:C:207:THR:CB	1:D:177:ILE:O	2.25	0.85
1:C:218:THR:O	1:D:279:HIS:ND1	2.08	0.85
1:A:275:LEU:HD23	1:F:216:LYS:C	2.02	0.85
1:A:235:VAL:HA	1:B:271:LEU:HD11	1.58	0.85
1:D:216:LYS:CB	1:E:278:ALA:CB	2.55	0.85
1:C:210:VAL:HG12	1:D:183:ILE:H	1.42	0.85
1:D:215:GLY:C	1:E:275:LEU:HD23	2.01	0.84
1:C:233:GLU:OE1	1:D:252:LYS:CD	2.26	0.84
1:A:210:VAL:HG12	1:B:182:ILE:CA	2.07	0.84
1:A:215:GLY:HA3	1:B:271:LEU:CD1	2.06	0.84
1:A:252:LYS:N	1:F:218:THR:N	2.25	0.84
1:B:214:ALA:HB3	1:C:270:LEU:HG	1.57	0.84
1:B:217:ALA:CB	1:C:436:VAL:CG2	2.35	0.84
1:A:216:LYS:CA	1:B:274:ARG:C	2.47	0.84
1:B:207:THR:CB	1:C:177:ILE:HB	2.05	0.84
1:C:219:TRP:CZ2	1:D:282:SER:C	2.54	0.84
1:B:217:ALA:HB3	1:C:436:VAL:HG21	1.59	0.84
1:B:241:GLU:OE2	1:C:178:PHE:CB	2.24	0.84
1:A:220:VAL:HB	1:B:437:THR:HG22	1.60	0.84
1:E:214:ALA:N	1:F:274:ARG:HB2	1.91	0.84
1:E:232:GLY:CA	1:F:252:LYS:N	2.40	0.84
1:A:233:GLU:HG2	1:B:434:TYR:C	1.98	0.84
1:C:216:LYS:HD2	1:D:278:ALA:HB2	1.59	0.84
1:C:221:ALA:CB	1:D:248:LYS:HB2	2.06	0.84
1:E:214:ALA:HB1	1:F:271:LEU:CG	2.08	0.83
1:C:221:ALA:CA	1:D:248:LYS:HB3	1.90	0.83
1:E:213:ASP:CG	1:F:274:ARG:CD	2.19	0.83
1:A:271:LEU:HD12	1:F:214:ALA:CA	2.08	0.83
1:B:237:GLY:CA	1:C:267:LEU:HD21	2.09	0.83
1:C:233:GLU:CD	1:D:252:LYS:HB2	2.03	0.83
1:A:435:TYR:CE2	1:F:233:GLU:OE2	2.32	0.83
1:A:212:PRO:HB2	1:B:184:ARG:CA	2.07	0.83
1:A:233:GLU:CB	1:B:434:TYR:H	1.90	0.83
1:B:241:GLU:OE1	1:C:178:PHE:HD2	1.62	0.83
1:E:207:THR:OG1	1:F:177:ILE:C	2.20	0.83
1:B:207:THR:HB	1:C:177:ILE:CG2	2.08	0.83
1:C:214:ALA:HB1	1:D:271:LEU:CB	2.09	0.83
1:C:220:VAL:CG1	1:D:250:ALA:HB3	2.09	0.83
1:E:241:GLU:CG	1:F:179:SER:CB	2.28	0.83
1:B:215:GLY:HA2	1:C:275:LEU:HG	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ALA:N	1:F:219:TRP:CG	2.25	0.82
1:C:234:GLU:CB	1:D:275:LEU:CD1	2.57	0.82
1:C:221:ALA:HA	1:D:248:LYS:HB2	0.83	0.82
1:D:211:GLU:CB	1:E:182:ILE:HG12	2.09	0.82
1:E:207:THR:H	1:F:177:ILE:CG2	1.92	0.82
1:A:210:VAL:CG1	1:B:182:ILE:CA	2.51	0.82
1:A:233:GLU:HG2	1:B:433:ALA:C	2.05	0.82
1:B:220:VAL:HG22	1:C:437:THR:HA	1.58	0.82
1:E:228:ASP:CG	1:F:252:LYS:HZ2	1.87	0.82
1:A:220:VAL:CG2	1:B:252:LYS:HG3	1.86	0.82
1:B:215:GLY:CA	1:C:271:LEU:HD12	2.08	0.82
1:C:210:VAL:HG13	1:D:182:ILE:CA	2.04	0.82
1:E:222:ALA:HB3	1:F:439:ARG:HH22	1.37	0.82
1:A:182:ILE:CB	1:F:211:GLU:C	2.50	0.82
1:A:207:THR:CB	1:B:177:ILE:H	1.91	0.82
1:C:216:LYS:HG3	1:D:278:ALA:HB1	1.60	0.82
1:A:219:TRP:CG	1:B:279:HIS:HE1	1.97	0.82
1:A:271:LEU:HD11	1:F:235:VAL:C	1.99	0.82
1:E:217:ALA:CB	1:F:279:HIS:CA	2.54	0.82
1:A:218:THR:CB	1:B:251:ALA:HB1	1.62	0.82
1:B:214:ALA:C	1:C:274:ARG:CG	2.50	0.82
1:D:220:VAL:CG2	1:E:251:ALA:N	2.43	0.82
1:E:207:THR:HB	1:F:178:PHE:O	1.79	0.82
1:A:271:LEU:HA	1:F:214:ALA:CA	2.08	0.82
1:B:230:THR:OG1	1:C:252:LYS:HD2	1.80	0.82
1:C:219:TRP:CG	1:D:249:LEU:HD22	2.15	0.82
1:D:216:LYS:N	1:E:275:LEU:HD23	1.95	0.82
1:A:204:LYS:HB2	1:B:174:TYR:HE2	1.45	0.81
1:C:212:PRO:HB2	1:D:184:ARG:HA	1.62	0.81
1:B:234:GLU:O	1:C:275:LEU:CD2	2.27	0.81
1:C:219:TRP:HB3	1:D:249:LEU:HA	1.62	0.81
1:C:220:VAL:HB	1:D:250:ALA:C	2.04	0.81
1:C:233:GLU:OE1	1:D:252:LYS:CG	2.27	0.81
1:D:208:MET:CB	1:E:179:SER:HA	2.10	0.81
1:A:250:ALA:HB2	1:F:220:VAL:O	1.81	0.81
1:B:219:TRP:CD2	1:C:249:LEU:HD23	2.14	0.81
1:A:435:TYR:CD2	1:F:233:GLU:OE2	2.33	0.81
1:B:316:ALA:O	1:C:353:TYR:OH	1.98	0.81
1:C:233:GLU:HB3	1:D:253:SER:C	2.06	0.81
1:A:253:SER:N	1:F:233:GLU:HG3	1.95	0.81
1:A:361:GLU:CD	1:B:363:GLN:OE1	2.23	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ALA:H	1:C:275:LEU:CG	1.92	0.81
1:B:232:GLY:CA	1:C:252:LYS:HB3	2.10	0.81
1:D:219:TRP:CG	1:E:249:LEU:HD22	2.16	0.81
1:C:234:GLU:N	1:D:253:SER:HA	1.94	0.81
1:D:233:GLU:CG	1:E:434:TYR:O	2.29	0.81
1:E:207:THR:CB	1:F:177:ILE:HG22	2.11	0.81
1:A:185:ASP:OD1	1:F:213:ASP:CB	2.29	0.81
1:A:219:TRP:HH2	1:B:248:LYS:HB2	1.46	0.81
1:C:213:ASP:CB	1:D:274:ARG:HD3	2.11	0.81
1:B:216:LYS:H	1:C:275:LEU:CD2	1.94	0.81
1:A:219:TRP:CG	1:B:249:LEU:HB3	1.84	0.80
1:C:220:VAL:H	1:D:249:LEU:CA	1.94	0.80
1:C:233:GLU:HG2	1:D:254:PHE:HB2	1.63	0.80
1:D:233:GLU:CD	1:E:433:ALA:HB1	2.07	0.80
1:E:205:ILE:HG23	1:F:177:ILE:CB	2.10	0.80
1:A:207:THR:HG21	1:B:176:THR:HG22	1.61	0.80
1:A:218:THR:HG22	1:B:252:LYS:H	1.45	0.80
1:A:252:LYS:HD2	1:F:231:THR:O	1.80	0.80
1:B:207:THR:HB	1:C:177:ILE:CB	1.96	0.80
1:D:207:THR:N	1:E:177:ILE:CB	1.83	0.80
1:D:232:GLY:HA2	1:E:252:LYS:CE	2.09	0.80
1:C:360:GLU:HB2	1:D:362:TRP:O	1.80	0.80
1:D:219:TRP:CZ2	1:E:282:SER:O	2.34	0.80
1:C:217:ALA:H	1:D:275:LEU:HD11	1.47	0.80
1:C:219:TRP:HB3	1:D:249:LEU:CB	2.12	0.80
1:C:233:GLU:CB	1:D:253:SER:CA	2.54	0.80
1:A:236:LYS:N	1:B:271:LEU:HD11	1.94	0.80
1:A:352:ALA:CB	1:F:332:ARG:NE	2.40	0.80
1:E:233:GLU:H	1:F:252:LYS:HB2	1.40	0.80
1:B:235:VAL:HG13	1:C:255:ILE:HG21	1.63	0.80
1:C:219:TRP:CD1	1:D:249:LEU:CD1	2.64	0.80
1:D:206:LEU:CA	1:E:177:ILE:HB	2.12	0.80
1:B:209:LEU:O	1:C:181:ARG:O	1.88	0.80
1:C:212:PRO:HA	1:D:182:ILE:HD13	1.63	0.80
1:C:232:GLY:O	1:D:251:ALA:HB1	1.82	0.80
1:E:208:MET:HE3	1:F:181:ARG:HD2	1.63	0.80
1:B:216:LYS:CB	1:C:274:ARG:O	2.30	0.80
1:C:221:ALA:C	1:D:248:LYS:CB	2.56	0.80
1:D:232:GLY:C	1:E:252:LYS:C	2.39	0.80
1:A:217:ALA:HB1	1:B:436:VAL:CG2	2.12	0.79
1:A:231:THR:O	1:B:252:LYS:CB	2.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:HIS:CE1	1:F:219:TRP:HD1	1.93	0.79
1:C:221:ALA:C	1:D:248:LYS:HG2	2.06	0.79
1:A:217:ALA:O	1:B:279:HIS:CB	2.30	0.79
1:A:271:LEU:CD1	1:F:214:ALA:C	2.51	0.79
1:D:206:LEU:HA	1:E:177:ILE:CB	2.12	0.79
1:D:231:THR:OG1	1:E:252:LYS:HG2	1.81	0.79
1:E:234:GLU:CA	1:F:253:SER:HB3	2.12	0.79
1:D:235:VAL:CB	1:E:255:ILE:CB	2.60	0.79
1:A:211:GLU:H	1:B:181:ARG:C	1.88	0.79
1:C:233:GLU:HB3	1:D:254:PHE:H	1.45	0.79
1:A:217:ALA:HB3	1:B:276:ILE:N	1.98	0.79
1:B:212:PRO:HB2	1:C:183:ILE:O	1.71	0.79
1:E:225:TYR:CB	1:F:422:GLU:OE2	2.31	0.79
1:A:216:LYS:N	1:B:275:LEU:CG	2.45	0.79
1:A:275:LEU:CD2	1:F:215:GLY:C	2.53	0.79
1:A:235:VAL:HA	1:B:271:LEU:CD2	2.12	0.79
1:B:214:ALA:C	1:C:274:ARG:CB	2.55	0.79
1:E:241:GLU:HG3	1:F:179:SER:HB3	0.79	0.79
1:A:206:LEU:CA	1:B:177:ILE:CG1	2.62	0.78
1:A:219:TRP:HA	1:B:279:HIS:ND1	1.97	0.78
1:B:210:VAL:CB	1:C:182:ILE:HA	2.14	0.78
1:D:233:GLU:OE1	1:E:434:TYR:N	2.13	0.78
1:A:219:TRP:CA	1:B:279:HIS:ND1	2.46	0.78
1:A:206:LEU:CA	1:B:177:ILE:HG13	2.13	0.78
1:A:252:LYS:HD3	1:F:233:GLU:OE2	1.82	0.78
1:D:232:GLY:O	1:E:252:LYS:CA	2.31	0.78
1:D:235:VAL:HG22	1:E:255:ILE:HD12	1.63	0.78
1:A:216:LYS:N	1:B:275:LEU:HG	1.98	0.78
1:A:222:ALA:CA	1:B:439:ARG:NH1	2.46	0.78
1:A:252:LYS:HE2	1:F:230:THR:OG1	1.82	0.78
1:A:274:ARG:HB2	1:F:214:ALA:O	1.83	0.78
1:A:212:PRO:CB	1:B:184:ARG:HA	2.12	0.78
1:E:232:GLY:CA	1:F:252:LYS:CG	2.61	0.78
1:E:219:TRP:CB	1:F:249:LEU:HA	2.09	0.78
1:A:218:THR:CG2	1:B:252:LYS:N	2.47	0.77
1:A:349:SER:OG	1:F:315:LYS:O	2.00	0.77
1:B:214:ALA:HB3	1:C:270:LEU:CB	2.13	0.77
1:E:222:ALA:CB	1:F:439:ARG:NH2	2.40	0.77
1:E:207:THR:N	1:F:177:ILE:HG22	1.99	0.77
1:E:214:ALA:HB3	1:F:271:LEU:O	1.85	0.77
1:B:210:VAL:HG13	1:C:182:ILE:CA	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:CA	1:D:275:LEU:HA	2.15	0.77
1:C:216:LYS:O	1:D:278:ALA:C	2.27	0.77
1:E:205:ILE:HG23	1:F:177:ILE:HB	1.65	0.77
1:D:237:GLY:C	1:E:267:LEU:HD11	2.10	0.77
1:A:274:ARG:NH1	1:F:212:PRO:CD	2.39	0.77
1:D:236:LYS:N	1:E:271:LEU:CD1	2.41	0.77
1:A:215:GLY:H	1:B:271:LEU:HD13	1.50	0.77
1:C:216:LYS:CA	1:D:275:LEU:HD12	2.14	0.77
1:D:222:ALA:HB3	1:E:437:THR:OG1	1.85	0.77
1:E:207:THR:HG22	1:F:179:SER:CA	2.14	0.77
1:E:219:TRP:CZ2	1:F:282:SER:O	2.37	0.77
1:C:234:GLU:N	1:D:253:SER:CA	2.47	0.77
1:C:316:ALA:CB	1:D:352:ALA:HB1	2.15	0.77
1:A:174:TYR:CZ	1:F:204:LYS:HB2	2.11	0.76
1:A:210:VAL:CA	1:B:181:ARG:O	2.28	0.76
1:A:207:THR:O	1:B:177:ILE:HG22	1.81	0.76
1:A:217:ALA:HB1	1:B:436:VAL:HG21	1.66	0.76
1:B:214:ALA:HB3	1:C:270:LEU:CG	2.14	0.76
1:C:215:GLY:C	1:D:275:LEU:CA	2.54	0.76
1:C:212:PRO:HB2	1:D:184:ARG:C	2.09	0.76
1:A:181:ARG:CA	1:F:211:GLU:OE2	2.33	0.76
1:A:331:ARG:HH12	1:B:355:ASP:HB2	1.44	0.76
1:B:231:THR:O	1:C:252:LYS:CB	2.34	0.76
1:C:383:TYR:HA	1:D:371:ASP:HB3	1.67	0.76
1:A:176:THR:CG2	1:F:205:ILE:HG21	2.14	0.76
1:A:217:ALA:HB2	1:B:275:LEU:HB2	1.66	0.76
1:A:275:LEU:CD2	1:F:216:LYS:C	2.56	0.76
1:B:212:PRO:HB3	1:C:183:ILE:CA	2.15	0.76
1:A:185:ASP:OD1	1:F:213:ASP:HB2	1.85	0.76
1:E:221:ALA:CA	1:F:248:LYS:CB	2.61	0.76
1:E:228:ASP:CG	1:F:252:LYS:NZ	2.43	0.76
1:A:207:THR:O	1:B:177:ILE:CG2	2.21	0.76
1:A:215:GLY:C	1:B:274:ARG:HB3	2.11	0.76
1:A:275:LEU:HD21	1:F:216:LYS:N	1.94	0.76
1:C:232:GLY:HA3	1:D:252:LYS:CG	2.16	0.76
1:D:237:GLY:HA2	1:E:267:LEU:HD13	1.65	0.76
1:E:219:TRP:CG	1:F:249:LEU:HD22	2.21	0.76
1:A:235:VAL:HB	1:B:271:LEU:HD21	1.64	0.75
1:A:268:LEU:HG	1:F:235:VAL:HG21	1.68	0.75
1:C:220:VAL:HG21	1:D:251:ALA:HA	1.68	0.75
1:B:204:LYS:HB2	1:C:175:GLU:OE1	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PRO:HB3	1:C:182:ILE:C	2.11	0.75
1:C:216:LYS:N	1:D:275:LEU:CD1	2.28	0.75
1:C:219:TRP:CG	1:D:249:LEU:HD13	2.21	0.75
1:D:211:GLU:O	1:E:182:ILE:HG12	1.72	0.75
1:A:275:LEU:HD21	1:F:234:GLU:HB2	1.69	0.75
1:C:223:SER:N	1:D:439:ARG:NH1	2.29	0.75
1:D:232:GLY:O	1:E:252:LYS:CB	2.35	0.75
1:E:207:THR:OG1	1:F:177:ILE:HB	1.87	0.75
1:E:228:ASP:OD1	1:F:252:LYS:NZ	2.19	0.75
1:A:226:GLY:HA3	1:B:424:GLU:CD	2.10	0.75
1:D:220:VAL:CB	1:E:251:ALA:N	2.47	0.75
1:E:233:GLU:HG3	1:F:252:LYS:HB3	1.67	0.75
1:B:209:LEU:N	1:C:180:GLN:N	2.23	0.75
1:E:219:TRP:HZ2	1:F:282:SER:O	1.69	0.75
1:D:216:LYS:O	1:E:275:LEU:C	2.30	0.75
1:D:219:TRP:HZ2	1:E:286:ALA:HB2	1.43	0.75
1:C:212:PRO:O	1:D:274:ARG:NH2	2.19	0.74
1:C:331:ARG:NH1	1:D:376:GLN:HE21	1.83	0.74
1:E:221:ALA:CA	1:F:248:LYS:HB3	2.15	0.74
1:B:232:GLY:HA3	1:C:254:PHE:HD1	1.50	0.74
1:C:234:GLU:H	1:D:253:SER:CB	2.00	0.74
1:E:234:GLU:N	1:F:253:SER:HA	1.14	0.74
1:A:215:GLY:H	1:B:271:LEU:HD12	0.91	0.74
1:A:215:GLY:C	1:B:274:ARG:CB	2.60	0.74
1:A:252:LYS:HB2	1:F:232:GLY:O	1.88	0.74
1:C:235:VAL:CG2	1:D:271:LEU:HD21	2.16	0.74
1:E:207:THR:HB	1:F:177:ILE:HG22	1.68	0.74
1:E:227:THR:HB	1:F:435:TYR:CE1	2.22	0.74
1:A:222:ALA:O	1:B:439:ARG:NH1	2.20	0.74
1:B:220:VAL:HG23	1:C:437:THR:CG2	1.96	0.74
1:C:219:TRP:HA	1:D:249:LEU:C	2.12	0.74
1:D:208:MET:HB3	1:E:179:SER:HA	1.67	0.74
1:A:218:THR:HG23	1:B:252:LYS:H	1.51	0.74
1:A:220:VAL:HB	1:B:437:THR:CG2	2.17	0.74
1:C:208:MET:HB2	1:D:179:SER:CA	2.18	0.74
1:C:219:TRP:CB	1:D:249:LEU:HB3	2.18	0.74
1:D:207:THR:OG1	1:E:176:THR:C	2.30	0.74
1:D:235:VAL:HG23	1:E:255:ILE:HD12	1.69	0.74
1:D:446:PHE:HZ	1:E:183:ILE:HD11	1.51	0.74
1:A:176:THR:CA	1:F:205:ILE:HG23	2.12	0.74
1:B:210:VAL:CG1	1:C:183:ILE:H	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ASP:OD1	1:F:274:ARG:NE	2.21	0.74
1:B:234:GLU:HG2	1:C:252:LYS:O	1.87	0.73
1:B:280:ALA:HA	1:B:283:ILE:HD12	1.69	0.73
1:C:208:MET:CA	1:D:179:SER:CA	2.65	0.73
1:C:227:THR:CB	1:D:435:TYR:OH	2.34	0.73
1:C:331:ARG:CZ	1:D:376:GLN:HE21	1.99	0.73
1:C:234:GLU:N	1:D:253:SER:HB3	2.03	0.73
1:C:383:TYR:HD2	1:D:371:ASP:HB2	1.53	0.73
1:D:215:GLY:H	1:E:271:LEU:HG	1.49	0.73
1:D:237:GLY:CA	1:E:267:LEU:CD1	2.37	0.73
1:A:227:THR:N	1:B:435:TYR:CE1	2.55	0.73
1:A:252:LYS:HE3	1:F:227:THR:OG1	1.88	0.73
1:D:332:ARG:NH1	1:E:351:ASP:OD2	2.21	0.73
1:E:210:VAL:CB	1:F:182:ILE:HA	2.16	0.73
1:A:218:THR:HG22	1:B:252:LYS:N	2.04	0.73
1:A:220:VAL:HG13	1:B:252:LYS:CE	2.17	0.73
1:E:219:TRP:HB3	1:F:249:LEU:CB	2.19	0.73
1:B:214:ALA:HB3	1:C:271:LEU:N	2.03	0.73
1:E:217:ALA:HB1	1:F:279:HIS:HB2	0.73	0.73
1:A:220:VAL:CB	1:B:437:THR:CG2	2.65	0.73
1:A:220:VAL:C	1:B:437:THR:HG22	2.13	0.73
1:A:352:ALA:HB1	1:F:332:ARG:HE	1.52	0.73
1:E:234:GLU:O	1:F:253:SER:HB2	1.88	0.73
1:E:235:VAL:HG12	1:F:271:LEU:HD21	1.70	0.73
1:D:446:PHE:HZ	1:E:183:ILE:CD1	2.02	0.73
1:E:211:GLU:HG2	1:F:182:ILE:HD12	0.87	0.73
1:A:331:ARG:NH1	1:B:355:ASP:CB	2.13	0.72
1:B:216:LYS:N	1:C:275:LEU:CG	2.52	0.72
1:C:216:LYS:CG	1:D:278:ALA:CB	2.62	0.72
1:C:216:LYS:C	1:D:275:LEU:HD12	2.12	0.72
1:D:233:GLU:OE2	1:E:433:ALA:C	2.31	0.72
1:A:331:ARG:NH2	1:B:355:ASP:CG	2.46	0.72
1:C:208:MET:HA	1:D:179:SER:CA	2.19	0.72
1:C:234:GLU:N	1:D:253:SER:CB	2.52	0.72
1:D:235:VAL:CG1	1:E:255:ILE:CA	2.42	0.72
1:E:234:GLU:CA	1:F:253:SER:CB	2.67	0.72
1:C:219:TRP:CG	1:D:249:LEU:HB3	2.23	0.72
1:C:360:GLU:CB	1:D:362:TRP:O	2.37	0.72
1:D:214:ALA:C	1:E:274:ARG:HB2	2.14	0.72
1:A:203:SER:OG	1:B:175:GLU:OE1	2.05	0.72
1:E:210:VAL:HB	1:F:183:ILE:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:LYS:C	1:C:267:LEU:HD21	2.15	0.72
1:C:234:GLU:CB	1:D:275:LEU:HD11	2.09	0.72
1:C:383:TYR:CB	1:D:371:ASP:HB3	2.19	0.72
1:E:217:ALA:HB3	1:F:279:HIS:CB	2.05	0.71
1:A:219:TRP:CH2	1:B:248:LYS:CB	2.73	0.71
1:C:219:TRP:HA	1:D:249:LEU:CA	2.20	0.71
1:C:383:TYR:HB3	1:D:371:ASP:HB3	1.71	0.71
1:A:215:GLY:HA3	1:B:271:LEU:CG	2.21	0.71
1:C:205:ILE:O	1:D:177:ILE:HG12	1.90	0.71
1:C:220:VAL:CB	1:D:250:ALA:CB	2.24	0.71
1:E:213:ASP:HA	1:F:274:ARG:HD2	0.72	0.71
1:A:218:THR:CG2	1:B:251:ALA:HB1	2.20	0.71
1:A:275:LEU:HD21	1:F:234:GLU:CB	2.21	0.71
1:B:207:THR:OG1	1:C:177:ILE:CA	2.24	0.71
1:B:214:ALA:CB	1:C:270:LEU:CG	2.68	0.71
1:A:230:THR:OG1	1:B:252:LYS:HD2	1.89	0.71
1:E:214:ALA:CA	1:F:274:ARG:CB	2.67	0.71
1:A:185:ASP:OD1	1:F:213:ASP:HB3	1.91	0.71
1:B:210:VAL:HG13	1:C:182:ILE:C	2.14	0.71
1:C:212:PRO:CA	1:D:182:ILE:HD13	2.17	0.71
1:C:219:TRP:HB3	1:D:249:LEU:CA	2.20	0.71
1:D:232:GLY:C	1:E:252:LYS:O	2.32	0.71
1:A:216:LYS:HZ2	1:B:277:GLU:C	1.87	0.71
1:A:227:THR:H	1:B:435:TYR:HE1	1.38	0.71
1:A:237:GLY:HA2	1:B:267:LEU:HD13	1.71	0.71
1:D:213:ASP:C	1:E:274:ARG:HG3	2.14	0.71
1:C:219:TRP:HA	1:D:249:LEU:HB3	1.73	0.70
1:D:206:LEU:CA	1:E:177:ILE:CB	2.68	0.70
1:A:275:LEU:CD2	1:F:234:GLU:HB2	2.21	0.70
1:B:214:ALA:CB	1:C:271:LEU:N	2.55	0.70
1:B:215:GLY:HA2	1:C:271:LEU:HD12	1.72	0.70
1:B:214:ALA:CB	1:C:270:LEU:C	2.63	0.70
1:C:217:ALA:HB1	1:D:279:HIS:CG	2.27	0.70
1:B:233:GLU:OE1	1:C:433:ALA:C	2.32	0.70
1:C:219:TRP:CB	1:D:249:LEU:CB	2.69	0.70
1:E:227:THR:CB	1:F:435:TYR:OH	2.39	0.70
1:C:207:THR:HB	1:D:177:ILE:C	2.16	0.70
1:C:316:ALA:HB2	1:D:352:ALA:HB1	1.73	0.70
1:D:215:GLY:O	1:E:274:ARG:HB3	1.91	0.70
1:E:208:MET:CE	1:F:181:ARG:HB2	2.22	0.70
1:D:219:TRP:HB3	1:E:249:LEU:HD22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:THR:CG2	1:F:178:PHE:O	2.40	0.70
1:C:220:VAL:CA	1:D:250:ALA:HB3	2.19	0.70
1:A:234:GLU:O	1:B:275:LEU:CD1	2.40	0.69
1:D:219:TRP:CZ2	1:E:286:ALA:CB	2.68	0.69
1:E:220:VAL:HG11	1:F:435:TYR:CZ	2.24	0.69
1:A:176:THR:HG23	1:F:205:ILE:HD13	1.73	0.69
1:B:212:PRO:HB2	1:C:184:ARG:N	2.08	0.69
1:A:178:PHE:CA	1:F:207:THR:HG22	2.21	0.69
1:A:222:ALA:HB2	1:B:437:THR:CG2	2.20	0.69
1:A:217:ALA:CB	1:B:275:LEU:CA	2.69	0.69
1:A:217:ALA:H	1:B:275:LEU:HD23	1.53	0.69
1:C:227:THR:HB	1:D:435:TYR:CE1	2.26	0.69
1:A:235:VAL:CA	1:B:271:LEU:HD11	2.22	0.69
1:D:232:GLY:C	1:E:252:LYS:CB	2.65	0.69
1:E:214:ALA:C	1:F:274:ARG:CB	2.61	0.69
1:A:178:PHE:HA	1:F:207:THR:CG2	2.22	0.69
1:A:220:VAL:CG1	1:B:252:LYS:HE3	2.19	0.69
1:B:217:ALA:CA	1:C:275:LEU:CD2	2.44	0.69
1:C:221:ALA:C	1:D:248:LYS:HB3	2.16	0.69
1:A:178:PHE:O	1:F:208:MET:CB	2.41	0.69
1:A:232:GLY:O	1:B:252:LYS:C	2.36	0.69
1:B:241:GLU:CD	1:C:178:PHE:HD2	2.00	0.69
1:B:216:LYS:HB2	1:C:274:ARG:O	1.93	0.69
1:D:207:THR:N	1:E:177:ILE:CA	2.45	0.69
1:D:235:VAL:HG11	1:E:255:ILE:CB	2.23	0.69
1:A:252:LYS:H	1:F:218:THR:N	1.87	0.68
1:A:252:LYS:HG3	1:F:220:VAL:CG2	2.23	0.68
1:A:271:LEU:HD12	1:F:215:GLY:H	1.55	0.68
1:B:214:ALA:O	1:C:274:ARG:HG3	1.92	0.68
1:D:235:VAL:CG2	1:E:255:ILE:CB	2.32	0.68
1:C:331:ARG:NH2	1:D:376:GLN:NE2	2.40	0.68
1:D:234:GLU:HG3	1:E:253:SER:HB3	1.74	0.68
1:A:220:VAL:HG23	1:B:251:ALA:CA	2.24	0.68
1:D:219:TRP:HZ2	1:E:282:SER:O	1.72	0.68
1:A:213:ASP:O	1:B:274:ARG:NH2	2.16	0.68
1:A:219:TRP:HH2	1:B:248:LYS:CB	2.06	0.68
1:B:316:ALA:HB1	1:C:353:TYR:CE1	2.28	0.68
1:C:210:VAL:CG1	1:D:182:ILE:CA	2.67	0.68
1:C:216:LYS:O	1:D:278:ALA:HB3	1.92	0.68
1:E:220:VAL:HG21	1:F:251:ALA:CA	2.23	0.68
1:A:252:LYS:CG	1:F:220:VAL:CG2	2.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:GLY:C	1:E:274:ARG:HB2	2.19	0.68
1:E:214:ALA:O	1:F:274:ARG:C	2.37	0.68
1:D:216:LYS:C	1:E:275:LEU:CA	2.46	0.68
1:A:219:TRP:HA	1:B:279:HIS:CE1	2.29	0.68
1:A:222:ALA:CA	1:B:439:ARG:HH12	2.04	0.68
1:A:252:LYS:N	1:F:217:ALA:HB1	2.09	0.68
1:E:225:TYR:HA	1:F:422:GLU:CD	2.18	0.68
1:C:205:ILE:O	1:D:177:ILE:CG1	2.42	0.68
1:C:219:TRP:NE1	1:D:249:LEU:HD13	2.07	0.68
1:E:214:ALA:HB1	1:F:271:LEU:CB	2.24	0.68
1:B:216:LYS:H	1:C:275:LEU:CG	2.06	0.67
1:C:235:VAL:HG22	1:D:271:LEU:CD1	1.97	0.67
1:B:207:THR:HG21	1:C:178:PHE:HA	1.75	0.67
1:A:222:ALA:CB	1:B:437:THR:HG21	2.22	0.67
1:E:209:LEU:HB2	1:F:180:GLN:N	2.10	0.67
1:A:210:VAL:HG13	1:B:182:ILE:CA	2.17	0.67
1:D:234:GLU:CG	1:E:253:SER:HB3	1.99	0.67
1:B:216:LYS:N	1:C:275:LEU:HG	2.09	0.67
1:A:234:GLU:CB	1:B:275:LEU:CD2	2.70	0.67
1:D:206:LEU:CA	1:E:177:ILE:CG1	2.65	0.67
1:E:207:THR:H	1:F:177:ILE:HG21	1.55	0.67
1:E:235:VAL:HG13	1:F:253:SER:HB2	1.76	0.67
1:E:241:GLU:HG3	1:F:179:SER:CA	2.22	0.67
1:C:219:TRP:HD1	1:D:249:LEU:HB3	1.58	0.66
1:D:213:ASP:C	1:E:274:ARG:CG	2.68	0.66
1:E:217:ALA:HB2	1:F:275:LEU:O	1.95	0.66
1:C:218:THR:HG22	1:D:251:ALA:HB2	0.74	0.66
1:D:215:GLY:HA2	1:E:275:LEU:CD2	2.24	0.66
1:A:217:ALA:CB	1:B:436:VAL:HG21	2.25	0.66
1:A:235:VAL:HA	1:B:271:LEU:CD1	2.25	0.66
1:E:222:ALA:HB1	1:F:439:ARG:HH22	1.58	0.66
1:E:225:TYR:HB3	1:F:422:GLU:OE2	1.94	0.66
1:A:217:ALA:CB	1:B:275:LEU:O	2.36	0.66
1:A:236:LYS:N	1:B:271:LEU:HD13	1.97	0.66
1:C:220:VAL:HB	1:D:250:ALA:HB3	0.67	0.66
1:E:219:TRP:NE1	1:F:282:SER:C	2.50	0.66
1:A:218:THR:HG23	1:B:252:LYS:N	2.10	0.66
1:B:214:ALA:C	1:C:274:ARG:HG3	2.20	0.66
1:E:227:THR:O	1:F:252:LYS:CG	2.43	0.66
1:E:218:THR:HG23	1:F:250:ALA:O	1.96	0.66
1:D:216:LYS:HD2	1:E:274:ARG:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:ASP:CB	1:F:252:LYS:HZ3	1.89	0.66
1:A:235:VAL:C	1:B:271:LEU:HD11	2.20	0.66
1:A:275:LEU:O	1:F:216:LYS:O	2.13	0.66
1:A:362:TRP:O	1:F:360:GLU:OE1	2.13	0.66
1:C:220:VAL:CB	1:D:250:ALA:O	2.42	0.66
1:C:232:GLY:HA2	1:D:251:ALA:CA	2.11	0.66
1:C:232:GLY:O	1:D:251:ALA:CB	2.40	0.66
1:D:235:VAL:HG11	1:E:255:ILE:HA	0.75	0.66
1:B:214:ALA:N	1:C:270:LEU:HG	2.09	0.66
1:D:213:ASP:HB2	1:E:274:ARG:NH2	2.11	0.66
1:A:176:THR:HG23	1:F:205:ILE:CG2	2.21	0.65
1:A:361:GLU:CD	1:B:363:GLN:CD	2.64	0.65
1:E:205:ILE:HG22	1:F:177:ILE:CG1	2.09	0.65
1:A:204:LYS:CB	1:B:174:TYR:HE2	2.09	0.65
1:A:217:ALA:CA	1:B:275:LEU:O	2.44	0.65
1:A:362:TRP:CH2	1:B:362:TRP:HD1	1.85	0.65
1:B:212:PRO:O	1:C:182:ILE:HD11	1.95	0.65
1:A:184:ARG:C	1:F:212:PRO:O	2.40	0.65
1:A:254:PHE:CD2	1:F:233:GLU:OE1	2.50	0.65
1:A:274:ARG:HB2	1:F:214:ALA:C	2.20	0.65
1:E:228:ASP:HB3	1:F:252:LYS:CE	2.23	0.65
1:B:406:VAL:HG13	1:B:410:ASN:HB2	1.79	0.65
1:C:219:TRP:CZ2	1:D:286:ALA:HB2	2.30	0.65
1:C:232:GLY:O	1:D:252:LYS:O	2.05	0.65
1:E:207:THR:CB	1:F:178:PHE:O	2.45	0.65
1:E:209:LEU:CB	1:F:180:GLN:C	2.69	0.65
1:D:220:VAL:HG23	1:E:250:ALA:C	2.22	0.65
1:C:219:TRP:CB	1:D:249:LEU:HA	2.27	0.65
1:C:331:ARG:NE	1:D:376:GLN:HE22	1.93	0.65
1:B:212:PRO:O	1:C:182:ILE:CD1	2.40	0.65
1:D:216:LYS:HG3	1:E:278:ALA:CA	2.19	0.65
1:D:220:VAL:HG23	1:E:251:ALA:N	2.10	0.64
1:D:216:LYS:O	1:E:275:LEU:O	2.14	0.64
1:E:208:MET:HE3	1:F:181:ARG:HB2	1.79	0.64
1:E:227:THR:CB	1:F:435:TYR:HH	2.10	0.64
1:A:217:ALA:CA	1:B:275:LEU:C	2.69	0.64
1:C:214:ALA:HB3	1:D:271:LEU:N	2.12	0.64
1:C:234:GLU:C	1:D:253:SER:HB3	2.22	0.64
1:C:332:ARG:NH1	1:D:351:ASP:OD2	2.30	0.64
1:B:210:VAL:HG12	1:C:183:ILE:H	1.56	0.64
1:A:215:GLY:CA	1:B:271:LEU:CG	2.72	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:HB3	1:F:233:GLU:OE2	1.98	0.64
1:A:215:GLY:HA3	1:B:271:LEU:HG	1.78	0.64
1:B:211:GLU:N	1:C:181:ARG:C	2.56	0.64
1:C:219:TRP:CA	1:D:249:LEU:CA	2.75	0.64
1:D:213:ASP:C	1:E:270:LEU:HG	2.22	0.64
1:A:180:GLN:H	1:F:208:MET:HE3	1.62	0.64
1:A:213:ASP:H	1:B:182:ILE:HD11	1.62	0.64
1:C:234:GLU:C	1:D:253:SER:CB	2.71	0.64
1:D:235:VAL:HG21	1:E:255:ILE:HG13	1.68	0.64
1:A:230:THR:OG1	1:B:252:LYS:CD	2.47	0.63
1:B:232:GLY:C	1:C:252:LYS:HB3	2.22	0.63
1:D:212:PRO:HB2	1:E:184:ARG:HA	1.81	0.63
1:A:216:LYS:HD2	1:B:274:ARG:O	1.98	0.63
1:A:274:ARG:CB	1:F:215:GLY:O	2.46	0.63
1:C:383:TYR:CA	1:D:371:ASP:HB3	2.27	0.63
1:A:215:GLY:HA3	1:B:271:LEU:HD12	1.61	0.63
1:A:235:VAL:CB	1:B:271:LEU:CD2	2.51	0.63
1:D:237:GLY:HA2	1:E:267:LEU:CG	2.27	0.63
1:A:206:LEU:HA	1:B:177:ILE:HG12	1.78	0.63
1:A:270:LEU:C	1:F:214:ALA:HB3	2.23	0.63
1:A:220:VAL:CG1	1:B:437:THR:HG22	2.21	0.63
1:A:254:PHE:CB	1:F:233:GLU:H	2.05	0.63
1:D:233:GLU:CD	1:E:434:TYR:O	2.42	0.63
1:E:214:ALA:HB2	1:F:271:LEU:CA	1.98	0.63
1:A:220:VAL:HG12	1:B:437:THR:HG22	1.75	0.63
1:C:232:GLY:CA	1:D:251:ALA:CA	2.75	0.63
1:A:218:THR:HG22	1:B:252:LYS:O	1.99	0.63
1:B:235:VAL:CG1	1:C:255:ILE:CG1	2.70	0.63
1:D:214:ALA:O	1:E:274:ARG:HB2	1.98	0.63
1:E:250:ALA:HA	1:E:279:HIS:HE1	1.64	0.63
1:A:213:ASP:H	1:B:182:ILE:CD1	2.11	0.62
1:D:220:VAL:HB	1:E:251:ALA:N	1.95	0.62
1:E:207:THR:OG1	1:F:177:ILE:CB	2.47	0.62
1:C:227:THR:O	1:D:252:LYS:CD	2.34	0.62
1:D:216:LYS:HG3	1:E:278:ALA:HB2	0.64	0.62
1:E:210:VAL:HA	1:F:182:ILE:N	2.09	0.62
1:D:207:THR:H	1:E:177:ILE:CG2	2.02	0.62
1:D:210:VAL:HG12	1:E:182:ILE:CB	2.13	0.62
1:A:220:VAL:CG1	1:B:252:LYS:CE	2.77	0.62
1:C:219:TRP:CA	1:D:249:LEU:HA	2.30	0.62
1:B:220:VAL:HG12	1:C:252:LYS:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:O	1:D:275:LEU:O	2.16	0.62
1:D:220:VAL:HG23	1:E:251:ALA:CA	2.29	0.62
1:A:219:TRP:CB	1:B:279:HIS:CE1	2.83	0.62
1:B:237:GLY:CA	1:C:267:LEU:HD11	2.29	0.62
1:C:216:LYS:H	1:D:275:LEU:CA	1.99	0.62
1:D:215:GLY:CA	1:E:271:LEU:HG	2.28	0.62
1:D:216:LYS:CA	1:E:278:ALA:CB	2.77	0.62
1:D:446:PHE:CZ	1:E:183:ILE:HD11	2.33	0.62
1:B:235:VAL:HG12	1:C:255:ILE:HG12	1.80	0.62
1:E:209:LEU:HB3	1:F:180:GLN:C	2.25	0.62
1:B:237:GLY:HA2	1:C:267:LEU:HD11	1.80	0.62
1:D:235:VAL:N	1:E:254:PHE:O	2.33	0.62
1:A:204:LYS:HB2	1:B:174:TYR:CE2	2.32	0.61
1:A:222:ALA:HB3	1:B:439:ARG:NH1	2.15	0.61
1:B:210:VAL:HG11	1:C:183:ILE:N	2.13	0.61
1:C:213:ASP:N	1:D:274:ARG:HD2	2.14	0.61
1:A:274:ARG:NH1	1:F:212:PRO:HD2	2.15	0.61
1:A:217:ALA:C	1:B:275:LEU:O	2.43	0.61
1:C:208:MET:CB	1:D:179:SER:CA	2.78	0.61
1:D:216:LYS:CA	1:E:278:ALA:HB3	2.30	0.61
1:D:383:TYR:C	1:E:371:ASP:HB3	2.25	0.61
1:E:219:TRP:C	1:F:250:ALA:C	2.61	0.61
1:E:219:TRP:CD1	1:F:249:LEU:HB3	2.35	0.61
1:A:215:GLY:N	1:B:271:LEU:HA	2.15	0.61
1:C:216:LYS:HD2	1:D:278:ALA:CB	2.21	0.61
1:E:220:VAL:N	1:F:250:ALA:O	2.34	0.61
1:D:213:ASP:CA	1:E:274:ARG:NH2	2.63	0.61
1:D:219:TRP:CB	1:E:249:LEU:HD22	2.30	0.61
1:C:210:VAL:HG12	1:D:183:ILE:N	2.14	0.61
1:D:210:VAL:HG23	1:E:179:SER:OG	2.00	0.61
1:D:220:VAL:O	1:E:249:LEU:C	2.43	0.61
1:D:383:TYR:O	1:E:371:ASP:HB3	2.01	0.61
1:E:219:TRP:N	1:F:250:ALA:O	2.33	0.61
1:E:219:TRP:O	1:F:250:ALA:O	2.19	0.61
1:E:241:GLU:OE1	1:F:179:SER:HB3	2.01	0.61
1:A:216:LYS:N	1:B:275:LEU:N	2.38	0.61
1:E:207:THR:CB	1:F:177:ILE:O	2.48	0.61
1:C:219:TRP:CZ2	1:D:286:ALA:CB	2.84	0.60
1:C:220:VAL:N	1:D:249:LEU:HA	2.16	0.60
1:A:214:ALA:C	1:B:274:ARG:CB	2.62	0.60
1:D:235:VAL:HG12	1:E:254:PHE:C	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:ALA:CB	1:F:271:LEU:CB	2.79	0.60
1:A:221:ALA:O	1:B:439:ARG:NE	2.34	0.60
1:A:331:ARG:HH22	1:B:355:ASP:CB	2.13	0.60
1:C:221:ALA:O	1:D:248:LYS:CB	2.50	0.60
1:C:331:ARG:NE	1:D:376:GLN:NE2	2.45	0.60
1:A:362:TRP:CB	1:F:360:GLU:OE1	2.50	0.60
1:B:220:VAL:HG12	1:C:252:LYS:CG	2.32	0.60
1:D:237:GLY:HA2	1:E:267:LEU:CD2	2.31	0.60
1:A:215:GLY:C	1:B:274:ARG:HB2	2.27	0.60
1:A:271:LEU:N	1:F:214:ALA:CB	2.55	0.60
1:A:331:ARG:NH2	1:B:355:ASP:HB3	2.15	0.60
1:B:217:ALA:HB2	1:C:275:LEU:CB	2.19	0.60
1:D:217:ALA:N	1:E:278:ALA:HB1	1.77	0.60
1:E:234:GLU:N	1:F:252:LYS:O	2.33	0.60
1:B:209:LEU:H	1:C:180:GLN:H	0.74	0.60
1:B:232:GLY:O	1:C:252:LYS:C	2.37	0.60
1:C:234:GLU:H	1:D:253:SER:CA	2.13	0.59
1:D:220:VAL:CG2	1:E:250:ALA:C	2.68	0.59
1:D:213:ASP:HA	1:E:274:ARG:NH2	2.16	0.59
1:A:227:THR:O	1:B:252:LYS:NZ	2.21	0.59
1:C:207:THR:HG22	1:D:177:ILE:O	2.00	0.59
1:C:383:TYR:HD2	1:D:371:ASP:CB	2.15	0.59
1:E:206:LEU:C	1:F:177:ILE:HG21	2.26	0.59
1:C:227:THR:HG21	1:D:435:TYR:OH	2.02	0.59
1:A:275:LEU:HD22	1:F:217:ALA:CA	2.31	0.59
1:C:218:THR:HG23	1:D:250:ALA:O	2.02	0.59
1:A:271:LEU:CA	1:F:214:ALA:C	2.63	0.59
1:B:207:THR:CG2	1:C:178:PHE:CA	2.80	0.59
1:E:207:THR:CB	1:F:177:ILE:C	2.75	0.59
1:A:177:ILE:H	1:F:205:ILE:HG23	1.67	0.59
1:A:249:LEU:CB	1:F:219:TRP:CD1	2.80	0.59
1:C:316:ALA:HB1	1:D:352:ALA:HB1	1.84	0.59
1:A:213:ASP:C	1:B:274:ARG:NH2	2.48	0.59
1:D:218:THR:O	1:E:279:HIS:ND1	2.36	0.59
1:A:220:VAL:CA	1:B:437:THR:HG22	2.33	0.59
1:B:215:GLY:C	1:C:275:LEU:HG	2.28	0.59
1:D:220:VAL:HG21	1:E:251:ALA:C	2.28	0.59
1:B:214:ALA:HB2	1:C:270:LEU:HD23	1.83	0.59
1:C:210:VAL:CG1	1:D:183:ILE:N	2.61	0.58
1:C:220:VAL:CB	1:D:250:ALA:CA	2.68	0.58
1:E:214:ALA:N	1:F:274:ARG:HB3	1.91	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:ALA:CB	1:F:275:LEU:O	2.51	0.58
1:A:227:THR:N	1:B:435:TYR:HE1	1.99	0.58
1:A:249:LEU:C	1:F:219:TRP:HB3	2.20	0.58
1:B:207:THR:OG1	1:C:177:ILE:N	2.35	0.58
1:B:209:LEU:CA	1:C:180:GLN:H	2.16	0.58
1:C:209:LEU:C	1:D:179:SER:OG	2.32	0.58
1:D:221:ALA:HA	1:E:248:LYS:CB	2.27	0.58
1:B:243:HIS:CE1	1:C:176:THR:HG23	2.38	0.58
1:C:219:TRP:HB3	1:D:249:LEU:CG	2.33	0.58
1:C:321:LEU:HD23	1:C:321:LEU:H	1.67	0.58
1:D:219:TRP:CE2	1:E:249:LEU:HD13	2.38	0.58
1:C:216:LYS:C	1:D:275:LEU:O	2.46	0.58
1:A:222:ALA:CB	1:B:439:ARG:HH12	2.16	0.58
1:C:216:LYS:O	1:D:278:ALA:CB	2.51	0.58
1:C:219:TRP:HA	1:D:249:LEU:CB	2.33	0.58
1:C:232:GLY:CA	1:D:251:ALA:HA	2.24	0.58
1:B:212:PRO:HB2	1:C:184:ARG:HA	1.85	0.58
1:C:219:TRP:C	1:D:250:ALA:O	2.46	0.58
1:D:235:VAL:CG1	1:E:254:PHE:C	2.76	0.58
1:B:207:THR:CG2	1:C:178:PHE:HA	2.32	0.58
1:B:234:GLU:CB	1:C:275:LEU:HD21	2.34	0.58
1:D:213:ASP:CA	1:E:274:ARG:CG	2.81	0.58
1:E:209:LEU:N	1:F:180:GLN:H	1.92	0.58
1:A:361:GLU:HG2	1:B:363:GLN:HG2	1.82	0.58
1:C:227:THR:CG2	1:D:435:TYR:OH	2.51	0.58
1:D:237:GLY:N	1:E:267:LEU:HD11	2.16	0.58
1:A:235:VAL:HG11	1:B:254:PHE:O	2.02	0.57
1:A:236:LYS:O	1:B:271:LEU:HD13	2.03	0.57
1:A:274:ARG:HB3	1:F:215:GLY:O	2.04	0.57
1:A:331:ARG:CZ	1:B:355:ASP:CB	2.76	0.57
1:A:361:GLU:HB3	1:B:363:GLN:OE1	2.00	0.57
1:A:435:TYR:HD2	1:F:233:GLU:OE2	1.82	0.57
1:B:215:GLY:H	1:C:271:LEU:CD1	2.05	0.57
1:C:233:GLU:CD	1:D:252:LYS:CB	2.67	0.57
1:D:222:ALA:CB	1:E:437:THR:OG1	2.52	0.57
1:E:214:ALA:CB	1:F:274:ARG:HB2	2.34	0.57
1:E:241:GLU:OE1	1:F:179:SER:N	2.37	0.57
1:A:249:LEU:C	1:F:219:TRP:CD1	2.83	0.57
1:B:205:ILE:HG23	1:C:177:ILE:CG1	2.34	0.57
1:B:234:GLU:HB2	1:C:275:LEU:HD21	1.83	0.57
1:C:220:VAL:N	1:D:249:LEU:CA	2.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ALA:HB3	1:D:439:ARG:HH12	1.68	0.57
1:B:207:THR:CB	1:C:177:ILE:HG22	2.33	0.57
1:B:212:PRO:HB2	1:C:184:ARG:CA	2.35	0.57
1:A:185:ASP:N	1:F:212:PRO:O	2.37	0.57
1:A:232:GLY:O	1:B:252:LYS:O	2.22	0.57
1:A:271:LEU:CD1	1:F:236:LYS:CA	2.68	0.57
1:B:233:GLU:HA	1:C:434:TYR:O	2.04	0.57
1:A:252:LYS:HG3	1:F:220:VAL:HG22	1.85	0.57
1:B:233:GLU:OE1	1:C:433:ALA:HA	2.01	0.57
1:E:213:ASP:CG	1:F:274:ARG:CG	2.76	0.57
1:E:241:GLU:HG3	1:F:179:SER:HB2	1.70	0.57
1:A:362:TRP:HZ2	1:B:362:TRP:CG	2.16	0.57
1:C:207:THR:HB	1:D:177:ILE:CA	2.35	0.57
1:C:232:GLY:CA	1:D:252:LYS:HG3	2.27	0.57
1:E:205:ILE:HG23	1:F:177:ILE:HG13	1.84	0.57
1:E:207:THR:CG2	1:F:179:SER:N	2.66	0.57
1:E:214:ALA:CB	1:F:271:LEU:C	2.67	0.57
1:C:222:ALA:HB3	1:D:439:ARG:NH1	2.20	0.56
1:C:383:TYR:HA	1:D:371:ASP:CB	2.35	0.56
1:E:207:THR:HG22	1:F:178:PHE:C	2.28	0.56
1:E:221:ALA:O	1:F:248:LYS:CG	2.44	0.56
1:A:220:VAL:O	1:B:437:THR:HG22	2.05	0.56
1:A:235:VAL:HG23	1:B:271:LEU:HD22	0.59	0.56
1:B:287:PHE:CE2	1:B:413:MET:HE2	2.40	0.56
1:E:207:THR:HG21	1:F:179:SER:N	2.19	0.56
1:C:234:GLU:O	1:D:253:SER:HB2	2.05	0.56
1:A:212:PRO:O	1:B:184:ARG:CA	2.54	0.56
1:B:207:THR:H	1:C:177:ILE:CG2	2.18	0.56
1:B:208:MET:C	1:C:179:SER:HA	2.08	0.56
1:B:209:LEU:CA	1:C:180:GLN:N	2.63	0.56
1:C:316:ALA:HB2	1:D:352:ALA:CB	2.35	0.56
1:A:222:ALA:CB	1:B:439:ARG:NH1	2.69	0.56
1:A:226:GLY:CA	1:B:424:GLU:CD	2.75	0.56
1:B:218:THR:OG1	1:C:251:ALA:HA	1.91	0.56
1:C:215:GLY:H	1:D:271:LEU:HG	1.69	0.56
1:C:216:LYS:H	1:D:275:LEU:CG	2.19	0.56
1:E:227:THR:N	1:F:435:TYR:CD2	2.73	0.56
1:A:331:ARG:NH2	1:B:355:ASP:CB	2.69	0.56
1:E:207:THR:H	1:F:177:ILE:HG22	1.63	0.56
1:A:235:VAL:HA	1:B:271:LEU:CG	2.36	0.56
1:D:446:PHE:CZ	1:E:183:ILE:CD1	2.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:PHE:CZ	1:F:233:GLU:OE1	2.58	0.56
1:A:434:TYR:H	1:F:233:GLU:CG	2.06	0.56
1:A:435:TYR:CE1	1:F:226:GLY:HA2	2.40	0.56
1:B:233:GLU:CB	1:C:434:TYR:HB2	2.28	0.56
1:C:218:THR:O	1:D:279:HIS:HE1	1.83	0.56
1:C:232:GLY:CA	1:D:252:LYS:CB	2.78	0.56
1:E:217:ALA:HB1	1:F:279:HIS:CG	2.39	0.56
1:B:316:ALA:HB1	1:C:353:TYR:CZ	2.41	0.55
1:D:209:LEU:HB3	1:E:178:PHE:HB2	1.88	0.55
1:E:210:VAL:CA	1:F:182:ILE:CA	2.33	0.55
1:A:252:LYS:CA	1:F:217:ALA:HB1	2.36	0.55
1:B:233:GLU:CA	1:C:434:TYR:O	2.49	0.55
1:D:211:GLU:CB	1:E:182:ILE:CG1	2.79	0.55
1:E:204:LYS:NZ	1:F:175:GLU:HB3	2.21	0.55
1:E:213:ASP:CG	1:F:274:ARG:HB3	2.32	0.55
1:B:220:VAL:HG11	1:C:436:VAL:H	1.72	0.55
1:B:230:THR:OG1	1:C:252:LYS:CD	2.54	0.55
1:E:219:TRP:HE1	1:F:283:ILE:N	2.02	0.55
1:C:217:ALA:HB3	1:D:279:HIS:HB2	0.55	0.55
1:C:220:VAL:HG11	1:D:435:TYR:HE1	1.71	0.55
1:E:207:THR:CA	1:F:177:ILE:HG22	2.36	0.55
1:B:241:GLU:OE2	1:C:178:PHE:CA	2.55	0.55
1:C:212:PRO:CB	1:D:184:ARG:HA	2.35	0.55
1:D:215:GLY:CA	1:E:275:LEU:HD21	2.33	0.55
1:A:434:TYR:O	1:F:233:GLU:HG2	2.02	0.55
1:A:219:TRP:CA	1:B:279:HIS:CE1	2.90	0.55
1:C:207:THR:O	1:D:177:ILE:CB	2.55	0.55
1:C:219:TRP:CA	1:D:249:LEU:HB3	2.36	0.55
1:E:228:ASP:HA	1:F:252:LYS:HD3	1.88	0.55
1:E:232:GLY:HA2	1:F:252:LYS:N	2.19	0.55
1:A:252:LYS:CB	1:F:232:GLY:O	2.55	0.54
1:B:235:VAL:CG1	1:C:255:ILE:CG2	2.67	0.54
1:B:237:GLY:O	1:C:274:ARG:NH2	2.40	0.54
1:A:182:ILE:CA	1:F:211:GLU:C	2.73	0.54
1:B:216:LYS:N	1:C:275:LEU:HD23	2.16	0.54
1:D:182:ILE:HD12	1:D:182:ILE:O	2.06	0.54
1:C:234:GLU:CB	1:D:275:LEU:HD13	2.36	0.54
1:E:241:GLU:OE1	1:F:179:SER:CB	2.56	0.54
1:A:219:TRP:CH2	1:B:248:LYS:HB2	2.32	0.54
1:C:208:MET:CA	1:D:179:SER:HA	2.35	0.54
1:D:235:VAL:CA	1:E:254:PHE:O	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PRO:C	1:B:184:ARG:HA	2.32	0.54
1:C:216:LYS:C	1:D:278:ALA:CB	2.75	0.54
1:C:331:ARG:NH2	1:D:376:GLN:HE22	2.03	0.54
1:C:332:ARG:CD	1:D:355:ASP:OD2	2.51	0.54
1:D:216:LYS:O	1:E:275:LEU:CB	2.53	0.54
1:D:235:VAL:HA	1:E:271:LEU:HD11	0.66	0.54
1:C:217:ALA:CA	1:D:279:HIS:HB2	2.21	0.54
1:E:214:ALA:HB3	1:F:274:ARG:HB2	1.88	0.54
1:B:205:ILE:CG2	1:C:177:ILE:HG12	2.37	0.54
1:B:232:GLY:CA	1:C:254:PHE:HD1	2.20	0.54
1:D:219:TRP:HZ2	1:E:286:ALA:CB	2.14	0.54
1:A:435:TYR:HE2	1:F:233:GLU:OE2	1.87	0.54
1:B:220:VAL:CG2	1:C:437:THR:HA	2.35	0.54
1:B:241:GLU:OE1	1:C:178:PHE:CD2	2.52	0.54
1:C:215:GLY:C	1:D:275:LEU:N	2.65	0.54
1:C:234:GLU:C	1:D:253:SER:HB2	2.32	0.54
1:D:235:VAL:HB	1:E:254:PHE:C	2.27	0.54
1:E:210:VAL:HB	1:F:183:ILE:N	2.23	0.54
1:D:216:LYS:C	1:E:275:LEU:O	2.51	0.53
1:E:208:MET:CA	1:F:180:GLN:H	2.20	0.53
1:A:178:PHE:CG	1:F:207:THR:HG21	2.21	0.53
1:A:214:ALA:O	1:B:271:LEU:CA	2.47	0.53
1:D:235:VAL:C	1:E:271:LEU:CD1	2.82	0.53
1:B:207:THR:O	1:C:177:ILE:HG22	2.09	0.53
1:D:236:LYS:C	1:E:267:LEU:HD11	2.33	0.53
1:A:220:VAL:CG1	1:B:437:THR:HG23	2.36	0.53
1:A:204:LYS:CB	1:B:174:TYR:CE2	2.92	0.53
1:A:435:TYR:CE2	1:F:233:GLU:CD	2.87	0.53
1:F:256:THR:HG22	1:F:431:ARG:HA	1.91	0.53
1:D:216:LYS:CA	1:E:275:LEU:CA	2.78	0.53
1:D:220:VAL:CG2	1:E:251:ALA:CA	2.86	0.53
1:B:236:LYS:HE2	1:C:274:ARG:HD2	1.91	0.53
1:C:217:ALA:HB3	1:D:279:HIS:HB3	1.67	0.53
1:A:212:PRO:O	1:B:184:ARG:HA	2.09	0.53
1:D:220:VAL:O	1:E:250:ALA:N	2.41	0.53
1:A:177:ILE:N	1:F:205:ILE:HG23	2.23	0.53
1:C:207:THR:N	1:D:177:ILE:HB	2.24	0.53
1:D:218:THR:HG21	1:E:252:LYS:H	1.73	0.53
1:A:233:GLU:HB3	1:B:434:TYR:H	1.74	0.52
1:A:271:LEU:CA	1:F:214:ALA:HB1	2.18	0.52
1:D:213:ASP:CB	1:E:274:ARG:NH2	2.71	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:GLU:HB2	1:D:275:LEU:HD13	1.84	0.52
1:D:218:THR:C	1:E:251:ALA:CA	2.67	0.52
1:A:360:GLU:OE1	1:B:364:ASP:N	2.41	0.52
1:D:214:ALA:O	1:E:274:ARG:CB	2.57	0.52
1:A:182:ILE:HA	1:F:211:GLU:C	2.32	0.52
1:A:252:LYS:C	1:F:217:ALA:HB1	2.34	0.52
1:E:220:VAL:HG21	1:F:251:ALA:N	2.21	0.52
1:A:213:ASP:N	1:B:182:ILE:CD1	2.72	0.52
1:E:214:ALA:CB	1:F:271:LEU:O	2.58	0.52
1:C:235:VAL:CG2	1:D:255:ILE:HD12	2.30	0.52
1:E:219:TRP:CB	1:F:249:LEU:HB3	2.40	0.52
1:E:220:VAL:CG1	1:F:435:TYR:CZ	2.90	0.52
1:C:216:LYS:CB	1:D:278:ALA:CB	2.87	0.52
1:D:218:THR:C	1:E:250:ALA:C	2.75	0.52
1:E:207:THR:CG2	1:F:179:SER:HA	2.28	0.52
1:A:361:GLU:N	1:B:363:GLN:HG2	2.25	0.52
1:D:237:GLY:C	1:E:267:LEU:CD1	2.77	0.52
1:E:211:GLU:OE2	1:F:182:ILE:HD12	2.07	0.52
1:A:207:THR:HB	1:B:176:THR:C	2.29	0.52
1:B:215:GLY:N	1:C:271:LEU:CA	2.48	0.52
1:E:219:TRP:CB	1:F:249:LEU:CA	2.77	0.52
1:E:360:GLU:HB2	1:F:363:GLN:HA	1.92	0.52
1:E:216:LYS:N	1:F:275:LEU:HD12	2.16	0.51
1:A:212:PRO:O	1:B:184:ARG:CB	2.57	0.51
1:A:252:LYS:CE	1:F:227:THR:OG1	2.56	0.51
1:B:205:ILE:HG23	1:C:177:ILE:HG12	1.92	0.51
1:B:237:GLY:HA2	1:C:267:LEU:HD21	1.90	0.51
1:C:220:VAL:N	1:D:250:ALA:CA	2.70	0.51
1:C:233:GLU:CB	1:D:253:SER:C	2.79	0.51
1:D:234:GLU:C	1:E:254:PHE:O	2.52	0.51
1:E:222:ALA:HA	1:F:435:TYR:OH	2.10	0.51
1:A:216:LYS:CB	1:B:275:LEU:HD23	2.41	0.51
1:C:235:VAL:CB	1:D:271:LEU:HD21	2.40	0.51
1:D:212:PRO:CG	1:E:183:ILE:O	2.55	0.51
1:D:216:LYS:N	1:E:275:LEU:HA	2.25	0.51
1:B:219:TRP:CE3	1:C:249:LEU:HD23	2.45	0.51
1:B:214:ALA:O	1:C:271:LEU:CA	2.58	0.51
1:E:204:LYS:HD2	1:F:175:GLU:HB3	1.92	0.51
1:A:271:LEU:HD13	1:F:236:LYS:C	2.36	0.51
1:C:217:ALA:HB2	1:D:275:LEU:HG	1.92	0.51
1:E:219:TRP:NE1	1:F:282:SER:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:ALA:HB2	1:D:450:VAL:HG13	1.92	0.51
1:B:219:TRP:HA	1:C:279:HIS:CE1	2.45	0.51
1:C:232:GLY:HA3	1:D:252:LYS:CB	2.39	0.51
1:A:252:LYS:CE	1:F:230:THR:OG1	2.57	0.51
1:C:222:ALA:CB	1:D:439:ARG:HH12	2.24	0.51
1:E:209:LEU:HB2	1:F:180:GLN:CA	2.40	0.51
1:E:215:GLY:HA3	1:F:275:LEU:HB2	1.92	0.51
1:A:360:GLU:OE1	1:B:363:GLN:C	2.53	0.51
1:B:220:VAL:CB	1:C:436:VAL:O	2.58	0.51
1:C:216:LYS:H	1:D:275:LEU:CB	2.22	0.51
1:D:235:VAL:CG1	1:E:255:ILE:CB	2.83	0.51
1:E:219:TRP:CE2	1:F:282:SER:O	2.64	0.51
1:B:234:GLU:O	1:C:275:LEU:CG	2.59	0.50
1:E:233:GLU:CG	1:F:252:LYS:HB3	2.39	0.50
1:C:383:TYR:CD2	1:D:371:ASP:CB	2.94	0.50
1:A:275:LEU:CA	1:F:216:LYS:HA	2.31	0.50
1:B:220:VAL:CG1	1:C:436:VAL:H	2.24	0.50
1:C:360:GLU:HB3	1:D:362:TRP:O	2.12	0.50
1:E:223:SER:N	1:F:439:ARG:HH22	2.10	0.50
1:A:252:LYS:CG	1:F:220:VAL:HG22	2.40	0.50
1:A:252:LYS:C	1:F:217:ALA:CB	2.84	0.50
1:B:214:ALA:O	1:C:271:LEU:C	2.55	0.50
1:C:219:TRP:CD1	1:D:249:LEU:CB	2.85	0.50
1:E:211:GLU:HB3	1:F:270:LEU:HD11	1.93	0.50
1:E:228:ASP:HB3	1:F:252:LYS:CD	2.40	0.50
1:A:234:GLU:C	1:B:275:LEU:HD21	2.37	0.50
1:B:235:VAL:HG12	1:C:255:ILE:CG1	2.41	0.50
1:C:217:ALA:N	1:D:275:LEU:HD11	2.15	0.50
1:E:219:TRP:CA	1:F:250:ALA:O	2.58	0.50
1:E:221:ALA:C	1:F:248:LYS:HB3	2.36	0.50
1:A:271:LEU:HD13	1:F:236:LYS:CB	2.41	0.50
1:A:271:LEU:HD11	1:F:236:LYS:HG3	1.94	0.50
1:D:205:ILE:O	1:E:177:ILE:HG12	2.12	0.50
1:D:232:GLY:CA	1:E:252:LYS:CE	2.61	0.50
1:A:219:TRP:CB	1:B:279:HIS:ND1	2.75	0.49
1:A:219:TRP:N	1:B:279:HIS:ND1	2.60	0.49
1:B:214:ALA:CA	1:C:271:LEU:HA	2.39	0.49
1:C:212:PRO:HA	1:D:182:ILE:CD1	2.36	0.49
1:D:221:ALA:CA	1:E:248:LYS:HB3	2.29	0.49
1:D:236:LYS:O	1:E:267:LEU:HD11	2.13	0.49
1:E:228:ASP:HA	1:F:252:LYS:CD	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LYS:O	1:F:217:ALA:CA	2.51	0.49
1:C:216:LYS:CE	1:D:278:ALA:HA	2.34	0.49
1:C:368:VAL:HG23	1:C:375:LEU:HD13	1.95	0.49
1:D:234:GLU:CA	1:E:254:PHE:H	2.22	0.49
1:E:208:MET:HE2	1:F:181:ARG:HB2	1.94	0.49
1:A:212:PRO:CB	1:B:184:ARG:CA	2.83	0.49
1:B:210:VAL:HG11	1:C:183:ILE:H	1.76	0.49
1:D:237:GLY:HA2	1:E:267:LEU:HD21	1.94	0.49
1:B:209:LEU:C	1:C:180:GLN:O	2.49	0.49
1:A:206:LEU:HB3	1:B:177:ILE:HG21	1.95	0.49
1:A:207:THR:HG21	1:B:176:THR:CG2	2.36	0.49
1:A:214:ALA:HB3	1:B:271:LEU:N	2.27	0.49
1:A:360:GLU:OE1	1:B:362:TRP:C	2.53	0.49
1:B:214:ALA:HB2	1:C:270:LEU:CD2	2.43	0.49
1:C:207:THR:O	1:D:177:ILE:HB	2.13	0.49
1:C:220:VAL:O	1:D:249:LEU:N	2.46	0.49
1:E:213:ASP:OD1	1:F:274:ARG:NH2	2.45	0.49
1:A:178:PHE:CD1	1:F:207:THR:CG2	2.93	0.49
1:C:220:VAL:HG21	1:D:251:ALA:CA	2.40	0.49
1:D:236:LYS:O	1:E:267:LEU:HG	2.12	0.49
1:E:207:THR:CG2	1:F:179:SER:CA	2.89	0.49
1:A:331:ARG:NH2	1:B:355:ASP:OD2	2.45	0.49
1:C:219:TRP:CG	1:D:249:LEU:CD2	2.93	0.49
1:C:225:TYR:O	1:D:435:TYR:CD2	2.66	0.49
1:E:213:ASP:OD1	1:F:274:ARG:CG	2.55	0.49
1:E:241:GLU:CD	1:F:179:SER:CB	2.72	0.49
1:B:215:GLY:HA2	1:C:271:LEU:CD1	2.42	0.48
1:A:182:ILE:HA	1:F:211:GLU:CA	2.33	0.48
1:B:220:VAL:HG22	1:C:437:THR:CA	2.35	0.48
1:E:219:TRP:CG	1:F:249:LEU:HB3	2.48	0.48
1:D:207:THR:OG1	1:E:176:THR:CA	2.60	0.48
1:E:223:SER:H	1:F:439:ARG:HH22	1.59	0.48
1:A:216:LYS:C	1:B:275:LEU:HD23	2.36	0.48
1:A:219:TRP:CG	1:B:279:HIS:CE1	2.83	0.48
1:C:211:GLU:CB	1:D:182:ILE:HG12	2.26	0.48
1:B:279:HIS:CD2	1:B:283:ILE:HD11	2.49	0.48
1:C:219:TRP:CE2	1:D:249:LEU:HD13	2.48	0.48
1:C:220:VAL:CG2	1:D:251:ALA:HA	2.41	0.48
1:D:235:VAL:CB	1:E:271:LEU:CD1	2.92	0.48
1:A:274:ARG:HB2	1:F:215:GLY:O	2.12	0.48
1:E:212:PRO:O	1:F:274:ARG:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:VAL:HG13	1:C:251:ALA:N	2.29	0.48
1:C:356:LEU:HD11	1:C:367:GLN:HE22	1.78	0.48
1:D:233:GLU:HG2	1:E:252:LYS:HB2	1.96	0.48
1:E:214:ALA:O	1:F:275:LEU:N	2.47	0.48
1:D:209:LEU:CB	1:E:178:PHE:CB	2.87	0.48
1:D:215:GLY:HA3	1:E:271:LEU:O	2.14	0.48
1:D:218:THR:O	1:E:251:ALA:HB2	1.59	0.48
1:E:226:GLY:HA2	1:F:435:TYR:HD2	1.78	0.48
1:B:216:LYS:CD	1:C:274:ARG:O	2.62	0.48
1:D:219:TRP:CD2	1:E:249:LEU:HD22	2.49	0.48
1:A:177:ILE:N	1:F:207:THR:OG1	2.47	0.48
1:A:220:VAL:HG23	1:B:251:ALA:N	2.28	0.48
1:B:218:THR:N	1:C:251:ALA:C	2.68	0.48
1:C:205:ILE:O	1:D:177:ILE:HG13	2.11	0.48
1:D:212:PRO:HB3	1:E:182:ILE:CD1	2.35	0.48
1:A:181:ARG:HA	1:F:211:GLU:OE2	2.13	0.47
1:A:216:LYS:NZ	1:B:277:GLU:O	2.19	0.47
1:A:254:PHE:CG	1:F:233:GLU:N	2.82	0.47
1:A:437:THR:HG22	1:F:220:VAL:HB	1.96	0.47
1:C:233:GLU:N	1:D:252:LYS:CB	2.48	0.47
1:E:207:THR:HG21	1:F:178:PHE:CA	2.43	0.47
1:B:214:ALA:HB3	1:C:270:LEU:HB3	1.96	0.47
1:D:222:ALA:C	1:E:439:ARG:NH1	2.50	0.47
1:E:219:TRP:CB	1:F:249:LEU:CB	2.90	0.47
1:A:271:LEU:HB3	1:F:235:VAL:HG23	1.86	0.47
1:B:243:HIS:CE1	1:C:176:THR:CG2	2.97	0.47
1:F:424:GLU:HG2	1:F:426:GLN:H	1.79	0.47
1:B:234:GLU:HB2	1:C:275:LEU:HD22	1.93	0.47
1:E:234:GLU:O	1:F:275:LEU:HD13	2.14	0.47
1:B:212:PRO:HA	1:C:182:ILE:HD12	0.51	0.47
1:C:219:TRP:CG	1:D:249:LEU:CB	2.97	0.47
1:E:223:SER:N	1:F:439:ARG:HH12	2.13	0.47
1:A:253:SER:H	1:F:233:GLU:CG	1.89	0.47
1:A:271:LEU:CD1	1:F:214:ALA:HB1	2.45	0.47
1:A:360:GLU:O	1:B:362:TRP:HB2	2.15	0.47
1:A:361:GLU:CA	1:B:363:GLN:HG2	2.45	0.47
1:B:207:THR:CB	1:C:177:ILE:CG2	2.83	0.47
1:C:233:GLU:CB	1:D:254:PHE:N	2.64	0.47
1:D:234:GLU:O	1:E:253:SER:CB	2.61	0.47
1:D:237:GLY:CA	1:E:267:LEU:HD21	2.45	0.47
1:E:209:LEU:N	1:F:180:GLN:N	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:VAL:HG11	1:F:435:TYR:HE1	0.68	0.47
1:A:211:GLU:N	1:B:181:ARG:O	2.48	0.47
1:B:237:GLY:C	1:C:274:ARG:HH22	2.22	0.47
1:A:218:THR:CG2	1:B:251:ALA:CB	2.87	0.47
1:C:208:MET:HB2	1:D:179:SER:CB	2.44	0.47
1:C:234:GLU:C	1:D:275:LEU:HD13	2.40	0.47
1:B:237:GLY:HA3	1:C:267:LEU:HD11	1.97	0.47
1:C:347:ILE:HD11	1:C:401:GLU:H	1.79	0.47
1:E:207:THR:HG22	1:F:178:PHE:O	2.13	0.47
1:E:219:TRP:HB3	1:F:249:LEU:CD2	2.45	0.47
1:A:176:THR:HA	1:F:205:ILE:HG21	1.78	0.46
1:D:215:GLY:HA2	1:E:275:LEU:HD21	1.92	0.46
1:A:177:ILE:HG21	1:F:206:LEU:HB3	1.07	0.46
1:C:332:ARG:HD3	1:D:355:ASP:CG	2.39	0.46
1:A:226:GLY:HA2	1:B:435:TYR:HE1	1.79	0.46
1:A:253:SER:N	1:F:233:GLU:CG	2.53	0.46
1:B:219:TRP:CG	1:C:249:LEU:CD2	2.98	0.46
1:B:241:GLU:CD	1:C:178:PHE:CD2	2.86	0.46
1:A:222:ALA:N	1:B:439:ARG:NH1	2.64	0.46
1:A:435:TYR:HE2	1:F:233:GLU:CD	2.23	0.46
1:D:236:LYS:O	1:E:267:LEU:CD1	2.64	0.46
1:E:406:VAL:O	1:E:410:ASN:HB2	2.16	0.46
1:A:218:THR:CB	1:B:251:ALA:CB	2.49	0.46
1:B:365:VAL:HB	1:C:369:GLY:HA3	1.97	0.46
1:A:176:THR:CB	1:F:205:ILE:HG21	2.46	0.46
1:B:234:GLU:CB	1:C:275:LEU:CD2	2.83	0.46
1:D:235:VAL:HB	1:E:255:ILE:CB	2.35	0.46
1:E:207:THR:HG22	1:F:179:SER:N	2.30	0.46
1:F:220:VAL:HG12	1:F:222:ALA:H	1.81	0.46
1:A:219:TRP:CG	1:B:250:ALA:C	2.94	0.46
1:A:223:SER:N	1:B:439:ARG:HH12	2.08	0.46
1:B:220:VAL:HG11	1:C:436:VAL:N	2.31	0.46
1:C:220:VAL:O	1:D:249:LEU:C	2.58	0.46
1:D:232:GLY:C	1:E:252:LYS:HB2	2.39	0.46
1:A:362:TRP:HB2	1:F:360:GLU:OE1	2.16	0.46
1:A:274:ARG:O	1:F:216:LYS:HD2	2.16	0.45
1:A:361:GLU:HB3	1:F:360:GLU:HG2	1.97	0.45
1:D:207:THR:CB	1:E:176:THR:C	2.86	0.45
1:E:210:VAL:HA	1:F:181:ARG:C	2.35	0.45
1:D:205:ILE:O	1:E:177:ILE:CG1	2.63	0.45
1:E:199:LEU:HD12	1:E:200:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:HD21	1:F:234:GLU:HB3	1.95	0.45
1:B:214:ALA:CA	1:C:270:LEU:HG	2.47	0.45
1:B:219:TRP:CG	1:C:249:LEU:HD23	2.52	0.45
1:E:213:ASP:CG	1:F:274:ARG:CB	2.90	0.45
1:A:180:GLN:O	1:F:208:MET:CE	2.65	0.45
1:A:217:ALA:N	1:B:275:LEU:HD23	2.09	0.45
1:A:250:ALA:N	1:F:219:TRP:HD1	2.04	0.45
1:A:275:LEU:HD22	1:F:234:GLU:HB2	1.98	0.45
1:A:352:ALA:CB	1:F:332:ARG:HD3	2.37	0.45
1:D:216:LYS:C	1:E:275:LEU:C	2.84	0.45
1:A:233:GLU:CG	1:B:434:TYR:CA	2.63	0.45
1:A:275:LEU:HD21	1:F:215:GLY:CA	2.47	0.45
1:B:255:ILE:HD11	1:B:432:ASP:HB3	1.99	0.45
1:D:217:ALA:HA	1:E:275:LEU:O	2.15	0.45
1:C:213:ASP:HA	1:D:274:ARG:HD3	0.45	0.45
1:D:383:TYR:C	1:E:371:ASP:CB	2.88	0.45
1:E:210:VAL:HA	1:F:182:ILE:HA	0.55	0.45
1:C:217:ALA:CB	1:D:279:HIS:CG	2.83	0.45
1:D:219:TRP:HB3	1:E:249:LEU:CD2	2.46	0.45
1:A:352:ALA:CA	1:F:332:ARG:CD	2.94	0.45
1:A:213:ASP:N	1:B:182:ILE:HD11	2.29	0.45
1:A:217:ALA:HB1	1:B:436:VAL:HG23	1.94	0.45
1:D:444:ARG:HH11	1:D:447:ALA:HB2	1.82	0.45
1:E:209:LEU:CB	1:F:180:GLN:CA	2.94	0.45
1:A:178:PHE:CE1	1:F:207:THR:HG21	2.48	0.44
1:B:236:LYS:C	1:C:267:LEU:CD2	2.89	0.44
1:C:406:VAL:HG13	1:C:410:ASN:HB2	1.99	0.44
1:E:233:GLU:H	1:F:252:LYS:HB3	1.64	0.44
1:A:178:PHE:HE2	1:F:241:GLU:OE1	2.01	0.44
1:B:222:ALA:HB3	1:C:248:LYS:CD	2.43	0.44
1:C:219:TRP:CB	1:D:249:LEU:CA	2.85	0.44
1:D:321:LEU:HD13	1:D:329:LYS:NZ	2.32	0.44
1:D:208:MET:HA	1:E:179:SER:HA	1.90	0.44
1:D:216:LYS:C	1:E:278:ALA:CB	2.52	0.44
1:A:439:ARG:HH12	1:F:222:ALA:HB3	1.82	0.44
1:B:207:THR:N	1:C:177:ILE:HB	2.32	0.44
1:A:209:LEU:HD12	1:B:178:PHE:HB2	2.00	0.44
1:A:220:VAL:HG11	1:B:252:LYS:HE2	1.99	0.44
1:A:348:VAL:HG13	1:A:349:SER:N	2.33	0.44
1:B:227:THR:HG22	1:B:229:THR:H	1.82	0.44
1:C:220:VAL:N	1:D:250:ALA:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ILE:H	1:D:347:ILE:HG13	1.66	0.44
1:E:215:GLY:HA3	1:F:275:LEU:CB	2.46	0.44
1:A:252:LYS:HG2	1:F:220:VAL:HG21	1.99	0.44
1:D:216:LYS:CG	1:E:278:ALA:HB1	2.16	0.44
1:E:213:ASP:OD1	1:F:274:ARG:CZ	2.66	0.44
1:D:216:LYS:HA	1:E:275:LEU:HA	1.91	0.44
1:F:249:LEU:HD21	1:F:295:LYS:HA	2.00	0.44
1:A:219:TRP:HB2	1:B:279:HIS:ND1	2.33	0.44
1:B:339:LEU:HD13	1:B:405:ILE:HD11	1.99	0.44
1:D:190:LEU:HB3	1:D:284:GLU:HG3	2.00	0.44
1:D:219:TRP:CD1	1:E:249:LEU:HD13	2.53	0.44
1:E:208:MET:CA	1:F:180:GLN:N	2.79	0.44
1:E:226:GLY:HA2	1:F:435:TYR:CD2	2.53	0.44
1:B:234:GLU:CA	1:C:275:LEU:HD21	2.44	0.43
1:D:235:VAL:CB	1:E:255:ILE:CA	2.93	0.43
1:E:220:VAL:HG12	1:F:435:TYR:OH	2.19	0.43
1:A:216:LYS:HD2	1:B:278:ALA:H	1.58	0.43
1:A:360:GLU:C	1:B:363:GLN:HG2	2.42	0.43
1:B:220:VAL:CG2	1:C:437:THR:CA	2.94	0.43
1:B:234:GLU:OE2	1:C:253:SER:HA	2.19	0.43
1:B:211:GLU:O	1:C:182:ILE:N	2.41	0.43
1:A:434:TYR:C	1:F:233:GLU:HG2	2.43	0.43
1:B:379:VAL:C	1:B:381:ARG:H	2.27	0.43
1:B:433:ALA:HB1	1:B:435:TYR:CE2	2.54	0.43
1:A:219:TRP:HB2	1:B:279:HIS:CE1	2.53	0.43
1:A:255:ILE:HG12	1:F:235:VAL:HG11	1.33	0.43
1:A:275:LEU:CD2	1:F:215:GLY:CA	2.95	0.43
1:A:178:PHE:CG	1:F:207:THR:CB	3.00	0.43
1:A:218:THR:HG23	1:B:251:ALA:C	2.43	0.43
1:A:271:LEU:CD1	1:F:214:ALA:CA	2.89	0.43
1:C:219:TRP:C	1:D:249:LEU:HA	2.44	0.43
1:B:316:ALA:HB1	1:C:353:TYR:OH	2.18	0.43
1:E:219:TRP:HA	1:F:279:HIS:HE1	1.83	0.43
1:F:271:LEU:C	1:F:271:LEU:HD23	2.43	0.43
1:A:208:MET:HB3	1:B:177:ILE:HG22	2.01	0.43
1:A:219:TRP:CG	1:B:249:LEU:CB	2.52	0.42
1:A:249:LEU:CA	1:F:219:TRP:CD1	3.02	0.42
1:A:268:LEU:HD21	1:A:434:TYR:CE1	2.54	0.42
1:C:216:LYS:H	1:D:275:LEU:HA	1.30	0.42
1:D:209:LEU:HB3	1:E:178:PHE:CB	2.49	0.42
1:D:214:ALA:C	1:E:274:ARG:CB	2.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ALA:CB	1:B:436:VAL:CG2	2.89	0.42
1:B:360:GLU:OE1	1:C:364:ASP:OD2	2.36	0.42
1:D:211:GLU:HB3	1:E:182:ILE:CG1	2.49	0.42
1:D:215:GLY:HA3	1:E:275:LEU:CG	2.48	0.42
1:D:235:VAL:CB	1:E:271:LEU:HD11	2.35	0.42
1:D:215:GLY:N	1:E:271:LEU:CG	2.60	0.42
1:C:212:PRO:O	1:D:274:ARG:CZ	2.68	0.42
1:D:216:LYS:HA	1:E:275:LEU:N	2.33	0.42
1:E:207:THR:HB	1:F:177:ILE:C	2.44	0.42
1:B:211:GLU:N	1:C:182:ILE:N	2.40	0.42
1:B:410:ASN:CG	1:B:411:PHE:H	2.27	0.42
1:E:211:GLU:CB	1:F:182:ILE:HB	2.47	0.42
1:C:214:ALA:HB1	1:D:271:LEU:HG	2.01	0.42
1:D:220:VAL:HG23	1:E:251:ALA:HA	2.01	0.42
1:E:305:GLU:HA	1:E:309:LYS:HA	2.02	0.42
1:B:214:ALA:C	1:C:271:LEU:C	2.86	0.42
1:B:219:TRP:CD2	1:C:249:LEU:CD2	2.95	0.42
1:A:271:LEU:CD1	1:F:215:GLY:H	2.21	0.42
1:D:222:ALA:CB	1:E:437:THR:CB	2.97	0.42
1:E:219:TRP:CD2	1:F:249:LEU:HD22	2.55	0.42
1:E:226:GLY:CA	1:F:435:TYR:HD2	2.33	0.42
1:C:219:TRP:CG	1:D:249:LEU:CD1	2.97	0.41
1:A:215:GLY:HA3	1:B:275:LEU:HG	2.03	0.41
1:B:207:THR:H	1:C:177:ILE:HG21	1.84	0.41
1:C:233:GLU:HG2	1:D:254:PHE:CB	2.41	0.41
1:E:400:ALA:H	1:E:455:TYR:HB3	1.85	0.41
1:A:178:PHE:CD1	1:F:207:THR:HG21	2.53	0.41
1:A:207:THR:CG2	1:B:176:THR:HG22	2.42	0.41
1:C:214:ALA:HB1	1:D:271:LEU:CG	2.51	0.41
1:C:219:TRP:CG	1:D:249:LEU:CG	3.03	0.41
1:D:256:THR:HG22	1:D:431:ARG:HG2	2.01	0.41
1:E:218:THR:HA	1:F:282:SER:OG	2.20	0.41
1:B:215:GLY:HA3	1:C:275:LEU:HG	1.97	0.41
1:B:230:THR:HG1	1:C:252:LYS:HD2	1.82	0.41
1:B:279:HIS:NE2	1:B:283:ILE:HD11	2.34	0.41
1:E:220:VAL:CG1	1:F:435:TYR:OH	2.68	0.41
1:A:252:LYS:CG	1:F:220:VAL:HG21	2.51	0.41
1:C:207:THR:HB	1:D:177:ILE:N	2.35	0.41
1:E:209:LEU:O	1:F:180:GLN:O	2.33	0.41
1:A:352:ALA:CA	1:F:332:ARG:HD3	2.50	0.41
1:A:254:PHE:HA	1:F:233:GLU:HB2	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:PRO:CB	1:C:182:ILE:HD12	1.95	0.41
1:C:207:THR:H	1:D:177:ILE:HB	1.82	0.41
1:E:228:ASP:CA	1:F:252:LYS:CD	2.98	0.41
1:A:177:ILE:HG13	1:F:206:LEU:HG	1.52	0.41
1:D:217:ALA:CA	1:E:275:LEU:O	2.69	0.41
1:D:322:VAL:HG22	1:D:325:LYS:HB2	2.03	0.41
1:A:183:ILE:N	1:F:212:PRO:HA	2.33	0.41
1:A:360:GLU:OE1	1:B:363:GLN:CA	2.68	0.41
1:B:214:ALA:CB	1:C:270:LEU:CB	2.94	0.41
1:B:232:GLY:CA	1:C:254:PHE:CD1	2.82	0.41
1:B:241:GLU:OE2	1:C:179:SER:N	2.49	0.41
1:B:243:HIS:HE1	1:C:176:THR:CG2	2.33	0.41
1:C:210:VAL:HG12	1:D:182:ILE:CA	2.48	0.41
1:C:234:GLU:CA	1:D:253:SER:HB3	2.51	0.41
1:C:419:VAL:HB	1:C:438:GLN:HE21	1.86	0.41
1:E:211:GLU:CG	1:F:182:ILE:CG2	2.99	0.41
1:A:216:LYS:O	1:B:274:ARG:O	2.39	0.41
1:A:217:ALA:N	1:B:275:LEU:HD22	2.04	0.41
1:B:207:THR:HG22	1:C:178:PHE:CA	2.49	0.41
1:E:228:ASP:HB3	1:F:252:LYS:HD3	2.02	0.41
1:A:207:THR:OG1	1:B:177:ILE:N	2.40	0.40
1:D:218:THR:O	1:E:251:ALA:CB	2.45	0.40
1:D:287:PHE:CZ	1:D:413:MET:HG3	2.56	0.40
1:A:252:LYS:HB3	1:F:233:GLU:CD	2.45	0.40
1:D:220:VAL:CG2	1:E:251:ALA:C	2.93	0.40
1:E:211:GLU:O	1:F:270:LEU:CD2	2.69	0.40
1:E:219:TRP:CA	1:F:249:LEU:CA	2.98	0.40
1:A:360:GLU:HG2	1:B:362:TRP:HA	1.76	0.40
1:B:192:VAL:HA	1:B:195:LEU:HD22	2.04	0.40
1:C:219:TRP:CZ2	1:D:286:ALA:HB3	2.56	0.40
1:C:316:ALA:CB	1:D:352:ALA:CB	2.93	0.40
1:A:208:MET:HB2	1:B:179:SER:HA	1.12	0.40
1:A:275:LEU:HG	1:F:215:GLY:HA3	2.04	0.40
1:A:331:ARG:HA	1:A:334:LEU:HD12	2.04	0.40
1:A:435:TYR:HE1	1:F:226:GLY:HA2	1.86	0.40
1:B:214:ALA:O	1:C:274:ARG:CG	2.58	0.40
1:B:222:ALA:HB3	1:C:248:LYS:HD2	2.04	0.40
1:C:207:THR:HB	1:D:177:ILE:H	1.87	0.40
1:D:209:LEU:HB3	1:E:178:PHE:CG	2.55	0.40
1:D:220:VAL:HB	1:E:251:ALA:H	1.81	0.40
1:E:219:TRP:HA	1:F:249:LEU:C	2.15	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:GLY:CA	1:F:252:LYS:CA	2.68	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	290/299 (97%)	246 (85%)	26 (9%)	18 (6%)	1	13
1	B	290/299 (97%)	230 (79%)	44 (15%)	16 (6%)	1	15
1	C	290/299 (97%)	233 (80%)	38 (13%)	19 (7%)	1	12
1	D	290/299 (97%)	242 (83%)	32 (11%)	16 (6%)	1	15
1	E	290/299 (97%)	238 (82%)	36 (12%)	16 (6%)	1	15
1	F	290/299 (97%)	237 (82%)	33 (11%)	20 (7%)	1	11
All	All	1740/1794 (97%)	1426 (82%)	209 (12%)	105 (6%)	2	13

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	VAL
1	A	223	SER
1	A	262	ASP
1	A	370	ASN
1	A	411	PHE
1	B	192	VAL
1	B	263	ALA
1	B	319	SER
1	B	357	LEU
1	B	427	ALA
1	C	263	ALA

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Mol	Chain	Res	Type
1	C	319	SER
1	C	371	ASP
1	D	192	VAL
1	D	394	PRO
1	D	397	ALA
1	E	192	VAL
1	E	195	LEU
1	E	319	SER
1	F	212	PRO
1	F	222	ALA
1	F	223	SER
1	F	231	THR
1	F	320	VAL
1	F	397	ALA
1	A	368	VAL
1	A	397	ALA
1	A	431	ARG
1	B	186	LEU
1	B	212	PRO
1	B	397	ALA
1	B	408	LYS
1	C	170	SER
1	C	186	LEU
1	C	320	VAL
1	C	363	GLN
1	C	364	ASP
1	C	367	GLN
1	D	175	GLU
1	D	319	SER
1	E	175	GLU
1	E	216	LYS
1	E	405	ILE
1	F	175	GLU
1	F	195	LEU
1	A	213	ASP
1	A	363	GLN
1	A	369	GLY
1	A	408	LYS
1	C	175	GLU
1	C	181	ARG
1	C	216	LYS
1	D	212	PRO

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Mol	Chain	Res	Type
1	D	369	GLY
1	E	320	VAL
1	E	357	LEU
1	E	369	GLY
1	F	228	ASP
1	F	363	GLN
1	F	431	ARG
1	A	186	LEU
1	A	212	PRO
1	A	364	ASP
1	B	233	GLU
1	B	307	SER
1	B	320	VAL
1	B	364	ASP
1	C	179	SER
1	C	397	ALA
1	D	195	LEU
1	D	262	ASP
1	D	320	VAL
1	D	363	GLN
1	D	367	GLN
1	D	370	ASN
1	E	427	ALA
1	F	168	GLU
1	F	181	ARG
1	F	369	GLY
1	F	427	ALA
1	B	369	GLY
1	C	195	LEU
1	C	212	PRO
1	C	366	ALA
1	C	394	PRO
1	D	230	THR
1	E	181	ARG
1	E	258	GLU
1	E	263	ALA
1	E	368	VAL
1	F	170	SER
1	F	364	ASP
1	A	263	ALA
1	D	222	ALA
1	D	427	ALA

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Mol	Chain	Res	Type
1	E	186	LEU
1	A	320	VAL
1	F	235	VAL
1	F	311	VAL
1	A	215	GLY
1	B	394	PRO
1	E	169	VAL
1	F	368	VAL
1	C	311	VAL
1	B	368	VAL

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	246/250 (98%)	231 (94%)	15 (6%)	17	38
1	B	246/250 (98%)	238 (97%)	8 (3%)	33	55
1	C	246/250 (98%)	230 (94%)	16 (6%)	15	37
1	D	246/250 (98%)	236 (96%)	10 (4%)	27	49
1	E	246/250 (98%)	237 (96%)	9 (4%)	30	51
1	F	246/250 (98%)	235 (96%)	11 (4%)	24	46
All	All	1476/1500 (98%)	1407 (95%)	69 (5%)	25	45

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	ILE
1	A	191	VAL
1	A	220	VAL
1	A	227	THR
1	A	228	ASP
1	A	236	LYS
1	A	268	LEU
1	A	281	VAL

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Mol	Chain	Res	Type
1	A	327	ILE
1	A	344	LEU
1	A	346	LEU
1	A	359	ASP
1	A	404	VAL
1	A	416	GLN
1	A	440	VAL
1	B	239	LEU
1	B	287	PHE
1	B	320	VAL
1	B	321	LEU
1	B	344	LEU
1	B	346	LEU
1	B	379	VAL
1	B	420	THR
1	C	173	SER
1	C	183	ILE
1	C	202	SER
1	C	206	LEU
1	C	216	LYS
1	C	233	GLU
1	C	239	LEU
1	C	267	LEU
1	C	355	ASP
1	C	360	GLU
1	C	387	VAL
1	C	390	SER
1	C	405	ILE
1	C	416	GLN
1	C	436	VAL
1	C	440	VAL
1	D	191	VAL
1	D	227	THR
1	D	239	LEU
1	D	262	ASP
1	D	291	ASP
1	D	321	LEU
1	D	322	VAL
1	D	347	ILE
1	D	416	GLN
1	D	441	ASN
1	E	233	GLU

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Mol	Chain	Res	Type
1	E	239	LEU
1	E	254	PHE
1	E	262	ASP
1	E	268	LEU
1	E	274	ARG
1	E	321	LEU
1	E	378	GLN
1	E	444	ARG
1	F	172	GLU
1	F	180	GLN
1	F	182	ILE
1	F	208	MET
1	F	227	THR
1	F	243	HIS
1	F	246	THR
1	F	291	ASP
1	F	301	THR
1	F	347	ILE
1	F	367	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	HIS
1	A	279	HIS
1	A	337	HIS
1	A	378	GLN
1	A	416	GLN
1	A	441	ASN
1	B	180	GLN
1	B	243	HIS
1	B	279	HIS
1	B	448	ASN
1	C	337	HIS
1	C	367	GLN
1	C	426	GLN
1	C	438	GLN
1	C	448	ASN
1	D	376	GLN
1	D	416	GLN
1	D	443	GLN
1	E	363	GLN

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Mol	Chain	Res	Type
1	E	367	GLN
1	F	180	GLN
1	F	243	HIS
1	F	378	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](#)

There are no chain breaks in this entry.

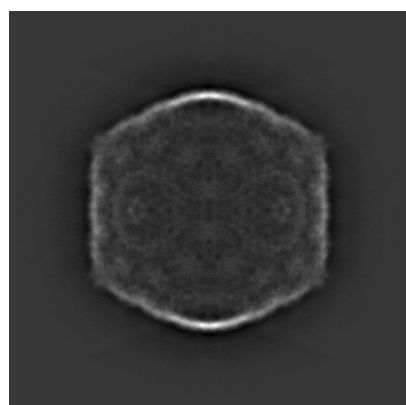
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8419. These allow visual inspection of the internal detail of the map and identification of artifacts.

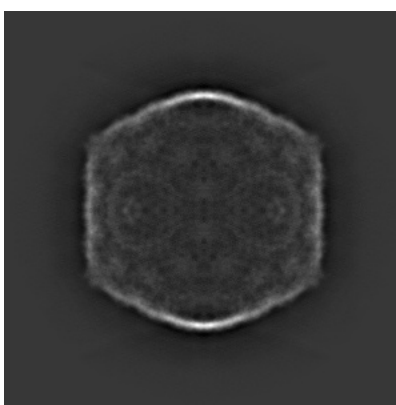
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

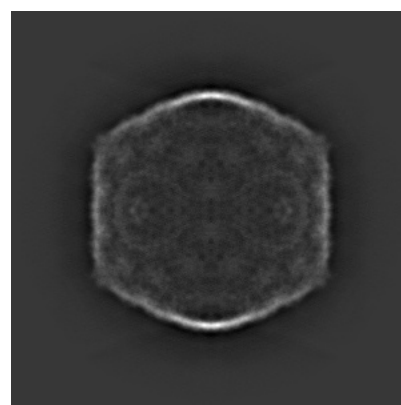
6.1.1 Primary map



X



Y

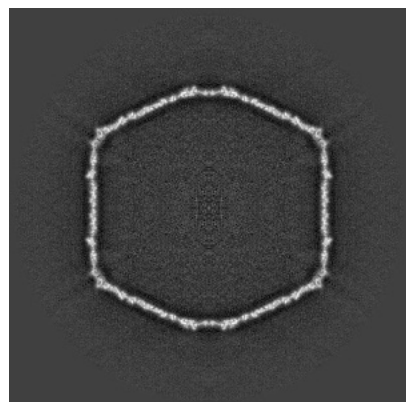


Z

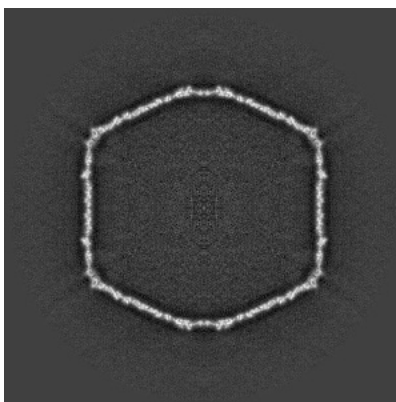
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

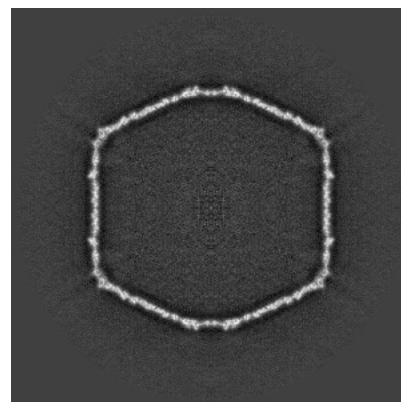
6.2.1 Primary map



X Index: 250



Y Index: 250

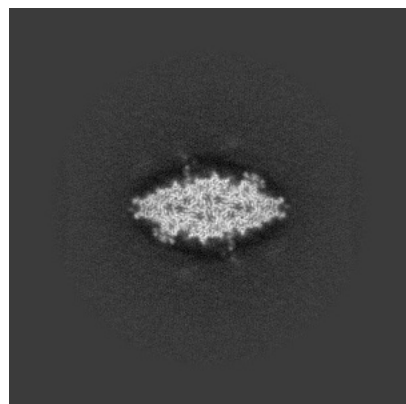


Z Index: 250

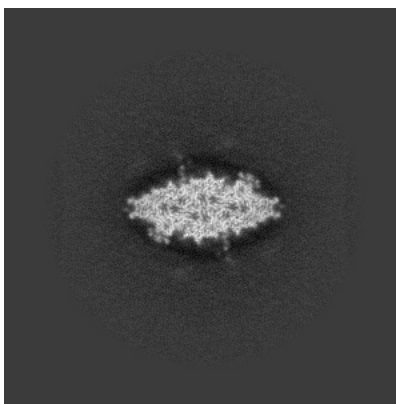
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

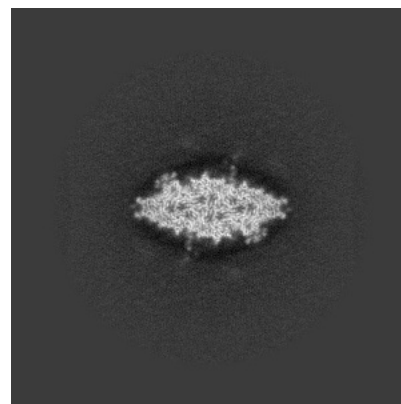
6.3.1 Primary map



X Index: 107



Y Index: 107

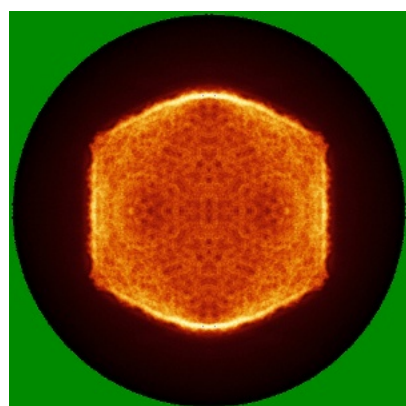


Z Index: 393

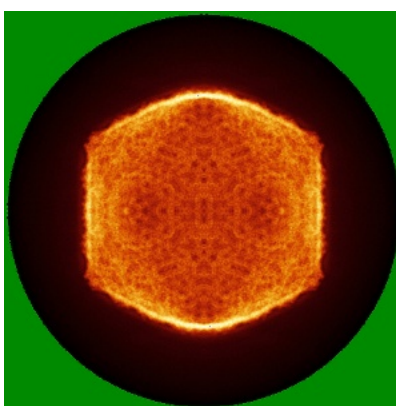
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

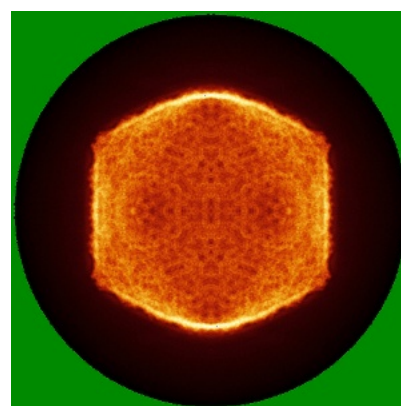
6.4.1 Primary map



X



Y

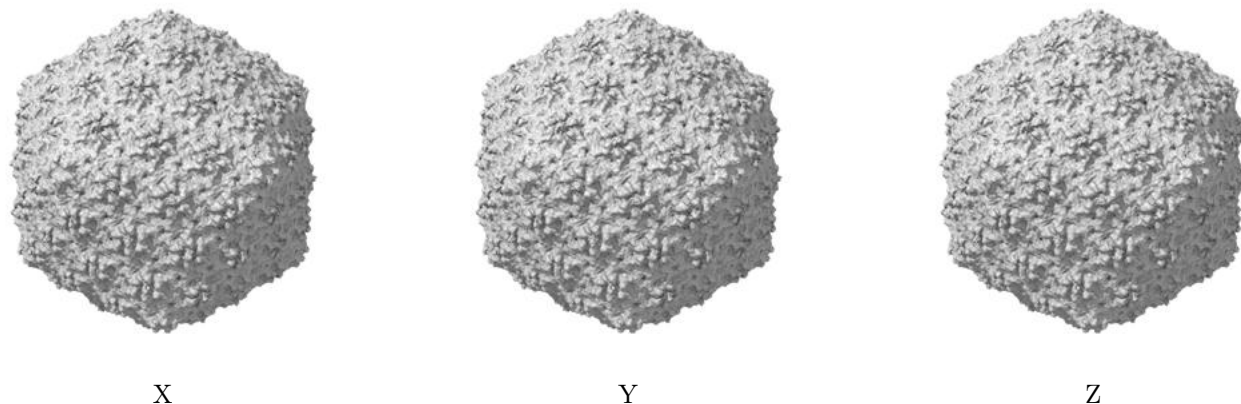


Z

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](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

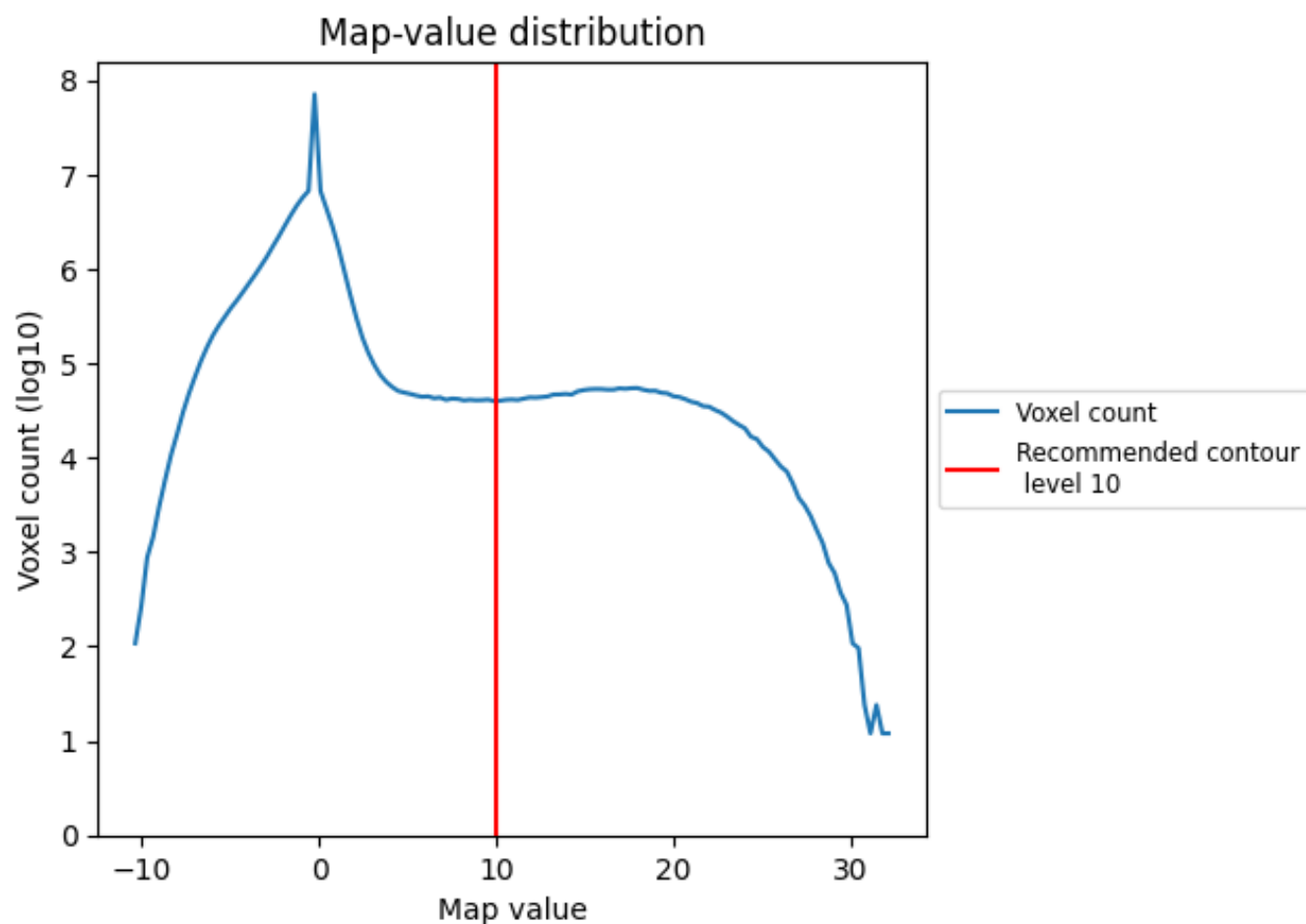
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

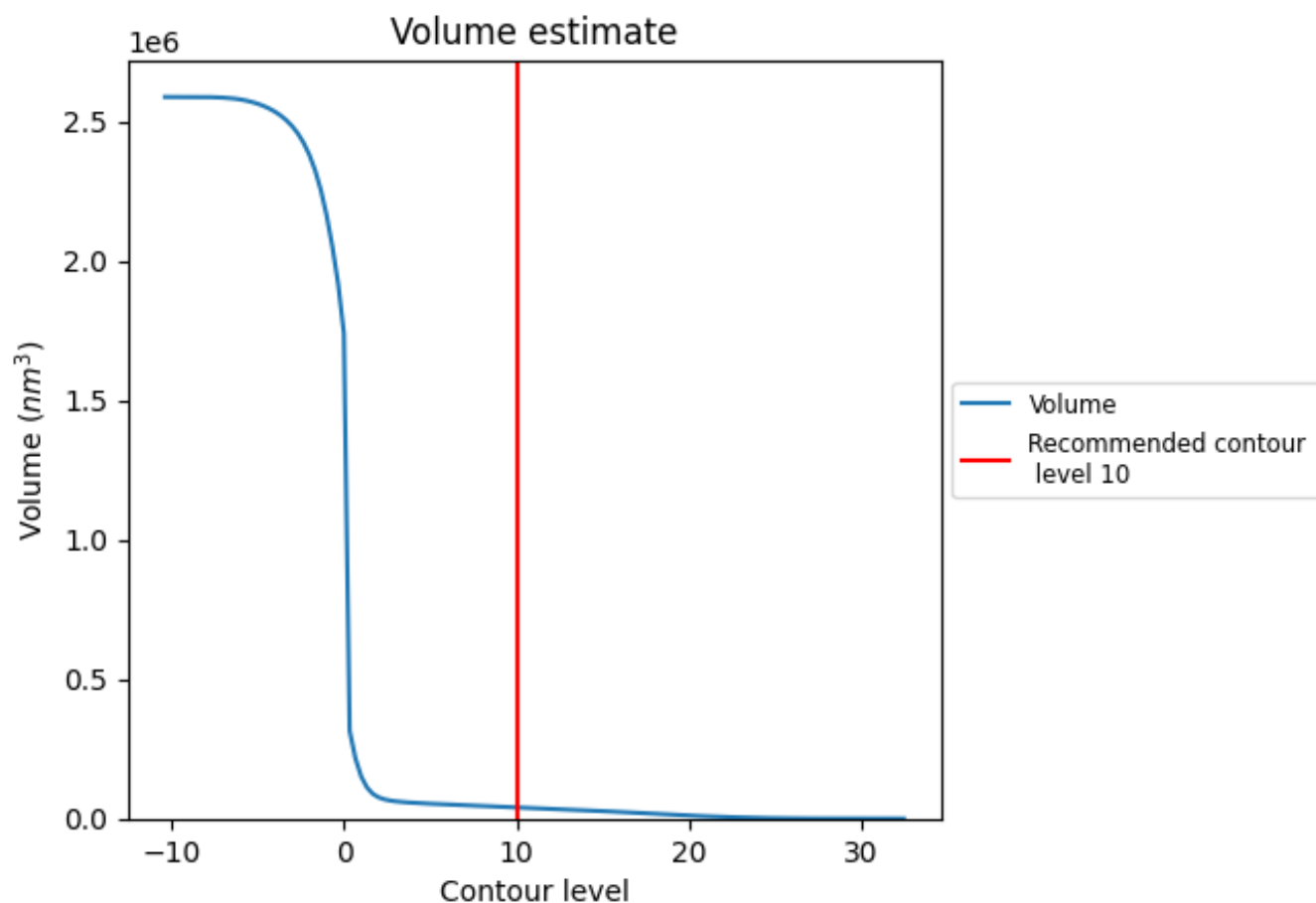
This section contains the results of statistical analysis of the map.

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.

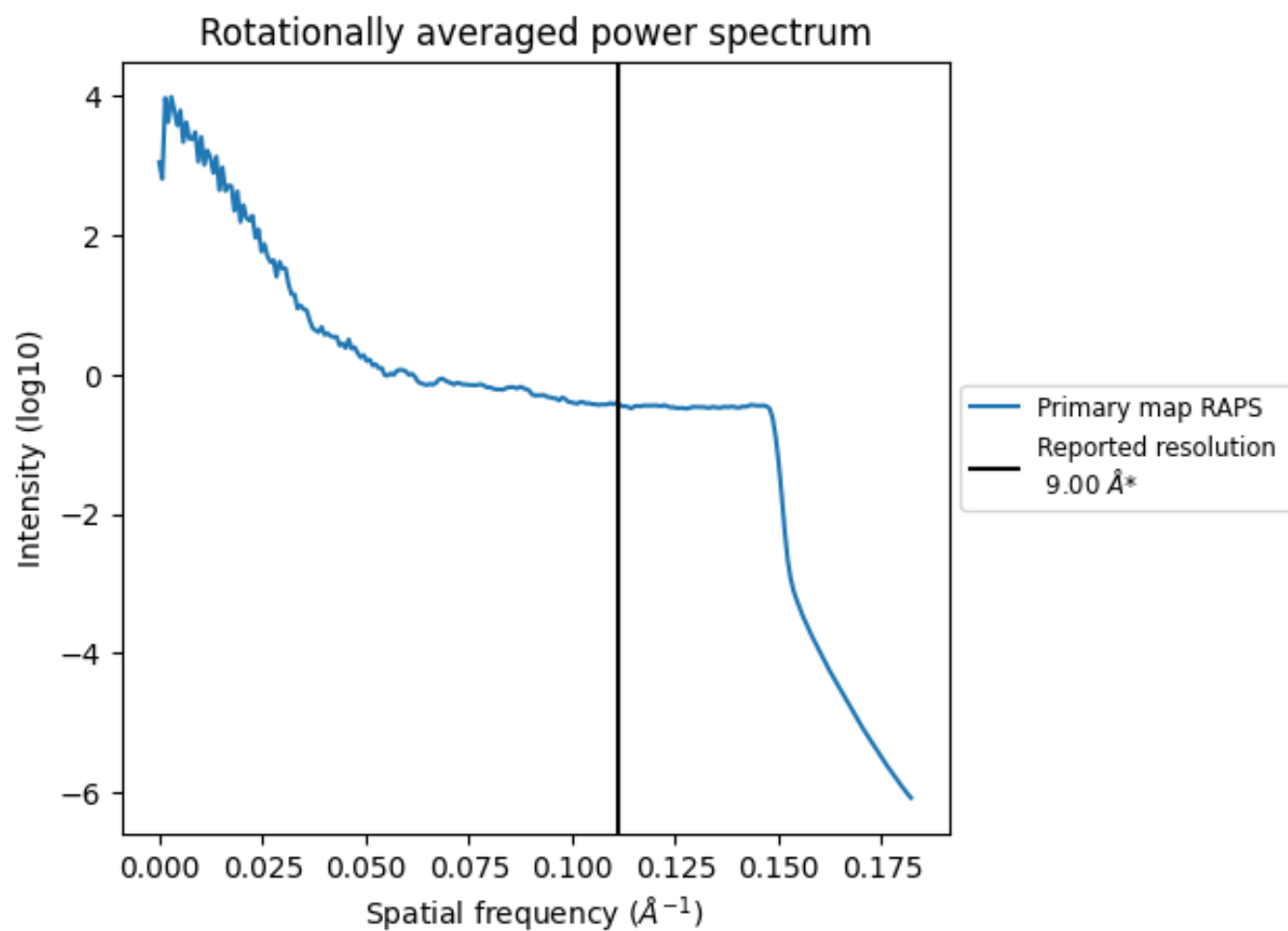
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 40373 nm³; this corresponds to an approximate mass of 36470 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 ⓘ

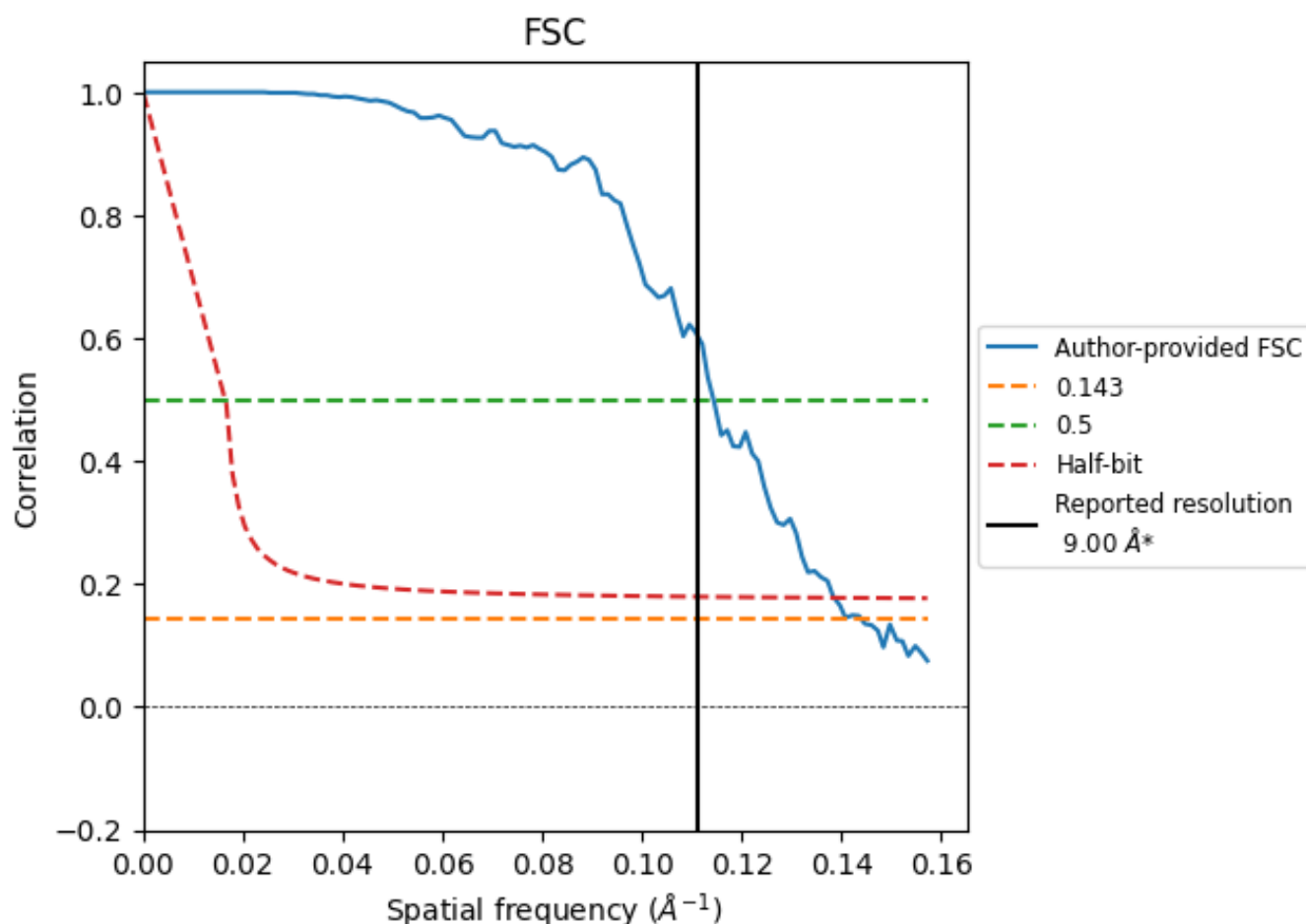


*Reported resolution corresponds to spatial frequency of 0.111 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.111 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	9.00	-
Author-provided FSC curve	6.94	8.74	7.22
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

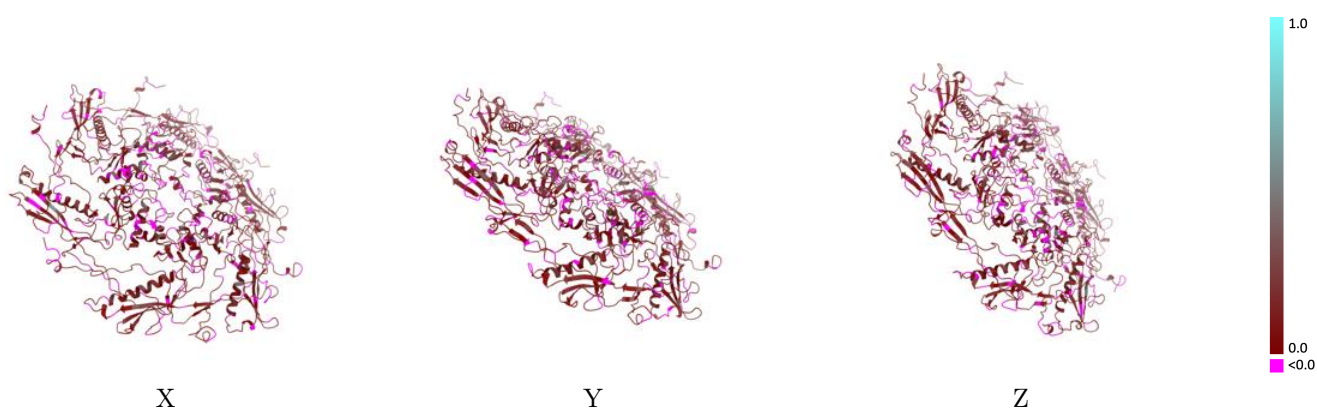
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8419 and PDB model 5TJT. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

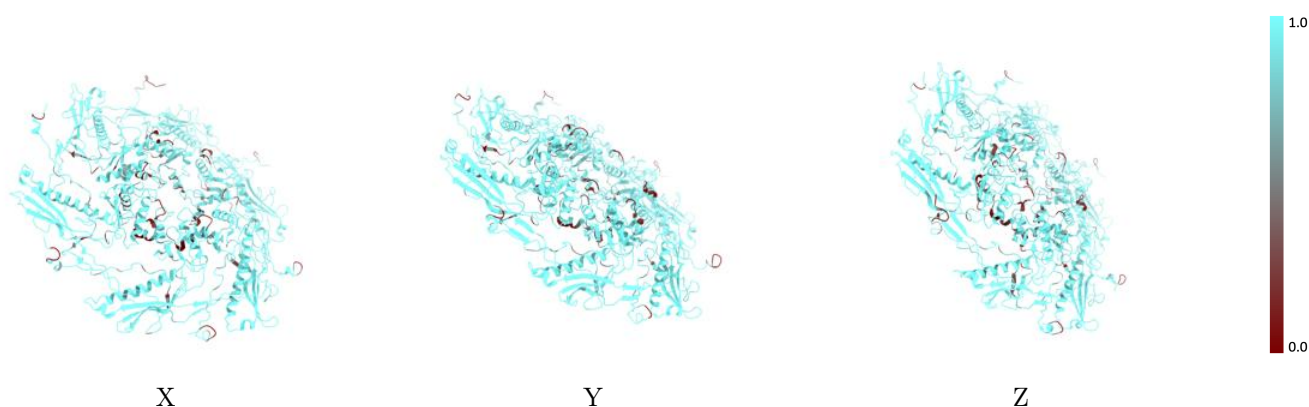
This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)



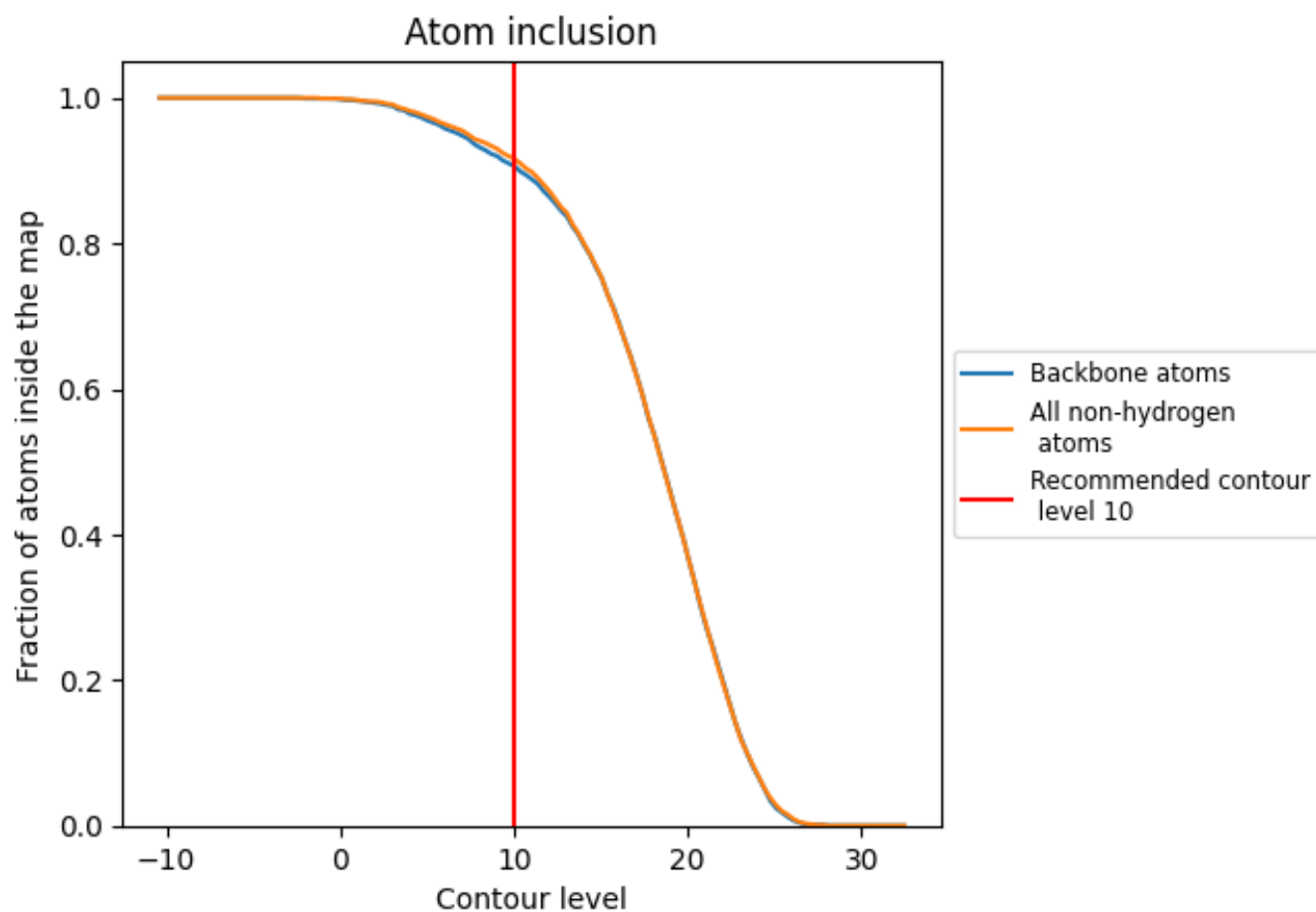
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (10).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (10) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9160	0.1060
A	0.9250	0.1090
B	0.9200	0.1010
C	0.9110	0.1070
D	0.9170	0.1030
E	0.9070	0.1100
F	0.9210	0.1090

1.0

0.0

<0.0