



## wwPDB EM Map/Model Validation Report ⓘ

Sep 26, 2016 – 11:23 AM EDT

PDB ID : 5GO9  
EMDB ID: : EMD-9528  
Title : Cryo-EM structure of RyR2 in closed state  
Authors : Peng, W.; Wu, J.P.; Yan, N.  
Deposited on : 2016-07-26  
Resolution : 4.40 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

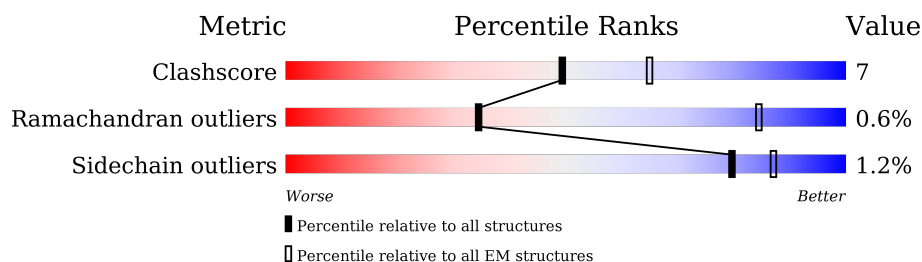
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	4968	54% 14% • 31%
1	B	4968	54% 14% • 31%
1	C	4968	54% 14% • 31%
1	D	4968	54% 14% • 31%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 105068 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3423	Total	C	N	O	S	0	0
			26266	16740	4498	4874	154		
1	B	3423	Total	C	N	O	S	0	0
			26266	16740	4498	4874	154		
1	C	3423	Total	C	N	O	S	0	0
			26266	16740	4498	4874	154		
1	D	3423	Total	C	N	O	S	0	0
			26266	16740	4498	4874	154		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total	Zn	0
			1	1	
2	A	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	



































G4956	D4869	R4755	E4660	PRO	ALA	LEU	ASN	LYS	GLU	E4108
D4957	A4870	T4756	E4660	THR	LYS	ILE	MET	MET	ARG	
C4958	F4871	I4757	R4664	ARG	GLU	PRO	PRO	THR	ALA	V4126
	G4872			SER	ASP	HIS	ASP	VAL	ASN	
K4961	E4873	H4763	I4667	SER	LYS	ASN	PRO	ARG	LYS	F4130
	L4874	M4764		SER	GLY	PRO	THR	ASP	GLU	Q4131
E4864	R4875	T4771	L4671	GLU	LYS	ASN	GLN	MET	GLU	
ASP			G4672	ASN	GLN	ALA	ASP	VAL	GLU	L4134
GLN	E4879	L4774	MET	ALA	LYS	ALA	GLY	GLU	SER	G4135
LEU	Q4880		ASP	ASN	ARG	LEU	VAL	ALA	GLU	R4136
ASN	V4881		LYS	PHE	GLN	SER	ARG	PHE	LYS	I4137
	K4882	Y4780	ALA	GLY	LEU	ASP	GLY	PHE	LYS	E4138
	E4883	L4781	ALA	SER	LEU	LEU	ASP	THR	LYS	I4139
D4884	Y4782		ALA	LEU	HIS	MET	GLY	THR	PRO	M4140
M4885	T4783	V4784	THR	ASP	THR	SER	ASP	TYR	GLU	G4141
E4886	T4784		ASP	SER	HIS	SER	GLU	TRP	GLU	S4142
T4887			PHE	SER	ARG	PRO	GLY	SER	GLN	A4143
K4888	R4791		SER	SER	TYR	ALA	GLY	VAL	GLY	K4144
C4889			ASP	PRO	GLY	PRO	ARG	PHE	PRO	R4145
F4890	E4798		ALA	ARG	GLU	ILE	LYS	MET	ARG	I4146
I4891	D4799		ARG	ILE	PRO	GLU	VAL	THR	MET	
C4892	G4800		ILE	ALA	VAL	VAL	LEU	LEU	PHE	S4157
G4893			LYS	ALA	VAL	GLN	GLY	LEU	GLY	R4158
I4894	D4804		LYS	PRO	PRO	GLN	GLY	HIS	PHE	
G4895			LYS	LYS	GLU	GLU	THR	ALA	LEU	I4161
	D4808		PRO	S4865	SER	LYS	LEU	ALA	SER	E4162
Y4898	D4809		LYS	S4866	ALA	PHE	PRO	ALA	VAL	R4163
	M4810		LYS	I4888	PHE	GLN	SER	SER	THR	R4164
N4915	L4811		ASP	I4888	TRP	GLU	GLU	VAL	VAL	
L4916	T4812		SER	K4610	LYS	GLN	ASP	SER	ARG	K4170
A4917	C4813		SER		LYS	LYS	LEU	ARG	SER	R4171
I4918			LEU		ILE	ALA	THR	GLY	ALA	
Y4919	Y4819		S4896	G4615	I4486	LYS	ASP	PHE	LEU	I4174
				L4616		GLU	LEU	SER	LEU	
F4922	R4823		W4709	Y4617	R4498	GLU	LYS	ARG	ALA	V4178
I4923				I4618	N4499	GLU	GLU	ILE	LEU	N4179
M4924	L4832		L4721		F4500	LYS	LEU	ILE	ARG	
Y4925			Y4722	Q4621		GLU	THR	GLY	TYR	M4187
	Y4840		L4723	T4627	M4503	GLU	GLU	GLY	ASN	E4188
			W4725	K4628	R4504	LYS	GLU	LEU	VAL	L4189
	R4844			G4629	M4505	GLU	SER	LEU	LEU	F4190
	I4845			W4630		GLU	ASP	THR	THR	V4191
E4931			M4729	W4631	I4514	ASN	LEU	GLY	LEU	
	D4848			D4632	M4515	LYS	LEU	GLY	MET	C4194
G4936			L4732	R4633		SER	SER	SER	ARG	
Q4937				I4636	L4518	GLU	ASP	LEU	MET	T4197
E4938	F4852		Y4735		L4519	PRO	ILE	VAL	LEU	
S4939	F4853		N4736			GLU	PHE	GLU	SER	M4201
Y4940	F4854		W4737	I4636	V4523	LYS	GLY	GLY	LEU	Q4202
V4941			F4738	S4640	S4524	ALA	LEU	LYS	SER	I4203
W4942	V4857		F4739		THR	GLU	ASP	LYS	SER	A4204
	I4858		F4740	N4643	SER	GLY	LEU	LYS	LEU	A4205
Y4945	L4859			Y4644	SER	GLU	LYS	ILE	LYS	Q4206
	A4861		L4745	Y4645	VAL	ASP	ARG	LYS	LYS	I4207
R4948			D4746	W4646	VAL	GLY	GLU	VAL	GLU	SER
C4949	A4861		I4747	D4647		GLU	GLY	ALA	MET	GLU
W4950	Q4864					LYS	GLY	GLU	LYS	GLU
	G4865		K4752	V4650		GLU	GLN	GLU	LYS	SER
F4953	L4866		T4753	K4651		LYS	GLU	LEU	ASP	SER
P4954	I4867		L4754	R4652		GLU	TYR	VAL	LEU	GLU
A4955	I4868					LYS	LYS	ALA	VAL	ASN



## 4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	48454	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	B	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	C	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	D	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
All	All	0.98	116/107004 (0.1%)	0.94	312/144596 (0.2%)

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	30
1	B	0	30
1	C	0	30
1	D	0	30
All	All	0	120

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	B	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	C	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	D	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	A	4950	TRP	CE3-CZ3	-9.89	1.21	1.38
1	B	4950	TRP	CE3-CZ3	-9.89	1.21	1.38
1	C	4950	TRP	CE3-CZ3	-9.89	1.21	1.38
1	D	4950	TRP	CE3-CZ3	-9.89	1.21	1.38
1	A	4190	PHE	CG-CD1	-8.95	1.25	1.38
1	B	4190	PHE	CG-CD1	-8.95	1.25	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4190	PHE	CG-CD1	-8.95	1.25	1.38
1	D	4190	PHE	CG-CD1	-8.95	1.25	1.38
1	A	4919	TYR	CG-CD1	-8.51	1.28	1.39
1	B	4919	TYR	CG-CD1	-8.51	1.28	1.39
1	C	4919	TYR	CG-CD1	-8.51	1.28	1.39
1	D	4919	TYR	CG-CD1	-8.51	1.28	1.39
1	A	4940	TYR	CG-CD1	-8.37	1.28	1.39
1	B	4940	TYR	CG-CD1	-8.37	1.28	1.39
1	C	4940	TYR	CG-CD1	-8.37	1.28	1.39
1	D	4940	TYR	CG-CD1	-8.37	1.28	1.39
1	A	4953	PHE	CG-CD2	-8.12	1.26	1.38
1	B	4953	PHE	CG-CD2	-8.12	1.26	1.38
1	C	4953	PHE	CG-CD2	-8.12	1.26	1.38
1	D	4953	PHE	CG-CD2	-8.12	1.26	1.38
1	A	4945	TYR	CE2-CZ	-7.18	1.29	1.38
1	B	4945	TYR	CE2-CZ	-7.18	1.29	1.38
1	C	4945	TYR	CE2-CZ	-7.18	1.29	1.38
1	D	4945	TYR	CE2-CZ	-7.18	1.29	1.38
1	A	4500	PHE	CG-CD1	-6.99	1.28	1.38
1	B	4500	PHE	CG-CD1	-6.99	1.28	1.38
1	C	4500	PHE	CG-CD1	-6.99	1.28	1.38
1	D	4500	PHE	CG-CD1	-6.99	1.28	1.38
1	A	4953	PHE	CE1-CZ	-6.97	1.24	1.37
1	B	4953	PHE	CE1-CZ	-6.97	1.24	1.37
1	C	4953	PHE	CE1-CZ	-6.97	1.24	1.37
1	D	4953	PHE	CE1-CZ	-6.97	1.24	1.37
1	A	4646	TRP	CG-CD1	-6.90	1.27	1.36
1	B	4646	TRP	CG-CD1	-6.90	1.27	1.36
1	C	4646	TRP	CG-CD1	-6.90	1.27	1.36
1	D	4646	TRP	CG-CD1	-6.90	1.27	1.36
1	A	4898	TYR	CG-CD2	-6.79	1.30	1.39
1	B	4898	TYR	CG-CD2	-6.79	1.30	1.39
1	C	4898	TYR	CG-CD2	-6.79	1.30	1.39
1	D	4898	TYR	CG-CD2	-6.79	1.30	1.39
1	A	4895	GLY	C-O	-6.48	1.13	1.23
1	B	4895	GLY	C-O	-6.48	1.13	1.23
1	C	4895	GLY	C-O	-6.48	1.13	1.23
1	D	4895	GLY	C-O	-6.48	1.13	1.23
1	A	4136	ARG	C-O	-6.46	1.11	1.23
1	B	4136	ARG	C-O	-6.46	1.11	1.23
1	C	4136	ARG	C-O	-6.46	1.11	1.23
1	D	4136	ARG	C-O	-6.46	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4919	TYR	CE1-CZ	-6.08	1.30	1.38
1	B	4919	TYR	CE1-CZ	-6.08	1.30	1.38
1	C	4919	TYR	CE1-CZ	-6.08	1.30	1.38
1	D	4919	TYR	CE1-CZ	-6.08	1.30	1.38
1	A	4138	GLU	CD-OE1	-5.87	1.19	1.25
1	B	4138	GLU	CD-OE1	-5.87	1.19	1.25
1	C	4138	GLU	CD-OE1	-5.87	1.19	1.25
1	D	4138	GLU	CD-OE1	-5.87	1.19	1.25
1	A	4922	PHE	CD2-CE2	-5.83	1.27	1.39
1	B	4922	PHE	CD2-CE2	-5.83	1.27	1.39
1	C	4922	PHE	CD2-CE2	-5.83	1.27	1.39
1	D	4922	PHE	CD2-CE2	-5.83	1.27	1.39
1	A	4950	TRP	CB-CG	-5.79	1.39	1.50
1	B	4950	TRP	CB-CG	-5.79	1.39	1.50
1	C	4950	TRP	CB-CG	-5.79	1.39	1.50
1	D	4950	TRP	CB-CG	-5.79	1.39	1.50
1	A	4854	PHE	CG-CD1	5.72	1.47	1.38
1	B	4854	PHE	CG-CD1	5.72	1.47	1.38
1	C	4854	PHE	CG-CD1	5.72	1.47	1.38
1	D	4854	PHE	CG-CD1	5.72	1.47	1.38
1	A	4954	PRO	CA-C	-5.71	1.41	1.52
1	B	4954	PRO	CA-C	-5.71	1.41	1.52
1	C	4954	PRO	CA-C	-5.71	1.41	1.52
1	D	4954	PRO	CA-C	-5.71	1.41	1.52
1	A	4925	TYR	CG-CD2	-5.62	1.31	1.39
1	B	4925	TYR	CG-CD2	-5.62	1.31	1.39
1	C	4925	TYR	CG-CD2	-5.62	1.31	1.39
1	D	4925	TYR	CG-CD2	-5.62	1.31	1.39
1	A	4735	TYR	CE2-CZ	-5.60	1.31	1.38
1	B	4735	TYR	CE2-CZ	-5.60	1.31	1.38
1	C	4735	TYR	CE2-CZ	-5.60	1.31	1.38
1	D	4735	TYR	CE2-CZ	-5.60	1.31	1.38
1	A	1825	PHE	CG-CD2	-5.56	1.30	1.38
1	B	1825	PHE	CG-CD2	-5.56	1.30	1.38
1	C	1825	PHE	CG-CD2	-5.56	1.30	1.38
1	D	1825	PHE	CG-CD2	-5.56	1.30	1.38
1	A	4890	PHE	CB-CG	-5.45	1.42	1.51
1	B	4890	PHE	CB-CG	-5.45	1.42	1.51
1	C	4890	PHE	CB-CG	-5.45	1.42	1.51
1	D	4890	PHE	CB-CG	-5.45	1.42	1.51
1	A	471	GLU	CG-CD	5.44	1.60	1.51
1	B	471	GLU	CG-CD	5.44	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	471	GLU	CG-CD	5.44	1.60	1.51
1	D	471	GLU	CG-CD	5.44	1.60	1.51
1	A	4958	CYS	CB-SG	-5.40	1.73	1.81
1	B	4958	CYS	CB-SG	-5.40	1.73	1.81
1	C	4958	CYS	CB-SG	-5.40	1.73	1.81
1	D	4958	CYS	CB-SG	-5.40	1.73	1.81
1	A	3781	TYR	CG-CD1	-5.39	1.32	1.39
1	B	3781	TYR	CG-CD1	-5.39	1.32	1.39
1	C	3781	TYR	CG-CD1	-5.39	1.32	1.39
1	D	3781	TYR	CG-CD1	-5.39	1.32	1.39
1	A	3700	CYS	CB-SG	5.37	1.91	1.82
1	B	3700	CYS	CB-SG	5.37	1.91	1.82
1	C	3700	CYS	CB-SG	5.37	1.91	1.82
1	D	3700	CYS	CB-SG	5.37	1.91	1.82
1	A	3890	TYR	CE2-CZ	5.27	1.45	1.38
1	B	3890	TYR	CE2-CZ	5.27	1.45	1.38
1	C	3890	TYR	CE2-CZ	5.27	1.45	1.38
1	D	3890	TYR	CE2-CZ	5.27	1.45	1.38
1	A	4735	TYR	CG-CD1	-5.18	1.32	1.39
1	B	4735	TYR	CG-CD1	-5.18	1.32	1.39
1	C	4735	TYR	CG-CD1	-5.18	1.32	1.39
1	D	4735	TYR	CG-CD1	-5.18	1.32	1.39

All (312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	B	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	C	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	D	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	A	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	C	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	D	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	4948	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	B	4948	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	C	4948	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	D	4948	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	A	2583	PRO	N-CA-CB	8.35	113.31	103.30
1	B	2583	PRO	N-CA-CB	8.35	113.31	103.30
1	C	2583	PRO	N-CA-CB	8.35	113.31	103.30
1	D	2583	PRO	N-CA-CB	8.35	113.31	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3104	PRO	N-CA-CB	8.32	113.29	103.30
1	B	3104	PRO	N-CA-CB	8.32	113.29	103.30
1	C	3104	PRO	N-CA-CB	8.32	113.29	103.30
1	D	3104	PRO	N-CA-CB	8.32	113.29	103.30
1	A	4844	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	B	4844	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	C	4844	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	D	4844	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	A	3778	MET	CG-SD-CE	7.94	112.90	100.20
1	B	3778	MET	CG-SD-CE	7.94	112.90	100.20
1	C	3778	MET	CG-SD-CE	7.94	112.90	100.20
1	D	3778	MET	CG-SD-CE	7.94	112.90	100.20
1	A	2495	PRO	N-CA-CB	7.79	112.64	103.30
1	B	2495	PRO	N-CA-CB	7.79	112.64	103.30
1	C	2495	PRO	N-CA-CB	7.79	112.64	103.30
1	D	2495	PRO	N-CA-CB	7.79	112.64	103.30
1	A	2736	ASP	CB-CG-OD2	7.77	125.30	118.30
1	B	2736	ASP	CB-CG-OD2	7.77	125.30	118.30
1	C	2736	ASP	CB-CG-OD2	7.77	125.30	118.30
1	D	2736	ASP	CB-CG-OD2	7.77	125.30	118.30
1	A	4139	ILE	CG1-CB-CG2	-7.39	95.15	111.40
1	B	4139	ILE	CG1-CB-CG2	-7.39	95.15	111.40
1	C	4139	ILE	CG1-CB-CG2	-7.39	95.15	111.40
1	D	4139	ILE	CG1-CB-CG2	-7.39	95.15	111.40
1	A	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	B	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	C	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	D	347	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	4885	MET	CG-SD-CE	-7.29	88.53	100.20
1	B	4885	MET	CG-SD-CE	-7.29	88.53	100.20
1	C	4885	MET	CG-SD-CE	-7.29	88.53	100.20
1	D	4885	MET	CG-SD-CE	-7.29	88.53	100.20
1	A	2598	PRO	N-CA-CB	7.25	112.00	103.30
1	B	2598	PRO	N-CA-CB	7.25	112.00	103.30
1	C	2598	PRO	N-CA-CB	7.25	112.00	103.30
1	D	2598	PRO	N-CA-CB	7.25	112.00	103.30
1	A	4505	MET	CB-CG-SD	7.13	133.79	112.40
1	B	4505	MET	CB-CG-SD	7.13	133.79	112.40
1	C	4505	MET	CB-CG-SD	7.13	133.79	112.40
1	D	4505	MET	CB-CG-SD	7.13	133.79	112.40
1	A	4745	LEU	CB-CG-CD2	7.06	123.01	111.00
1	B	4745	LEU	CB-CG-CD2	7.06	123.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4745	LEU	CB-CG-CD2	7.06	123.01	111.00
1	D	4745	LEU	CB-CG-CD2	7.06	123.01	111.00
1	A	2534	PRO	N-CA-CB	7.04	111.75	103.30
1	B	2534	PRO	N-CA-CB	7.04	111.75	103.30
1	C	2534	PRO	N-CA-CB	7.04	111.75	103.30
1	D	2534	PRO	N-CA-CB	7.04	111.75	103.30
1	A	3918	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	B	3918	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	C	3918	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	D	3918	PHE	CB-CG-CD2	-7.01	115.89	120.80
1	A	4859	LEU	CB-CG-CD2	6.97	122.84	111.00
1	B	4859	LEU	CB-CG-CD2	6.97	122.84	111.00
1	C	4859	LEU	CB-CG-CD2	6.97	122.84	111.00
1	D	4859	LEU	CB-CG-CD2	6.97	122.84	111.00
1	A	4859	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	B	4859	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	C	4859	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	D	4859	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	A	4136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	4136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	C	4136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	D	4136	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	2625	PRO	N-CA-CB	6.61	111.23	103.30
1	B	2625	PRO	N-CA-CB	6.61	111.23	103.30
1	C	2625	PRO	N-CA-CB	6.61	111.23	103.30
1	D	2625	PRO	N-CA-CB	6.61	111.23	103.30
1	A	4500	PHE	CB-CG-CD2	6.56	125.39	120.80
1	B	4500	PHE	CB-CG-CD2	6.56	125.39	120.80
1	C	4500	PHE	CB-CG-CD2	6.56	125.39	120.80
1	D	4500	PHE	CB-CG-CD2	6.56	125.39	120.80
1	A	3683	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	B	3683	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	C	3683	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	D	3683	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	A	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	B	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	C	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	D	2678	PRO	N-CA-CB	6.36	110.93	103.30
1	A	4938	GLU	OE1-CD-OE2	6.35	130.92	123.30
1	B	4938	GLU	OE1-CD-OE2	6.35	130.92	123.30
1	C	4938	GLU	OE1-CD-OE2	6.35	130.92	123.30
1	D	4938	GLU	OE1-CD-OE2	6.35	130.92	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4170	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	B	4170	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	C	4170	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	D	4170	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	A	4158	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	B	4158	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	C	4158	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	D	4158	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	A	3803	VAL	N-CA-C	-6.17	94.34	111.00
1	B	3803	VAL	N-CA-C	-6.17	94.34	111.00
1	C	3803	VAL	N-CA-C	-6.17	94.34	111.00
1	D	3803	VAL	N-CA-C	-6.17	94.34	111.00
1	A	2607	PRO	N-CA-CB	6.15	110.68	103.30
1	B	2607	PRO	N-CA-CB	6.15	110.68	103.30
1	C	2607	PRO	N-CA-CB	6.15	110.68	103.30
1	D	2607	PRO	N-CA-CB	6.15	110.68	103.30
1	A	2990	PRO	N-CA-CB	6.12	110.64	103.30
1	B	2990	PRO	N-CA-CB	6.12	110.64	103.30
1	C	2990	PRO	N-CA-CB	6.12	110.64	103.30
1	D	2990	PRO	N-CA-CB	6.12	110.64	103.30
1	A	2679	PRO	N-CA-CB	6.06	110.57	103.30
1	B	2679	PRO	N-CA-CB	6.06	110.57	103.30
1	C	2679	PRO	N-CA-CB	6.06	110.57	103.30
1	D	2679	PRO	N-CA-CB	6.06	110.57	103.30
1	A	4735	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	B	4735	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	C	4735	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	D	4735	TYR	CG-CD2-CE2	6.03	126.12	121.30
1	A	2783	MET	CG-SD-CE	5.97	109.76	100.20
1	B	2783	MET	CG-SD-CE	5.97	109.76	100.20
1	C	2783	MET	CG-SD-CE	5.97	109.76	100.20
1	D	2783	MET	CG-SD-CE	5.97	109.76	100.20
1	A	1303	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	B	1303	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	C	1303	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	D	1303	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	3948	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	B	3948	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	C	3948	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	D	3948	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	A	814	LEU	CA-CB-CG	5.81	128.67	115.30
1	B	814	LEU	CA-CB-CG	5.81	128.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	814	LEU	CA-CB-CG	5.81	128.67	115.30
1	D	814	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	4134	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	4134	LEU	CA-CB-CG	5.79	128.62	115.30
1	C	4134	LEU	CA-CB-CG	5.79	128.62	115.30
1	D	4134	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	4953	PHE	CB-CG-CD1	5.78	124.84	120.80
1	B	4953	PHE	CB-CG-CD1	5.78	124.84	120.80
1	C	4953	PHE	CB-CG-CD1	5.78	124.84	120.80
1	D	4953	PHE	CB-CG-CD1	5.78	124.84	120.80
1	A	2268	ARG	CB-CG-CD	5.63	126.25	111.60
1	B	2268	ARG	CB-CG-CD	5.63	126.25	111.60
1	C	2268	ARG	CB-CG-CD	5.63	126.25	111.60
1	D	2268	ARG	CB-CG-CD	5.63	126.25	111.60
1	A	2425	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	2425	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	2425	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	2425	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	2668	PRO	N-CA-CB	5.60	110.02	103.30
1	B	2668	PRO	N-CA-CB	5.60	110.02	103.30
1	C	2668	PRO	N-CA-CB	5.60	110.02	103.30
1	D	2668	PRO	N-CA-CB	5.60	110.02	103.30
1	A	4945	TYR	CB-CG-CD2	5.59	124.35	121.00
1	B	4945	TYR	CB-CG-CD2	5.59	124.35	121.00
1	C	4945	TYR	CB-CG-CD2	5.59	124.35	121.00
1	D	4945	TYR	CB-CG-CD2	5.59	124.35	121.00
1	A	836	HIS	CB-CA-C	-5.58	99.25	110.40
1	B	836	HIS	CB-CA-C	-5.58	99.25	110.40
1	C	836	HIS	CB-CA-C	-5.58	99.25	110.40
1	D	836	HIS	CB-CA-C	-5.58	99.25	110.40
1	A	4504	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	4504	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	4504	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	4504	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	3803	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	B	3803	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	C	3803	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	D	3803	VAL	CG1-CB-CG2	-5.49	102.11	110.90
1	A	4500	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	B	4500	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	C	4500	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	D	4500	PHE	CB-CG-CD1	-5.49	116.96	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4085	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	B	4085	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	C	4085	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	D	4085	VAL	CG1-CB-CG2	-5.48	102.14	110.90
1	A	2143	MET	CG-SD-CE	-5.45	91.48	100.20
1	B	2143	MET	CG-SD-CE	-5.45	91.48	100.20
1	C	2143	MET	CG-SD-CE	-5.45	91.48	100.20
1	D	2143	MET	CG-SD-CE	-5.45	91.48	100.20
1	A	1599	MET	CG-SD-CE	5.44	108.91	100.20
1	B	1599	MET	CG-SD-CE	5.44	108.91	100.20
1	C	1599	MET	CG-SD-CE	5.44	108.91	100.20
1	D	1599	MET	CG-SD-CE	5.44	108.91	100.20
1	A	4187	MET	CG-SD-CE	5.44	108.90	100.20
1	B	4187	MET	CG-SD-CE	5.44	108.90	100.20
1	C	4187	MET	CG-SD-CE	5.44	108.90	100.20
1	D	4187	MET	CG-SD-CE	5.44	108.90	100.20
1	A	1032	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	B	1032	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	C	1032	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	D	1032	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	A	4916	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	B	4916	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	C	4916	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	D	4916	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	A	4189	LEU	CA-CB-CG	5.36	127.63	115.30
1	B	4189	LEU	CA-CB-CG	5.36	127.63	115.30
1	C	4189	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	4189	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	4197	THR	CA-CB-CG2	-5.35	104.92	112.40
1	B	4197	THR	CA-CB-CG2	-5.35	104.92	112.40
1	C	4197	THR	CA-CB-CG2	-5.35	104.92	112.40
1	D	4197	THR	CA-CB-CG2	-5.35	104.92	112.40
1	A	1738	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	B	1738	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	C	1738	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	D	1738	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	A	4645	TYR	CB-CG-CD1	5.33	124.20	121.00
1	B	4645	TYR	CB-CG-CD1	5.33	124.20	121.00
1	C	4645	TYR	CB-CG-CD1	5.33	124.20	121.00
1	D	4645	TYR	CB-CG-CD1	5.33	124.20	121.00
1	A	2101	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	4940	TYR	CB-CG-CD2	5.29	124.17	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2101	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	4940	TYR	CB-CG-CD2	5.29	124.17	121.00
1	C	2101	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	4940	TYR	CB-CG-CD2	5.29	124.17	121.00
1	D	2101	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	D	4940	TYR	CB-CG-CD2	5.29	124.17	121.00
1	A	2166	LEU	CB-CG-CD1	-5.29	102.02	111.00
1	B	2166	LEU	CB-CG-CD1	-5.29	102.02	111.00
1	C	2166	LEU	CB-CG-CD1	-5.29	102.02	111.00
1	D	2166	LEU	CB-CG-CD1	-5.29	102.02	111.00
1	A	2517	LEU	CA-CB-CG	5.28	127.45	115.30
1	B	2517	LEU	CA-CB-CG	5.28	127.45	115.30
1	C	2517	LEU	CA-CB-CG	5.28	127.45	115.30
1	D	2517	LEU	CA-CB-CG	5.28	127.45	115.30
1	A	4823	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	B	4823	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	C	4823	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	D	4823	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	4924	MET	CG-SD-CE	-5.25	91.81	100.20
1	B	4924	MET	CG-SD-CE	-5.25	91.81	100.20
1	C	4924	MET	CG-SD-CE	-5.25	91.81	100.20
1	D	4924	MET	CG-SD-CE	-5.25	91.81	100.20
1	A	2736	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	B	2736	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	C	2736	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	D	2736	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	A	677	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	677	LEU	CA-CB-CG	5.22	127.30	115.30
1	C	677	LEU	CA-CB-CG	5.22	127.30	115.30
1	D	677	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	4945	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	B	4945	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	C	4945	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	D	4945	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	A	1824	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	4721	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	1824	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	4721	LEU	CA-CB-CG	5.20	127.26	115.30
1	C	1824	LEU	CA-CB-CG	5.20	127.26	115.30
1	C	4721	LEU	CA-CB-CG	5.20	127.26	115.30
1	D	1824	LEU	CA-CB-CG	5.20	127.26	115.30
1	D	4721	LEU	CA-CB-CG	5.20	127.26	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1942	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	B	1942	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	C	1942	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	D	1942	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	1729	MET	CG-SD-CE	5.16	108.45	100.20
1	B	1729	MET	CG-SD-CE	5.16	108.45	100.20
1	C	1729	MET	CG-SD-CE	5.16	108.45	100.20
1	D	1729	MET	CG-SD-CE	5.16	108.45	100.20
1	A	3837	THR	CA-CB-CG2	-5.15	105.19	112.40
1	B	3837	THR	CA-CB-CG2	-5.15	105.19	112.40
1	C	3837	THR	CA-CB-CG2	-5.15	105.19	112.40
1	D	3837	THR	CA-CB-CG2	-5.15	105.19	112.40
1	A	4941	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	B	4941	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	C	4941	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	D	4941	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	A	4086	LYS	CD-CE-NZ	5.14	123.53	111.70
1	B	4086	LYS	CD-CE-NZ	5.14	123.53	111.70
1	C	4086	LYS	CD-CE-NZ	5.14	123.53	111.70
1	D	4086	LYS	CD-CE-NZ	5.14	123.53	111.70
1	A	3802	SER	C-N-CA	5.13	134.52	121.70
1	B	3802	SER	C-N-CA	5.13	134.52	121.70
1	C	3802	SER	C-N-CA	5.13	134.52	121.70
1	D	3802	SER	C-N-CA	5.13	134.52	121.70
1	A	3945	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	B	3945	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	C	3945	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	D	3945	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	A	4845	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	B	4845	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	C	4845	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	D	4845	ILE	CG1-CB-CG2	-5.06	100.27	111.40
1	A	2059	LEU	CB-CG-CD1	5.03	119.54	111.00
1	B	2059	LEU	CB-CG-CD1	5.03	119.54	111.00
1	C	2059	LEU	CB-CG-CD1	5.03	119.54	111.00
1	D	2059	LEU	CB-CG-CD1	5.03	119.54	111.00
1	A	3918	PHE	CB-CG-CD1	5.02	124.31	120.80
1	B	3918	PHE	CB-CG-CD1	5.02	124.31	120.80
1	C	3918	PHE	CB-CG-CD1	5.02	124.31	120.80
1	D	3918	PHE	CB-CG-CD1	5.02	124.31	120.80
1	A	2203	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	B	2203	TYR	CB-CG-CD2	-5.01	118.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2203	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	D	2203	TYR	CB-CG-CD2	-5.01	118.00	121.00

There are no chirality outliers.

All (120) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1102	TYR	Peptide
1	A	1266	GLU	Peptide
1	A	1297	THR	Peptide
1	A	1475	LYS	Peptide
1	A	1579	VAL	Peptide
1	A	1635	GLU	Peptide
1	A	1739	PHE	Peptide
1	A	1808	ASP	Peptide
1	A	1835	HIS	Peptide
1	A	1847	GLU	Peptide
1	A	2075	VAL	Peptide
1	A	2077	GLU	Peptide
1	A	3767	LEU	Peptide
1	A	3805	ASP	Peptide
1	A	4070	CYS	Peptide
1	A	4144	LYS	Peptide
1	A	4163	LYS	Peptide
1	A	471	GLU	Peptide
1	A	4798	GLU	Peptide
1	A	4956	GLY	Peptide
1	A	4958	CYS	Peptide
1	A	657	PRO	Peptide
1	A	729	GLY	Peptide
1	A	775	VAL	Peptide
1	A	791	VAL	Peptide
1	A	818	GLY	Peptide
1	A	819	TYR	Peptide
1	A	838	ARG	Peptide
1	A	852	GLY	Mainchain,Peptide
1	B	1102	TYR	Peptide
1	B	1266	GLU	Peptide
1	B	1297	THR	Peptide
1	B	1475	LYS	Peptide
1	B	1579	VAL	Peptide
1	B	1635	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	1739	PHE	Peptide
1	B	1808	ASP	Peptide
1	B	1835	HIS	Peptide
1	B	1847	GLU	Peptide
1	B	2075	VAL	Peptide
1	B	2077	GLU	Peptide
1	B	3767	LEU	Peptide
1	B	3805	ASP	Peptide
1	B	4070	CYS	Peptide
1	B	4144	LYS	Peptide
1	B	4163	LYS	Peptide
1	B	471	GLU	Peptide
1	B	4798	GLU	Peptide
1	B	4956	GLY	Peptide
1	B	4958	CYS	Peptide
1	B	657	PRO	Peptide
1	B	729	GLY	Peptide
1	B	775	VAL	Peptide
1	B	791	VAL	Peptide
1	B	818	GLY	Peptide
1	B	819	TYR	Peptide
1	B	838	ARG	Peptide
1	B	852	GLY	Mainchain,Peptide
1	C	1102	TYR	Peptide
1	C	1266	GLU	Peptide
1	C	1297	THR	Peptide
1	C	1475	LYS	Peptide
1	C	1579	VAL	Peptide
1	C	1635	GLU	Peptide
1	C	1739	PHE	Peptide
1	C	1808	ASP	Peptide
1	C	1835	HIS	Peptide
1	C	1847	GLU	Peptide
1	C	2075	VAL	Peptide
1	C	2077	GLU	Peptide
1	C	3767	LEU	Peptide
1	C	3805	ASP	Peptide
1	C	4070	CYS	Peptide
1	C	4144	LYS	Peptide
1	C	4163	LYS	Peptide
1	C	471	GLU	Peptide
1	C	4798	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	C	4956	GLY	Peptide
1	C	4958	CYS	Peptide
1	C	657	PRO	Peptide
1	C	729	GLY	Peptide
1	C	775	VAL	Peptide
1	C	791	VAL	Peptide
1	C	818	GLY	Peptide
1	C	819	TYR	Peptide
1	C	838	ARG	Peptide
1	C	852	GLY	Mainchain,Peptide
1	D	1102	TYR	Peptide
1	D	1266	GLU	Peptide
1	D	1297	THR	Peptide
1	D	1475	LYS	Peptide
1	D	1579	VAL	Peptide
1	D	1635	GLU	Peptide
1	D	1739	PHE	Peptide
1	D	1808	ASP	Peptide
1	D	1835	HIS	Peptide
1	D	1847	GLU	Peptide
1	D	2075	VAL	Peptide
1	D	2077	GLU	Peptide
1	D	3767	LEU	Peptide
1	D	3805	ASP	Peptide
1	D	4070	CYS	Peptide
1	D	4144	LYS	Peptide
1	D	4163	LYS	Peptide
1	D	471	GLU	Peptide
1	D	4798	GLU	Peptide
1	D	4956	GLY	Peptide
1	D	4958	CYS	Peptide
1	D	657	PRO	Peptide
1	D	729	GLY	Peptide
1	D	775	VAL	Peptide
1	D	791	VAL	Peptide
1	D	818	GLY	Peptide
1	D	819	TYR	Peptide
1	D	838	ARG	Peptide
1	D	852	GLY	Mainchain,Peptide

## 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	26266	0	24898	409	0
1	B	26266	0	24898	421	0
1	C	26266	0	24898	414	0
1	D	26266	0	24898	401	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	105068	0	99592	1515	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 7.

All (1515) 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:A:4873:GLU:HA	1:B:4875:ARG:NH1	1.62	1.15
1:A:4875:ARG:NH1	1:D:4873:GLU:HA	1.62	1.14
1:B:4873:GLU:HA	1:C:4875:ARG:NH1	1.62	1.13
1:C:4873:GLU:OE1	1:D:4875:ARG:HD3	1.49	1.12
1:C:4873:GLU:HA	1:D:4875:ARG:NH1	1.62	1.12
1:B:4873:GLU:OE1	1:C:4875:ARG:HD3	1.49	1.11
1:A:4873:GLU:OE1	1:B:4875:ARG:HD3	1.49	1.11
1:A:4875:ARG:HD3	1:D:4873:GLU:OE1	1.49	1.10
1:A:4823:ARG:HA	1:D:4852:PHE:CZ	1.98	0.98
1:B:4852:PHE:CZ	1:C:4823:ARG:HA	1.98	0.98
1:A:4852:PHE:CZ	1:B:4823:ARG:HA	1.98	0.98
1:C:4852:PHE:CZ	1:D:4823:ARG:HA	1.98	0.98
1:D:4832:ILE:HG21	1:D:4844:ARG:HH21	1.44	0.83
1:B:4832:ILE:HG21	1:B:4844:ARG:HH21	1.44	0.82
1:C:4832:ILE:HG21	1:C:4844:ARG:HH21	1.44	0.82
1:A:4832:ILE:HG21	1:A:4844:ARG:HH21	1.44	0.80
1:A:4872:GLY:C	1:B:4875:ARG:HH22	1.86	0.79
1:A:4875:ARG:HH22	1:D:4872:GLY:C	1.86	0.78
1:A:4810:MET:HG2	1:B:4518:LEU:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4872:GLY:C	1:C:4875:ARG:HH22	1.86	0.78
1:B:4810:MET:HG2	1:C:4518:LEU:O	1.84	0.78
1:C:4872:GLY:C	1:D:4875:ARG:HH22	1.86	0.78
1:A:4518:LEU:O	1:D:4810:MET:HG2	1.84	0.77
1:C:4810:MET:HG2	1:D:4518:LEU:O	1.84	0.77
1:C:76:ARG:HG2	1:D:3891:TRP:HB3	1.68	0.75
1:B:708:GLY:HA2	1:B:714:GLY:HA3	1.69	0.74
1:B:76:ARG:HG2	1:C:3891:TRP:HB3	1.68	0.74
1:D:708:GLY:HA2	1:D:714:GLY:HA3	1.69	0.74
1:A:708:GLY:HA2	1:A:714:GLY:HA3	1.69	0.73
1:A:76:ARG:HG2	1:B:3891:TRP:HB3	1.68	0.73
1:A:3891:TRP:HB3	1:D:76:ARG:HG2	1.68	0.73
1:C:4872:GLY:C	1:D:4875:ARG:NH2	2.42	0.73
1:C:4873:GLU:OE1	1:D:4875:ARG:CD	2.35	0.73
1:B:4872:GLY:C	1:C:4875:ARG:NH2	2.42	0.73
1:C:708:GLY:HA2	1:C:714:GLY:HA3	1.69	0.72
1:B:4873:GLU:OE1	1:C:4875:ARG:CD	2.35	0.72
1:A:4872:GLY:C	1:B:4875:ARG:NH2	2.42	0.72
1:A:4875:ARG:NH2	1:D:4872:GLY:C	2.42	0.71
1:A:4875:ARG:NH1	1:D:4872:GLY:O	2.24	0.71
1:A:4157:SER:OG	1:A:4924:MET:SD	2.50	0.70
1:A:4872:GLY:O	1:B:4875:ARG:NH2	2.25	0.70
1:A:4872:GLY:O	1:B:4875:ARG:NH1	2.24	0.70
1:A:4875:ARG:NH2	1:D:4872:GLY:O	2.25	0.70
1:B:4157:SER:OG	1:B:4924:MET:SD	2.50	0.70
1:C:4872:GLY:O	1:D:4875:ARG:NH1	2.24	0.70
1:D:4157:SER:OG	1:D:4924:MET:SD	2.50	0.70
1:B:4872:GLY:O	1:C:4875:ARG:NH2	2.25	0.70
1:A:2419:ARG:NH1	1:D:189:GLU:OE1	2.25	0.70
1:B:189:GLU:OE1	1:C:2419:ARG:NH1	2.25	0.70
1:C:4873:GLU:CA	1:D:4875:ARG:NH1	2.51	0.69
1:B:4872:GLY:O	1:C:4875:ARG:NH1	2.24	0.69
1:A:189:GLU:OE1	1:B:2419:ARG:NH1	2.25	0.69
1:C:4157:SER:OG	1:C:4924:MET:SD	2.50	0.69
1:C:189:GLU:OE1	1:D:2419:ARG:NH1	2.25	0.69
1:B:4800:GLY:HA2	1:B:4804:ASP:HB3	1.74	0.68
1:A:4873:GLU:CA	1:B:4875:ARG:NH1	2.51	0.68
1:C:4872:GLY:O	1:D:4875:ARG:NH2	2.25	0.68
1:A:3986:MET:HG2	1:A:3996:ILE:HD11	1.75	0.68
1:D:3986:MET:HG2	1:D:3996:ILE:HD11	1.75	0.68
1:A:4875:ARG:NH1	1:D:4873:GLU:CA	2.51	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4011:VAL:HA	1:A:4014:ILE:HG12	1.76	0.68
1:A:1645:THR:HG22	1:A:1695:PRO:HG3	1.76	0.68
1:C:4011:VAL:HA	1:C:4014:ILE:HG12	1.76	0.68
1:B:4873:GLU:CA	1:C:4875:ARG:NH1	2.51	0.68
1:D:4800:GLY:HA2	1:D:4804:ASP:HB3	1.74	0.68
1:C:1645:THR:HG22	1:C:1695:PRO:HG3	1.76	0.67
1:C:4873:GLU:HA	1:D:4875:ARG:HH12	1.59	0.67
1:D:1138:ASP:HB2	1:D:1145:TRP:HE1	1.60	0.67
1:D:4011:VAL:HA	1:D:4014:ILE:HG12	1.76	0.67
1:A:1138:ASP:HB2	1:A:1145:TRP:HE1	1.60	0.67
1:C:1138:ASP:HB2	1:C:1145:TRP:HE1	1.60	0.67
1:C:4800:GLY:HA2	1:C:4804:ASP:HB3	1.74	0.67
1:A:4800:GLY:HA2	1:A:4804:ASP:HB3	1.74	0.67
1:B:1645:THR:HG22	1:B:1695:PRO:HG3	1.76	0.67
1:B:4873:GLU:HA	1:C:4875:ARG:HH12	1.59	0.67
1:C:3986:MET:HG2	1:C:3996:ILE:HD11	1.75	0.67
1:B:3986:MET:HG2	1:B:3996:ILE:HD11	1.75	0.67
1:B:4011:VAL:HA	1:B:4014:ILE:HG12	1.76	0.67
1:B:1138:ASP:HB2	1:B:1145:TRP:HE1	1.60	0.67
1:D:1645:THR:HG22	1:D:1695:PRO:HG3	1.76	0.67
1:D:35:LEU:HD13	1:D:49:LEU:HD22	1.77	0.66
1:A:299:HIS:HE2	1:A:301:THR:HG1	1.43	0.66
1:B:35:LEU:HD13	1:B:49:LEU:HD22	1.77	0.66
1:A:4875:ARG:CD	1:D:4873:GLU:OE1	2.35	0.65
1:A:4873:GLU:HA	1:B:4875:ARG:HH12	1.59	0.65
1:C:3875:THR:HG21	1:C:3924:TYR:HE2	1.62	0.65
1:A:35:LEU:HD13	1:A:49:LEU:HD22	1.77	0.65
1:B:248:PRO:HG2	1:B:257:ARG:HA	1.79	0.65
1:A:3875:THR:HG21	1:A:3924:TYR:HE2	1.62	0.65
1:A:248:PRO:HG2	1:A:257:ARG:HA	1.79	0.65
1:A:4873:GLU:OE1	1:B:4875:ARG:CD	2.35	0.65
1:C:35:LEU:HD13	1:C:49:LEU:HD22	1.77	0.65
1:D:248:PRO:HG2	1:D:257:ARG:HA	1.79	0.65
1:B:243:GLU:HA	1:B:264:GLY:HA2	1.79	0.65
1:B:1602:GLN:HE22	1:B:1642:LEU:HB3	1.62	0.65
1:A:1602:GLN:HE22	1:A:1642:LEU:HB3	1.62	0.65
1:B:299:HIS:HE2	1:B:301:THR:HG1	1.45	0.65
1:C:243:GLU:HA	1:C:264:GLY:HA2	1.79	0.65
1:C:248:PRO:HG2	1:C:257:ARG:HA	1.79	0.64
1:D:1602:GLN:HE22	1:D:1642:LEU:HB3	1.62	0.64
1:A:243:GLU:HA	1:A:264:GLY:HA2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1602:GLN:HE22	1:C:1642:LEU:HB3	1.62	0.64
1:D:3875:THR:HG21	1:D:3924:TYR:HE2	1.62	0.64
1:D:243:GLU:HA	1:D:264:GLY:HA2	1.79	0.64
1:B:1304:LEU:HB3	1:B:1541:PRO:HG2	1.80	0.64
1:B:3875:THR:HG21	1:B:3924:TYR:HE2	1.62	0.63
1:A:227:TYR:HE1	1:A:355:LYS:HG2	1.64	0.63
1:A:4868:ILE:HG12	1:D:4865:GLY:HA3	1.81	0.63
1:B:3845:GLN:HB2	1:B:3920:THR:HG22	1.81	0.63
1:D:188:SER:HB2	1:D:190:ARG:HH21	1.64	0.63
1:D:227:TYR:HE1	1:D:355:LYS:HG2	1.64	0.63
1:C:227:TYR:HE1	1:C:355:LYS:HG2	1.64	0.63
1:D:1304:LEU:HB3	1:D:1541:PRO:HG2	1.80	0.63
1:B:188:SER:HB2	1:B:190:ARG:HH21	1.64	0.62
1:A:188:SER:HB2	1:A:190:ARG:HH21	1.64	0.62
1:A:3922:THR:O	1:A:3926:GLN:N	2.32	0.62
1:A:4865:GLY:HA3	1:B:4868:ILE:HG12	1.81	0.62
1:C:188:SER:HB2	1:C:190:ARG:HH21	1.64	0.62
1:C:3922:THR:O	1:C:3926:GLN:N	2.32	0.62
1:A:1304:LEU:HB3	1:A:1541:PRO:HG2	1.80	0.62
1:A:3845:GLN:HB2	1:A:3920:THR:HG22	1.81	0.62
1:C:1304:LEU:HB3	1:C:1541:PRO:HG2	1.80	0.62
1:B:3922:THR:O	1:B:3926:GLN:N	2.32	0.62
1:B:227:TYR:HE1	1:B:355:LYS:HG2	1.64	0.62
1:D:3922:THR:O	1:D:3926:GLN:N	2.32	0.62
1:B:4865:GLY:HA3	1:C:4868:ILE:HG12	1.81	0.62
1:D:3845:GLN:HB2	1:D:3920:THR:HG22	1.81	0.62
1:C:4865:GLY:HA3	1:D:4868:ILE:HG12	1.81	0.62
1:B:1272:ARG:NH1	1:B:1587:HIS:O	2.34	0.61
1:D:1272:ARG:NH1	1:D:1587:HIS:O	2.34	0.61
1:D:299:HIS:HE2	1:D:301:THR:HG1	1.46	0.61
1:C:4072:GLU:HB3	1:C:4074:ASP:HB2	1.83	0.61
1:C:1272:ARG:NH1	1:C:1587:HIS:O	2.34	0.61
1:B:3841:PHE:HB3	1:B:3920:THR:HG21	1.82	0.61
1:A:4875:ARG:HH12	1:D:4873:GLU:HA	1.59	0.61
1:D:779:PHE:HB3	1:D:782:PHE:HE2	1.66	0.61
1:A:3841:PHE:HB3	1:A:3920:THR:HG21	1.82	0.60
1:B:4072:GLU:HB3	1:B:4074:ASP:HB2	1.83	0.60
1:D:3841:PHE:HB3	1:D:3920:THR:HG21	1.82	0.60
1:A:4140:MET:HG2	1:A:4146:ILE:HG12	1.82	0.60
1:B:1258:PHE:HB2	1:B:1593:HIS:HB3	1.83	0.60
1:D:4140:MET:HG2	1:D:4146:ILE:HG12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:HG22	1:A:34:LYS:HG2	1.83	0.60
1:A:779:PHE:HB3	1:A:782:PHE:HE2	1.66	0.60
1:C:3802:SER:OG	1:C:3833:ASP:O	2.18	0.60
1:C:779:PHE:HB3	1:C:782:PHE:HE2	1.66	0.60
1:A:954:ASP:HB3	1:A:1061:GLY:HA3	1.84	0.60
1:B:779:PHE:HB3	1:B:782:PHE:HE2	1.66	0.60
1:D:954:ASP:HB3	1:D:1061:GLY:HA3	1.84	0.60
1:A:1469:LEU:HG	1:A:1480:ILE:HD11	1.84	0.60
1:A:3802:SER:OG	1:A:3833:ASP:O	2.18	0.60
1:B:143:LEU:HD23	1:C:2426:SER:HB3	1.84	0.60
1:C:123:HIS:HD2	1:C:126:SER:H	1.50	0.60
1:C:3845:GLN:HB2	1:C:3920:THR:HG22	1.81	0.60
1:D:1469:LEU:HG	1:D:1480:ILE:HD11	1.84	0.60
1:D:802:PHE:HB2	1:D:1617:TRP:HB2	1.84	0.60
1:B:954:ASP:HB3	1:B:1061:GLY:HA3	1.84	0.60
1:C:802:PHE:HB2	1:C:1617:TRP:HB2	1.84	0.60
1:C:4140:MET:HG2	1:C:4146:ILE:HG12	1.82	0.60
1:D:25:THR:HG22	1:D:34:LYS:HG2	1.83	0.60
1:A:1258:PHE:HB2	1:A:1593:HIS:HB3	1.83	0.60
1:A:802:PHE:HB2	1:A:1617:TRP:HB2	1.84	0.60
1:C:1137:PHE:HA	1:C:1144:ARG:HA	1.82	0.60
1:A:1272:ARG:NH1	1:A:1587:HIS:O	2.34	0.60
1:B:123:HIS:HD2	1:B:126:SER:H	1.50	0.60
1:B:25:THR:HG22	1:B:34:LYS:HG2	1.83	0.60
1:B:4140:MET:HG2	1:B:4146:ILE:HG12	1.82	0.60
1:C:1258:PHE:HB2	1:C:1593:HIS:HB3	1.83	0.60
1:A:4072:GLU:HB3	1:A:4074:ASP:HB2	1.83	0.60
1:A:756:SER:HB3	1:A:769:ARG:HB2	1.84	0.60
1:B:4617:TYR:OH	1:B:4629:GLY:O	2.20	0.60
1:B:672:LYS:HA	1:B:760:ASP:HA	1.84	0.60
1:D:1113:MET:HG3	1:D:1156:TRP:HZ2	1.67	0.60
1:B:756:SER:HB3	1:B:769:ARG:HB2	1.84	0.59
1:D:123:HIS:HD2	1:D:126:SER:H	1.50	0.59
1:A:1137:PHE:HA	1:A:1144:ARG:HA	1.82	0.59
1:D:4072:GLU:HB3	1:D:4074:ASP:HB2	1.83	0.59
1:A:4617:TYR:OH	1:A:4629:GLY:O	2.20	0.59
1:A:672:LYS:HA	1:A:760:ASP:HA	1.84	0.59
1:B:1469:LEU:HG	1:B:1480:ILE:HD11	1.84	0.59
1:B:802:PHE:HB2	1:B:1617:TRP:HB2	1.84	0.59
1:C:954:ASP:HB3	1:C:1061:GLY:HA3	1.84	0.59
1:D:1137:PHE:HA	1:D:1144:ARG:HA	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3802:SER:OG	1:D:3833:ASP:O	2.18	0.59
1:A:559:ILE:HD13	1:A:593:HIS:HB3	1.85	0.59
1:B:1137:PHE:HA	1:B:1144:ARG:HA	1.82	0.59
1:D:1445:TRP:HE1	1:D:1508:GLY:HA3	1.67	0.59
1:C:3914:ALA:HA	1:C:3917:VAL:HG12	1.85	0.59
1:A:2426:SER:HB3	1:D:143:LEU:HD23	1.84	0.59
1:D:559:ILE:HD13	1:D:593:HIS:HB3	1.85	0.59
1:A:123:HIS:HD2	1:A:126:SER:H	1.50	0.59
1:A:143:LEU:HD23	1:B:2426:SER:HB3	1.84	0.59
1:A:3914:ALA:HA	1:A:3917:VAL:HG12	1.85	0.59
1:D:3914:ALA:HA	1:D:3917:VAL:HG12	1.85	0.59
1:C:143:LEU:HD23	1:D:2426:SER:HB3	1.84	0.59
1:D:3924:TYR:O	1:D:3932:ASN:ND2	2.36	0.59
1:B:3914:ALA:HA	1:B:3917:VAL:HG12	1.85	0.59
1:C:25:THR:HG22	1:C:34:LYS:HG2	1.83	0.59
1:C:3841:PHE:HB3	1:C:3920:THR:HG21	1.82	0.59
1:D:1258:PHE:HB2	1:D:1593:HIS:HB3	1.83	0.59
1:A:1113:MET:HG3	1:A:1156:TRP:HZ2	1.67	0.59
1:C:1469:LEU:HG	1:C:1480:ILE:HD11	1.84	0.59
1:C:756:SER:HB3	1:C:769:ARG:HB2	1.84	0.59
1:B:1113:MET:HG3	1:B:1156:TRP:HZ2	1.67	0.58
1:C:1113:MET:HG3	1:C:1156:TRP:HZ2	1.67	0.58
1:C:672:LYS:HA	1:C:760:ASP:HA	1.84	0.58
1:A:3924:TYR:O	1:A:3932:ASN:ND2	2.36	0.58
1:C:4883:GLU:O	1:C:4887:THR:HG23	2.04	0.58
1:B:1445:TRP:HE1	1:B:1508:GLY:HA3	1.67	0.58
1:C:1706:LEU:HD21	1:C:1787:LEU:HD21	1.85	0.58
1:B:3802:SER:OG	1:B:3833:ASP:O	2.18	0.58
1:C:4617:TYR:OH	1:C:4629:GLY:O	2.20	0.58
1:D:756:SER:HB3	1:D:769:ARG:HB2	1.84	0.58
1:A:1104:GLU:HA	1:A:1163:GLY:HA2	1.85	0.58
1:B:3924:TYR:O	1:B:3932:ASN:ND2	2.36	0.58
1:C:897:LYS:HD3	1:C:918:LEU:HD21	1.86	0.58
1:B:559:ILE:HD13	1:B:593:HIS:HB3	1.85	0.58
1:D:672:LYS:HA	1:D:760:ASP:HA	1.84	0.58
1:B:1706:LEU:HD21	1:B:1787:LEU:HD21	1.85	0.58
1:B:897:LYS:HD3	1:B:918:LEU:HD21	1.86	0.58
1:D:4617:TYR:OH	1:D:4629:GLY:O	2.20	0.58
1:A:247:VAL:O	1:A:272:ARG:NH1	2.36	0.58
1:C:559:ILE:HD13	1:C:593:HIS:HB3	1.85	0.58
1:A:4883:GLU:O	1:A:4887:THR:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:LYS:HD3	1:A:918:LEU:HD21	1.86	0.58
1:C:1104:GLU:HA	1:C:1163:GLY:HA2	1.85	0.58
1:D:4883:GLU:O	1:D:4887:THR:HG23	2.04	0.58
1:D:897:LYS:HD3	1:D:918:LEU:HD21	1.86	0.58
1:A:1445:TRP:HE1	1:A:1508:GLY:HA3	1.67	0.57
1:C:3924:TYR:O	1:C:3932:ASN:ND2	2.36	0.57
1:C:4915:ASN:O	1:C:4917:ALA:N	2.38	0.57
1:D:1104:GLU:HA	1:D:1163:GLY:HA2	1.85	0.57
1:A:1124:PRO:HB2	1:A:1252:SER:HB3	1.86	0.57
1:A:4915:ASN:O	1:A:4917:ALA:N	2.38	0.57
1:C:1445:TRP:HE1	1:C:1508:GLY:HA3	1.67	0.57
1:D:247:VAL:O	1:D:272:ARG:NH1	2.36	0.57
1:B:4915:ASN:O	1:B:4917:ALA:N	2.38	0.57
1:C:1114:ARG:HB2	1:C:1206:SER:HB3	1.86	0.57
1:D:1706:LEU:HD21	1:D:1787:LEU:HD21	1.85	0.57
1:B:1114:ARG:HB2	1:B:1206:SER:HB3	1.86	0.57
1:D:1124:PRO:HB2	1:D:1252:SER:HB3	1.86	0.57
1:D:4915:ASN:O	1:D:4917:ALA:N	2.38	0.57
1:B:4883:GLU:O	1:B:4887:THR:HG23	2.04	0.57
1:C:299:HIS:HE2	1:C:301:THR:HG1	1.51	0.57
1:C:530:LEU:HD23	1:C:533:LEU:HD12	1.87	0.57
1:C:1429:SER:HA	1:C:1507:ILE:HG12	1.87	0.57
1:D:1429:SER:HA	1:D:1507:ILE:HG12	1.87	0.57
1:A:530:LEU:HD23	1:A:533:LEU:HD12	1.87	0.57
1:C:1433:PHE:HD2	1:C:1551:ASN:HB3	1.70	0.57
1:D:530:LEU:HD23	1:D:533:LEU:HD12	1.87	0.57
1:A:1429:SER:HA	1:A:1507:ILE:HG12	1.87	0.57
1:B:1104:GLU:HA	1:B:1163:GLY:HA2	1.85	0.57
1:A:1706:LEU:HD21	1:A:1787:LEU:HD21	1.85	0.56
1:A:1433:PHE:HD2	1:A:1551:ASN:HB3	1.70	0.56
1:D:1442:TRP:HD1	1:D:1488:VAL:HG13	1.71	0.56
1:C:1442:TRP:HD1	1:C:1488:VAL:HG13	1.71	0.56
1:C:473:GLU:OE2	1:C:477:ASN:ND2	2.39	0.56
1:C:1124:PRO:HB2	1:C:1252:SER:HB3	1.86	0.56
1:C:1699:ARG:NH1	1:C:1816:PHE:O	2.39	0.56
1:B:4791:ARG:NE	1:C:4523:VAL:HG11	2.20	0.56
1:D:1433:PHE:HD2	1:D:1551:ASN:HB3	1.70	0.56
1:B:1429:SER:HA	1:B:1507:ILE:HG12	1.87	0.56
1:C:4015:LEU:HD22	1:C:4126:VAL:HG21	1.87	0.56
1:C:58:VAL:HG22	1:C:320:GLU:HA	1.87	0.56
1:D:473:GLU:OE2	1:D:477:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:TRP:HD1	1:A:1488:VAL:HG13	1.71	0.56
1:A:1114:ARG:HB2	1:A:1206:SER:HB3	1.86	0.56
1:B:4161:TRP:HD1	1:B:4201:MET:HE1	1.71	0.56
1:B:530:LEU:HD23	1:B:533:LEU:HD12	1.87	0.56
1:D:4015:LEU:HD22	1:D:4126:VAL:HG21	1.87	0.56
1:A:1121:GLY:O	1:A:1133:ARG:NH1	2.38	0.56
1:C:2060:GLN:NE2	1:C:2092:GLN:O	2.39	0.56
1:D:1114:ARG:HB2	1:D:1206:SER:HB3	1.86	0.56
1:A:4015:LEU:HD22	1:A:4126:VAL:HG21	1.87	0.56
1:B:58:VAL:HG22	1:B:320:GLU:HA	1.87	0.56
1:D:1121:GLY:O	1:D:1133:ARG:NH1	2.38	0.56
1:A:58:VAL:HG22	1:A:320:GLU:HA	1.87	0.56
1:B:1699:ARG:NH1	1:B:1816:PHE:O	2.39	0.56
1:B:4015:LEU:HD22	1:B:4126:VAL:HG21	1.87	0.56
1:A:4791:ARG:NE	1:B:4523:VAL:HG11	2.20	0.56
1:A:2060:GLN:NE2	1:A:2092:GLN:O	2.39	0.56
1:A:4618:ILE:HD12	1:A:4667:ILE:HD12	1.88	0.56
1:B:986:ILE:HD12	1:B:1059:GLY:HA2	1.88	0.56
1:C:4161:TRP:HD1	1:C:4201:MET:HE1	1.71	0.56
1:C:4618:ILE:HD12	1:C:4667:ILE:HD12	1.88	0.56
1:C:4791:ARG:NE	1:D:4523:VAL:HG11	2.20	0.56
1:B:1124:PRO:HB2	1:B:1252:SER:HB3	1.86	0.55
1:D:2060:GLN:NE2	1:D:2092:GLN:O	2.39	0.55
1:B:1433:PHE:HD2	1:B:1551:ASN:HB3	1.70	0.55
1:B:2060:GLN:NE2	1:B:2092:GLN:O	2.39	0.55
1:D:1272:ARG:NH2	1:D:1590:PHE:O	2.39	0.55
1:A:1272:ARG:NH2	1:A:1590:PHE:O	2.39	0.55
1:A:4523:VAL:HG11	1:D:4791:ARG:NE	2.20	0.55
1:B:375:GLN:HE21	1:B:392:ILE:HD13	1.72	0.55
1:B:473:GLU:OE2	1:B:477:ASN:ND2	2.39	0.55
1:C:1726:ILE:HD11	1:C:2121:LEU:HD11	1.89	0.55
1:D:1726:ILE:HD11	1:D:2121:LEU:HD11	1.89	0.55
1:A:2463:PRO:HB3	1:A:2516:ALA:HA	1.88	0.55
1:A:618:CYS:SG	1:A:629:GLN:NE2	2.80	0.55
1:A:986:ILE:HD12	1:A:1059:GLY:HA2	1.88	0.55
1:B:4618:ILE:HD12	1:B:4667:ILE:HD12	1.88	0.55
1:B:4819:TYR:O	1:B:4823:ARG:NH2	2.33	0.55
1:C:1272:ARG:NH2	1:C:1590:PHE:O	2.39	0.55
1:D:58:VAL:HG22	1:D:320:GLU:HA	1.87	0.55
1:A:1699:ARG:NH1	1:A:1816:PHE:O	2.39	0.55
1:A:375:GLN:HE21	1:A:392:ILE:HD13	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4618:ILE:HD12	1:D:4667:ILE:HD12	1.88	0.55
1:B:2843:GLU:OE1	1:B:2887:ARG:NH2	2.40	0.55
1:C:2843:GLU:OE1	1:C:2887:ARG:NH2	2.40	0.55
1:C:4840:TYR:O	1:C:4844:ARG:N	2.40	0.55
1:B:1272:ARG:NH2	1:B:1590:PHE:O	2.39	0.55
1:C:2463:PRO:HB3	1:C:2516:ALA:HA	1.88	0.55
1:C:247:VAL:O	1:C:272:ARG:NH1	2.36	0.55
1:B:1442:TRP:HD1	1:B:1488:VAL:HG13	1.71	0.55
1:B:618:CYS:SG	1:B:629:GLN:NE2	2.80	0.55
1:C:797:GLY:HA2	1:C:1622:LEU:HA	1.89	0.55
1:D:1699:ARG:NH1	1:D:1816:PHE:O	2.39	0.55
1:D:375:GLN:HE21	1:D:392:ILE:HD13	1.72	0.55
1:C:618:CYS:SG	1:C:629:GLN:NE2	2.80	0.55
1:D:2463:PRO:HB3	1:D:2516:ALA:HA	1.88	0.55
1:D:797:GLY:HA2	1:D:1622:LEU:HA	1.89	0.55
1:A:4514:ILE:HG21	1:A:4740:PHE:HE2	1.72	0.55
1:B:1726:ILE:HD11	1:B:2121:LEU:HD11	1.89	0.55
1:B:4514:ILE:HG21	1:B:4740:PHE:HE2	1.72	0.55
1:C:986:ILE:HD12	1:C:1059:GLY:HA2	1.88	0.55
1:C:4514:ILE:HG21	1:C:4740:PHE:HE2	1.72	0.55
1:A:1510:VAL:HG12	1:A:1511:VAL:HG23	1.89	0.54
1:A:473:GLU:OE2	1:A:477:ASN:ND2	2.39	0.54
1:B:3960:SER:HG	1:B:4070:CYS:HG	1.53	0.54
1:D:2158:GLN:O	1:D:3616:ARG:NH1	2.40	0.54
1:A:1156:TRP:HB3	1:A:1177:LEU:HD11	1.90	0.54
1:B:4840:TYR:O	1:B:4844:ARG:N	2.40	0.54
1:C:258:ARG:NH1	1:C:317:MET:SD	2.80	0.54
1:A:1726:ILE:HD11	1:A:2121:LEU:HD11	1.89	0.54
1:A:258:ARG:NH1	1:A:317:MET:SD	2.80	0.54
1:B:258:ARG:NH1	1:B:317:MET:SD	2.80	0.54
1:B:2158:GLN:O	1:B:3616:ARG:NH1	2.40	0.54
1:D:258:ARG:NH1	1:D:317:MET:SD	2.80	0.54
1:D:2843:GLU:OE1	1:D:2887:ARG:NH2	2.40	0.54
1:D:986:ILE:HD12	1:D:1059:GLY:HA2	1.88	0.54
1:A:2158:GLN:O	1:A:3616:ARG:NH1	2.40	0.54
1:C:2158:GLN:O	1:C:3616:ARG:NH1	2.40	0.54
1:C:375:GLN:HE21	1:C:392:ILE:HD13	1.72	0.54
1:D:4514:ILE:HG21	1:D:4740:PHE:HE2	1.72	0.54
1:D:618:CYS:SG	1:D:629:GLN:NE2	2.80	0.54
1:A:797:GLY:HA2	1:A:1622:LEU:HA	1.89	0.54
1:B:4046:LYS:HG3	1:B:4068:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1601:ASN:ND2	1:C:1643:GLU:OE2	2.41	0.54
1:A:2843:GLU:OE1	1:A:2887:ARG:NH2	2.40	0.54
1:B:1156:TRP:HB3	1:B:1177:LEU:HD11	1.90	0.54
1:B:1601:ASN:ND2	1:B:1643:GLU:OE2	2.41	0.54
1:B:247:VAL:O	1:B:272:ARG:NH1	2.36	0.54
1:C:1156:TRP:HB3	1:C:1177:LEU:HD11	1.90	0.54
1:C:4046:LYS:HG3	1:C:4068:LEU:HD22	1.90	0.54
1:D:1510:VAL:HG12	1:D:1511:VAL:HG23	1.89	0.54
1:A:1607:ASP:HB3	1:A:1608:VAL:HG23	1.90	0.54
1:B:1510:VAL:HG12	1:B:1511:VAL:HG23	1.89	0.54
1:B:228:LEU:HB3	1:B:289:ILE:HB	1.90	0.54
1:C:1607:ASP:HB3	1:C:1608:VAL:HG23	1.90	0.54
1:D:1156:TRP:HB3	1:D:1177:LEU:HD11	1.90	0.54
1:A:1601:ASN:ND2	1:A:1643:GLU:OE2	2.41	0.54
1:A:4161:TRP:HD1	1:A:4201:MET:HE1	1.71	0.54
1:C:228:LEU:HB3	1:C:289:ILE:HB	1.90	0.54
1:D:598:ILE:HG23	1:D:636:LEU:HD12	1.90	0.54
1:B:2463:PRO:HB3	1:B:2516:ALA:HA	1.88	0.54
1:B:797:GLY:HA2	1:B:1622:LEU:HA	1.89	0.54
1:B:1121:GLY:O	1:B:1133:ARG:NH1	2.38	0.54
1:B:1607:ASP:HB3	1:B:1608:VAL:HG23	1.90	0.54
1:D:1601:ASN:ND2	1:D:1643:GLU:OE2	2.41	0.54
1:A:4840:TYR:O	1:A:4844:ARG:N	2.40	0.53
1:C:1911:LEU:HD11	1:C:2063:ILE:HG12	1.90	0.53
1:C:26:ALA:HB3	1:C:33:GLN:HB3	1.90	0.53
1:D:4819:TYR:O	1:D:4823:ARG:NH2	2.33	0.53
1:C:3926:GLN:HE21	1:C:4936:GLY:H	1.56	0.53
1:C:4660:GLU:HG3	1:C:4664:ARG:HH21	1.73	0.53
1:B:598:ILE:HG23	1:B:636:LEU:HD12	1.90	0.53
1:D:4161:TRP:HD1	1:D:4201:MET:HE1	1.71	0.53
1:A:3926:GLN:HE21	1:A:4936:GLY:H	1.56	0.53
1:C:1121:GLY:O	1:C:1133:ARG:NH1	2.38	0.53
1:D:1607:ASP:HB3	1:D:1608:VAL:HG23	1.90	0.53
1:D:1726:ILE:HB	1:D:2109:ILE:HD11	1.91	0.53
1:D:4840:TYR:O	1:D:4844:ARG:N	2.40	0.53
1:D:636:LEU:HD21	1:D:643:LEU:HD21	1.90	0.53
1:C:3730:ALA:HA	1:C:3733:HIS:CE1	2.44	0.53
1:D:1911:LEU:HD11	1:D:2063:ILE:HG12	1.90	0.53
1:D:2488:LEU:O	1:D:2492:GLY:N	2.42	0.53
1:B:3730:ALA:HA	1:B:3733:HIS:CE1	2.44	0.53
1:C:61:ASP:OD2	1:C:417:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:598:ILE:HG23	1:C:636:LEU:HD12	1.90	0.53
1:D:26:ALA:HB3	1:D:33:GLN:HB3	1.90	0.53
1:D:4046:LYS:HG3	1:D:4068:LEU:HD22	1.90	0.53
1:A:1726:ILE:HB	1:A:2109:ILE:HD11	1.91	0.53
1:A:3730:ALA:HA	1:A:3733:HIS:CE1	2.44	0.53
1:A:3798:MET:HE1	1:A:3875:THR:HB	1.91	0.53
1:A:598:ILE:HG23	1:A:636:LEU:HD12	1.90	0.53
1:B:1726:ILE:HB	1:B:2109:ILE:HD11	1.91	0.53
1:B:61:ASP:OD2	1:B:417:ARG:NH2	2.42	0.53
1:C:1510:VAL:HG12	1:C:1511:VAL:HG23	1.89	0.53
1:D:4660:GLU:HG3	1:D:4664:ARG:HH21	1.73	0.53
1:B:677:LEU:HD11	1:B:792:VAL:HG21	1.91	0.53
1:B:4660:GLU:HG3	1:B:4664:ARG:HH21	1.73	0.53
1:C:4889:CYS:HB3	1:C:4892:CYS:SG	2.49	0.53
1:D:3798:MET:HE1	1:D:3875:THR:HB	1.91	0.53
1:D:4889:CYS:HB3	1:D:4892:CYS:SG	2.49	0.53
1:A:228:LEU:HB3	1:A:289:ILE:HB	1.90	0.52
1:A:2488:LEU:O	1:A:2492:GLY:N	2.42	0.52
1:A:2793:THR:OG1	1:A:2901:GLY:O	2.25	0.52
1:B:4889:CYS:HB3	1:B:4892:CYS:SG	2.49	0.52
1:D:228:LEU:HB3	1:D:289:ILE:HB	1.90	0.52
1:D:3729:GLN:O	1:D:3733:HIS:ND1	2.41	0.52
1:D:4108:GLU:HG3	1:D:4136:ARG:HH22	1.74	0.52
1:D:61:ASP:OD2	1:D:417:ARG:NH2	2.42	0.52
1:B:1094:TYR:OH	1:B:1808:ASP:OD1	2.28	0.52
1:B:4050:HIS:HB2	1:B:4068:LEU:HD11	1.91	0.52
1:B:636:LEU:HD21	1:B:643:LEU:HD21	1.90	0.52
1:C:677:LEU:HD11	1:C:792:VAL:HG21	1.91	0.52
1:B:1911:LEU:HD11	1:B:2063:ILE:HG12	1.90	0.52
1:B:3798:MET:HE1	1:B:3875:THR:HB	1.91	0.52
1:C:1094:TYR:OH	1:C:1808:ASP:OD1	2.28	0.52
1:C:3798:MET:HE1	1:C:3875:THR:HB	1.92	0.52
1:A:1911:LEU:HD11	1:A:2063:ILE:HG12	1.90	0.52
1:B:2488:LEU:O	1:B:2492:GLY:N	2.42	0.52
1:B:4791:ARG:CZ	1:C:4523:VAL:HG11	2.39	0.52
1:A:26:ALA:HB3	1:A:33:GLN:HB3	1.90	0.52
1:A:364:GLN:HE21	1:A:369:GLY:HA2	1.75	0.52
1:A:4889:CYS:HB3	1:A:4892:CYS:SG	2.49	0.52
1:C:2488:LEU:O	1:C:2492:GLY:N	2.42	0.52
1:A:4660:GLU:HG3	1:A:4664:ARG:HH21	1.73	0.52
1:A:4819:TYR:O	1:A:4823:ARG:NH2	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1487:MET:HB3	1:B:1520:PHE:HZ	1.75	0.52
1:B:26:ALA:HB3	1:B:33:GLN:HB3	1.90	0.52
1:B:3926:GLN:HE21	1:B:4936:GLY:H	1.56	0.52
1:C:4108:GLU:HG3	1:C:4136:ARG:HH22	1.74	0.52
1:A:1487:MET:HB3	1:A:1520:PHE:HZ	1.75	0.52
1:A:192:LEU:O	1:A:212:TRP:NE1	2.42	0.52
1:A:4046:LYS:HG3	1:A:4068:LEU:HD22	1.90	0.52
1:A:4791:ARG:CZ	1:B:4523:VAL:HG11	2.39	0.52
1:C:1726:ILE:HB	1:C:2109:ILE:HD11	1.91	0.52
1:C:636:LEU:HD21	1:C:643:LEU:HD21	1.90	0.52
1:D:3730:ALA:HA	1:D:3733:HIS:CE1	2.44	0.52
1:A:61:ASP:OD2	1:A:417:ARG:NH2	2.42	0.52
1:C:1938:GLN:HE22	1:C:3614:ARG:HA	1.75	0.52
1:A:1252:SER:HB2	1:A:1598:ARG:HB2	1.92	0.52
1:A:4108:GLU:HG3	1:A:4136:ARG:HH22	1.74	0.52
1:A:4523:VAL:HG11	1:D:4791:ARG:CZ	2.39	0.52
1:D:1094:TYR:OH	1:D:1808:ASP:OD1	2.28	0.52
1:D:1632:ILE:HD11	1:D:1637:ARG:HG2	1.92	0.52
1:C:4791:ARG:CZ	1:D:4523:VAL:HG11	2.39	0.52
1:A:1703:TYR:HD2	1:A:1820:PRO:HB2	1.75	0.52
1:A:476:GLN:NE2	1:A:3679:GLU:OE1	2.43	0.52
1:A:636:LEU:HD21	1:A:643:LEU:HD21	1.90	0.52
1:A:677:LEU:HD11	1:A:792:VAL:HG21	1.91	0.52
1:B:2192:LYS:O	1:B:2196:ASN:ND2	2.43	0.52
1:B:4108:GLU:HG3	1:B:4136:ARG:HH22	1.74	0.52
1:C:1632:ILE:HD11	1:C:1637:ARG:HG2	1.92	0.52
1:C:4050:HIS:HB2	1:C:4068:LEU:HD11	1.91	0.52
1:C:4873:GLU:HA	1:D:4875:ARG:HH11	1.68	0.52
1:D:3926:GLN:HE21	1:D:4936:GLY:H	1.56	0.52
1:A:4873:GLU:HA	1:B:4875:ARG:HH11	1.68	0.51
1:B:1252:SER:HB2	1:B:1598:ARG:HB2	1.92	0.51
1:D:1487:MET:HB3	1:D:1520:PHE:HZ	1.75	0.51
1:A:1938:GLN:HE22	1:A:3614:ARG:HA	1.75	0.51
1:B:1629:SER:HA	1:B:1640:ASP:HA	1.93	0.51
1:B:2103:LEU:HA	1:B:2106:THR:HG22	1.93	0.51
1:C:1487:MET:HB3	1:C:1520:PHE:HZ	1.75	0.51
1:C:2103:LEU:HA	1:C:2106:THR:HG22	1.93	0.51
1:C:2192:LYS:O	1:C:2196:ASN:ND2	2.43	0.51
1:D:4809:ASP:O	1:D:4813:CYS:N	2.39	0.51
1:A:1613:GLU:HB2	1:A:1618:LEU:H	1.76	0.51
1:B:1613:GLU:HB2	1:B:1618:LEU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:GLN:NE2	1:B:3679:GLU:OE1	2.43	0.51
1:D:1613:GLU:HB2	1:D:1618:LEU:H	1.76	0.51
1:D:1629:SER:HA	1:D:1640:ASP:HA	1.93	0.51
1:D:677:LEU:HD11	1:D:792:VAL:HG21	1.91	0.51
1:C:1629:SER:HA	1:C:1640:ASP:HA	1.93	0.51
1:C:1703:TYR:HD2	1:C:1820:PRO:HB2	1.75	0.51
1:C:4809:ASP:O	1:C:4813:CYS:N	2.39	0.51
1:D:476:GLN:NE2	1:D:3679:GLU:OE1	2.43	0.51
1:B:364:GLN:HE21	1:B:369:GLY:HA2	1.75	0.51
1:C:1613:GLU:HB2	1:C:1618:LEU:H	1.76	0.51
1:C:476:GLN:NE2	1:C:3679:GLU:OE1	2.43	0.51
1:C:3980:VAL:HA	1:C:3983:LEU:HD23	1.92	0.51
1:D:1703:TYR:HD2	1:D:1820:PRO:HB2	1.75	0.51
1:D:364:GLN:HE21	1:D:369:GLY:HA2	1.75	0.51
1:A:4050:HIS:HB2	1:A:4068:LEU:HD11	1.91	0.51
1:B:1654:HIS:O	1:B:1657:THR:OG1	2.26	0.51
1:B:23:GLN:HA	1:B:36:CYS:HA	1.92	0.51
1:B:4163:LYS:HB2	1:B:4164:PRO:HD3	1.92	0.51
1:C:4636:ILE:O	1:C:4651:LYS:NZ	2.44	0.51
1:D:1252:SER:HB2	1:D:1598:ARG:HB2	1.92	0.51
1:D:192:LEU:O	1:D:212:TRP:NE1	2.42	0.51
1:D:2192:LYS:O	1:D:2196:ASN:ND2	2.43	0.51
1:D:1938:GLN:HE22	1:D:3614:ARG:HA	1.75	0.51
1:D:4636:ILE:O	1:D:4651:LYS:NZ	2.44	0.51
1:A:1094:TYR:OH	1:A:1808:ASP:OD1	2.28	0.51
1:A:4163:LYS:HB2	1:A:4164:PRO:HD3	1.92	0.51
1:B:1576:LYS:NZ	1:B:1589:GLN:OE1	2.44	0.51
1:B:4636:ILE:O	1:B:4651:LYS:NZ	2.44	0.51
1:C:1252:SER:HB2	1:C:1598:ARG:HB2	1.92	0.51
1:C:364:GLN:HE21	1:C:369:GLY:HA2	1.75	0.51
1:B:1703:TYR:HD2	1:B:1820:PRO:HB2	1.75	0.51
1:A:4875:ARG:CZ	1:D:4872:GLY:O	2.59	0.51
1:A:1576:LYS:NZ	1:A:1589:GLN:OE1	2.44	0.51
1:A:2103:LEU:HA	1:A:2106:THR:HG22	1.93	0.51
1:A:4636:ILE:O	1:A:4651:LYS:NZ	2.44	0.51
1:C:4872:GLY:O	1:D:4875:ARG:CZ	2.59	0.51
1:A:2192:LYS:O	1:A:2196:ASN:ND2	2.43	0.51
1:B:4872:GLY:O	1:C:4875:ARG:CZ	2.59	0.51
1:C:4819:TYR:O	1:C:4823:ARG:NH2	2.33	0.51
1:D:2103:LEU:HA	1:D:2106:THR:HG22	1.93	0.51
1:D:4050:HIS:HB2	1:D:4068:LEU:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1632:ILE:HD11	1:B:1637:ARG:HG2	1.92	0.50
1:B:4052:ALA:O	1:B:4056:HIS:ND1	2.44	0.50
1:C:150:GLN:NE2	1:C:158:CYS:SG	2.80	0.50
1:C:4052:ALA:O	1:C:4056:HIS:ND1	2.44	0.50
1:D:1726:ILE:HG13	1:D:1757:LEU:HD23	1.93	0.50
1:D:4174:ILE:HG21	1:D:4885:MET:HE2	1.93	0.50
1:A:1629:SER:HA	1:A:1640:ASP:HA	1.93	0.50
1:A:2857:LYS:HE3	1:A:2861:LEU:HD11	1.93	0.50
1:B:260:VAL:HG12	1:B:391:ALA:HB3	1.92	0.50
1:B:3980:VAL:HA	1:B:3983:LEU:HD23	1.92	0.50
1:C:419:ILE:HD13	1:C:492:GLU:HG3	1.93	0.50
1:A:3980:VAL:HA	1:A:3983:LEU:HD23	1.92	0.50
1:A:1911:LEU:HD22	1:A:2088:LEU:HD13	1.94	0.50
1:A:260:VAL:HG12	1:A:391:ALA:HB3	1.92	0.50
1:C:1128:LEU:HD13	1:C:1206:SER:HB2	1.94	0.50
1:C:1654:HIS:O	1:C:1657:THR:OG1	2.26	0.50
1:C:23:GLN:HA	1:C:36:CYS:HA	1.92	0.50
1:C:4647:ASP:O	1:C:4650:VAL:HG23	2.12	0.50
1:A:1632:ILE:HD11	1:A:1637:ARG:HG2	1.92	0.50
1:A:3729:GLN:O	1:A:3733:HIS:ND1	2.41	0.50
1:A:812:LYS:HD3	1:A:813:PHE:HB2	1.93	0.50
1:B:1431:ARG:HB3	1:B:1554:GLN:HB2	1.94	0.50
1:B:150:GLN:NE2	1:B:158:CYS:SG	2.80	0.50
1:B:1726:ILE:HG13	1:B:1757:LEU:HD23	1.93	0.50
1:B:2857:LYS:HE3	1:B:2861:LEU:HD11	1.93	0.50
1:B:1938:GLN:HE22	1:B:3614:ARG:HA	1.75	0.50
1:D:1128:LEU:HD13	1:D:1206:SER:HB2	1.94	0.50
1:D:1911:LEU:HD22	1:D:2088:LEU:HD13	1.94	0.50
1:C:1576:LYS:NZ	1:C:1589:GLN:OE1	2.44	0.50
1:C:260:VAL:HG12	1:C:391:ALA:HB3	1.92	0.50
1:C:812:LYS:HD3	1:C:813:PHE:HB2	1.93	0.50
1:D:1228:THR:HA	1:D:1232:LEU:HD12	1.94	0.50
1:A:1726:ILE:HG13	1:A:1757:LEU:HD23	1.93	0.50
1:A:2783:MET:HG2	1:A:2788:TRP:HE3	1.77	0.50
1:D:23:GLN:HA	1:D:36:CYS:HA	1.92	0.50
1:A:2439:ILE:HD13	1:A:2465:HIS:HB3	1.94	0.50
1:B:1444:GLY:HA2	1:B:1487:MET:HB2	1.94	0.50
1:C:1228:THR:HA	1:C:1232:LEU:HD12	1.94	0.50
1:C:1726:ILE:HG13	1:C:1757:LEU:HD23	1.93	0.50
1:C:565:LEU:HG	1:C:604:HIS:CE1	2.47	0.50
1:A:23:GLN:HA	1:A:36:CYS:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4780:TYR:HA	1:A:4783:THR:HG22	1.94	0.50
1:B:419:ILE:HD13	1:B:492:GLU:HG3	1.93	0.50
1:C:4861:ALA:HA	1:C:4864:GLN:HB2	1.94	0.50
1:D:260:VAL:HG12	1:D:391:ALA:HB3	1.92	0.50
1:D:4163:LYS:HB2	1:D:4164:PRO:HD3	1.92	0.50
1:A:4052:ALA:O	1:A:4056:HIS:ND1	2.44	0.49
1:A:3961:GLN:NE2	1:A:4069:SER:OG	2.45	0.49
1:B:2439:ILE:HD13	1:B:2465:HIS:HB3	1.94	0.49
1:B:4647:ASP:O	1:B:4650:VAL:HG23	2.12	0.49
1:B:565:LEU:HG	1:B:604:HIS:CE1	2.47	0.49
1:C:1444:GLY:HA2	1:C:1487:MET:HB2	1.94	0.49
1:D:1576:LYS:NZ	1:D:1589:GLN:OE1	2.44	0.49
1:A:4811:LEU:HD23	1:B:4519:LEU:HG	1.94	0.49
1:A:4872:GLY:O	1:B:4875:ARG:CZ	2.59	0.49
1:B:4784:VAL:HG13	1:C:4738:PHE:CE2	2.47	0.49
1:B:4861:ALA:HA	1:B:4864:GLN:HB2	1.94	0.49
1:C:1911:LEU:HD22	1:C:2088:LEU:HD13	1.94	0.49
1:D:1654:HIS:O	1:D:1657:THR:OG1	2.26	0.49
1:D:2857:LYS:HE3	1:D:2861:LEU:HD11	1.93	0.49
1:D:719:GLY:H	1:D:722:LEU:HD12	1.77	0.49
1:A:4632:ASP:OD1	1:A:4709:TRP:NE1	2.42	0.49
1:A:4784:VAL:HG13	1:B:4738:PHE:CE2	2.47	0.49
1:B:2783:MET:HG2	1:B:2788:TRP:HE3	1.77	0.49
1:B:4811:LEU:HD23	1:C:4519:LEU:HG	1.94	0.49
1:C:4784:VAL:HG13	1:D:4738:PHE:CE2	2.47	0.49
1:D:3961:GLN:NE2	1:D:4069:SER:OG	2.45	0.49
1:D:4610:LYS:HB3	1:D:4616:LEU:HD22	1.94	0.49
1:A:1444:GLY:HA2	1:A:1487:MET:HB2	1.94	0.49
1:A:2521:LEU:HD22	1:A:2565:ALA:HB2	1.94	0.49
1:A:477:ASN:OD1	1:A:480:ARG:NH1	2.46	0.49
1:B:3961:GLN:NE2	1:B:4069:SER:OG	2.45	0.49
1:B:4780:TYR:HA	1:B:4783:THR:HG22	1.94	0.49
1:D:3980:VAL:HA	1:D:3983:LEU:HD23	1.92	0.49
1:A:4519:LEU:HG	1:D:4811:LEU:HD23	1.94	0.49
1:D:812:LYS:HD3	1:D:813:PHE:HB2	1.93	0.49
1:A:1228:THR:HA	1:A:1232:LEU:HD12	1.94	0.49
1:A:1431:ARG:HB3	1:A:1554:GLN:HB2	1.94	0.49
1:D:1444:GLY:HA2	1:D:1487:MET:HB2	1.94	0.49
1:D:2521:LEU:HD22	1:D:2565:ALA:HB2	1.94	0.49
1:A:288:HIS:ND1	1:A:349:MET:O	2.43	0.49
1:B:1911:LEU:HD22	1:B:2088:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2783:MET:HG2	1:C:2788:TRP:HE3	1.77	0.49
1:C:4163:LYS:HB2	1:C:4164:PRO:HD3	1.92	0.49
1:D:4003:MET:HG3	1:D:4004:LEU:HG	1.95	0.49
1:A:4647:ASP:O	1:A:4650:VAL:HG23	2.12	0.49
1:A:419:ILE:HD13	1:A:492:GLU:HG3	1.93	0.49
1:B:1184:ASP:HB3	1:B:1186:SER:H	1.78	0.49
1:B:1228:THR:HA	1:B:1232:LEU:HD12	1.94	0.49
1:C:2857:LYS:HE3	1:C:2861:LEU:HD11	1.93	0.49
1:D:227:TYR:CE1	1:D:355:LYS:HG2	2.47	0.49
1:D:4052:ALA:O	1:D:4056:HIS:ND1	2.44	0.49
1:D:477:ASN:OD1	1:D:480:ARG:NH1	2.46	0.49
1:A:1128:LEU:HD13	1:A:1206:SER:HB2	1.94	0.49
1:A:4610:LYS:HB3	1:A:4616:LEU:HD22	1.94	0.49
1:B:2521:LEU:HD22	1:B:2565:ALA:HB2	1.94	0.49
1:B:3729:GLN:O	1:B:3733:HIS:ND1	2.41	0.49
1:B:335:LYS:NZ	1:B:398:HIS:O	2.44	0.49
1:B:812:LYS:HD3	1:B:813:PHE:HB2	1.93	0.49
1:C:227:TYR:CE1	1:C:355:LYS:HG2	2.47	0.49
1:C:335:LYS:NZ	1:C:398:HIS:O	2.44	0.49
1:D:4647:ASP:O	1:D:4650:VAL:HG23	2.12	0.49
1:B:1473:LYS:HE2	1:B:1475:LYS:HE3	1.95	0.49
1:C:2439:ILE:HD13	1:C:2465:HIS:HB3	1.94	0.49
1:C:4610:LYS:HB3	1:C:4616:LEU:HD22	1.94	0.49
1:D:1086:ARG:HH22	1:D:1254:ARG:HB2	1.78	0.49
1:D:419:ILE:HD13	1:D:492:GLU:HG3	1.93	0.49
1:D:4780:TYR:HA	1:D:4783:THR:HG22	1.94	0.49
1:D:565:LEU:HG	1:D:604:HIS:CE1	2.47	0.49
1:A:1184:ASP:HB3	1:A:1186:SER:H	1.78	0.49
1:A:565:LEU:HG	1:A:604:HIS:CE1	2.47	0.49
1:B:2421:ARG:HH21	1:B:2425:ARG:HH21	1.61	0.49
1:B:719:GLY:H	1:B:722:LEU:HD12	1.77	0.49
1:C:1431:ARG:HB3	1:C:1554:GLN:HB2	1.94	0.49
1:C:2521:LEU:HD22	1:C:2565:ALA:HB2	1.94	0.49
1:C:4003:MET:HG3	1:C:4004:LEU:HG	1.95	0.49
1:D:1184:ASP:HB3	1:D:1186:SER:H	1.78	0.49
1:D:1431:ARG:HB3	1:D:1554:GLN:HB2	1.94	0.49
1:A:3663:ASP:OD2	1:A:3735:ARG:NH2	2.46	0.48
1:A:150:GLN:NE2	1:A:158:CYS:SG	2.80	0.48
1:A:4774:LEU:HD13	1:B:4754:LEU:HD21	1.95	0.48
1:B:1086:ARG:HB2	1:B:1207:LEU:HB2	1.95	0.48
1:B:1220:ASP:O	1:B:1223:THR:N	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:ASN:OD1	1:C:480:ARG:NH1	2.46	0.48
1:C:4174:ILE:HD13	1:C:4885:MET:HE1	1.96	0.48
1:D:2783:MET:HG2	1:D:2788:TRP:HE3	1.77	0.48
1:A:4191:VAL:HA	1:A:4194:CYS:HB2	1.96	0.48
1:A:4732:LEU:O	1:A:4736:ASN:N	2.44	0.48
1:A:4861:ALA:HA	1:A:4864:GLN:HB2	1.94	0.48
1:B:1128:LEU:HD13	1:B:1206:SER:HB2	1.94	0.48
1:B:2345:LEU:HD21	1:B:2434:VAL:HB	1.96	0.48
1:C:3663:ASP:OD2	1:C:3735:ARG:NH2	2.46	0.48
1:C:4780:TYR:HA	1:C:4783:THR:HG22	1.94	0.48
1:C:4764:ASN:ND2	1:C:4866:LEU:O	2.47	0.48
1:D:3663:ASP:OD2	1:D:3735:ARG:NH2	2.46	0.48
1:D:4861:ALA:HA	1:D:4864:GLN:HB2	1.94	0.48
1:A:1934:VAL:O	1:A:1938:GLN:N	2.43	0.48
1:A:2345:LEU:HD21	1:A:2434:VAL:HB	1.96	0.48
1:A:719:GLY:H	1:A:722:LEU:HD12	1.77	0.48
1:B:1184:ASP:OD2	1:B:1188:SER:OG	2.31	0.48
1:B:3663:ASP:OD2	1:B:3735:ARG:NH2	2.46	0.48
1:B:477:ASN:OD1	1:B:480:ARG:NH1	2.46	0.48
1:B:653:SER:OG	1:B:794:PHE:O	2.31	0.48
1:C:192:LEU:O	1:C:212:TRP:NE1	2.42	0.48
1:C:2723:ASN:OD1	1:C:2773:ARG:NH2	2.47	0.48
1:C:4774:LEU:HD13	1:D:4754:LEU:HD21	1.95	0.48
1:D:150:GLN:NE2	1:D:158:CYS:SG	2.80	0.48
1:D:2209:ARG:HG3	1:D:2251:ASN:HD21	1.79	0.48
1:D:2345:LEU:HD21	1:D:2434:VAL:HB	1.96	0.48
1:A:4003:MET:HG3	1:A:4004:LEU:HG	1.95	0.48
1:B:1086:ARG:HH22	1:B:1254:ARG:HB2	1.78	0.48
1:C:2421:ARG:HH21	1:C:2425:ARG:HH21	1.61	0.48
1:C:4811:LEU:HD23	1:D:4519:LEU:HG	1.94	0.48
1:D:1184:ASP:OD2	1:D:1188:SER:OG	2.31	0.48
1:A:4013:MET:O	1:A:4017:PHE:N	2.46	0.48
1:C:2345:LEU:HD21	1:C:2434:VAL:HB	1.96	0.48
1:D:1473:LYS:HE2	1:D:1475:LYS:HE3	1.95	0.48
1:C:4780:TYR:OH	1:D:4515:ASN:ND2	2.46	0.48
1:A:1220:ASP:O	1:A:1223:THR:N	2.35	0.48
1:A:1473:LYS:HE2	1:A:1475:LYS:HE3	1.95	0.48
1:A:2421:ARG:HH21	1:A:2425:ARG:HH21	1.61	0.48
1:C:374:TYR:HA	1:C:391:ALA:HA	1.96	0.48
1:C:3961:GLN:NE2	1:C:4069:SER:OG	2.45	0.48
1:C:719:GLY:H	1:C:722:LEU:HD12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:852:GLY:HA2	1:C:853:PRO:HA	1.69	0.48
1:D:2723:ASN:OD1	1:D:2773:ARG:NH2	2.47	0.48
1:A:1833:ILE:HG22	1:A:1834:PHE:H	1.79	0.48
1:A:428:ARG:O	1:A:432:GLY:N	2.46	0.48
1:A:4515:ASN:ND2	1:D:4780:TYR:OH	2.46	0.48
1:A:4780:TYR:OH	1:B:4515:ASN:ND2	2.46	0.48
1:C:2717:LYS:HB2	1:C:2792:ARG:HH22	1.79	0.48
1:D:4764:ASN:ND2	1:D:4866:LEU:O	2.47	0.48
1:A:4738:PHE:CE2	1:D:4784:VAL:HG13	2.47	0.48
1:A:4130:PHE:O	1:A:4134:LEU:N	2.45	0.48
1:B:2723:ASN:OD1	1:B:2773:ARG:NH2	2.47	0.48
1:B:4771:THR:OG1	1:C:4757:ILE:HD13	2.14	0.48
1:B:4780:TYR:OH	1:C:4515:ASN:ND2	2.46	0.48
1:D:2439:ILE:HD13	1:D:2465:HIS:HB3	1.94	0.48
1:B:1833:ILE:HG22	1:B:1834:PHE:H	1.79	0.48
1:B:192:LEU:O	1:B:212:TRP:NE1	2.42	0.48
1:B:3911:ILE:HG21	1:B:3971:GLU:HB3	1.96	0.48
1:B:4610:LYS:HB3	1:B:4616:LEU:HD22	1.94	0.48
1:C:1184:ASP:HB3	1:C:1186:SER:H	1.78	0.48
1:D:1086:ARG:HB2	1:D:1207:LEU:HB2	1.95	0.48
1:D:1626:GLN:O	1:D:1687:TYR:OH	2.32	0.48
1:B:4191:VAL:HA	1:B:4194:CYS:HB2	1.96	0.47
1:C:1473:LYS:HE2	1:C:1475:LYS:HE3	1.95	0.47
1:D:2717:LYS:HB2	1:D:2792:ARG:HH22	1.79	0.47
1:D:4013:MET:O	1:D:4017:PHE:N	2.46	0.47
1:D:4191:VAL:HA	1:D:4194:CYS:HB2	1.96	0.47
1:B:115:TYR:HB3	1:B:164:PRO:HD3	1.97	0.47
1:C:3729:GLN:O	1:C:3733:HIS:ND1	2.41	0.47
1:C:3911:ILE:HG21	1:C:3971:GLU:HB3	1.96	0.47
1:D:2421:ARG:HH21	1:D:2425:ARG:HH21	1.61	0.47
1:D:374:TYR:HA	1:D:391:ALA:HA	1.96	0.47
1:D:3911:ILE:HG21	1:D:3971:GLU:HB3	1.96	0.47
1:A:1086:ARG:HH22	1:A:1254:ARG:HB2	1.78	0.47
1:A:2723:ASN:OD1	1:A:2773:ARG:NH2	2.47	0.47
1:A:4764:ASN:ND2	1:A:4866:LEU:O	2.47	0.47
1:A:4771:THR:OG1	1:B:4757:ILE:HD13	2.14	0.47
1:D:2076:ILE:HG21	1:D:2081:LEU:HD22	1.97	0.47
1:D:3804:LEU:HD13	1:D:3910:ALA:HB2	1.96	0.47
1:A:115:TYR:HB3	1:A:164:PRO:HD3	1.97	0.47
1:A:3911:ILE:HG21	1:A:3971:GLU:HB3	1.96	0.47
1:B:4774:LEU:HD13	1:C:4754:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4764:ASN:ND2	1:B:4866:LEU:O	2.47	0.47
1:C:1086:ARG:HH22	1:C:1254:ARG:HB2	1.78	0.47
1:D:115:TYR:HB3	1:D:164:PRO:HD3	1.97	0.47
1:D:2793:THR:OG1	1:D:2901:GLY:O	2.25	0.47
1:A:1184:ASP:OD2	1:A:1188:SER:OG	2.31	0.47
1:A:2076:ILE:HG21	1:A:2081:LEU:HD22	1.97	0.47
1:A:374:TYR:HA	1:A:391:ALA:HA	1.96	0.47
1:B:4003:MET:HG3	1:B:4004:LEU:HG	1.95	0.47
1:C:590:LYS:HB2	1:C:593:HIS:HD2	1.80	0.47
1:C:718:VAL:HA	1:C:736:CYS:HB2	1.96	0.47
1:A:2717:LYS:HB2	1:A:2792:ARG:HH22	1.79	0.47
1:A:3804:LEU:HD13	1:A:3910:ALA:HB2	1.96	0.47
1:A:572:LEU:O	1:A:576:HIS:N	2.47	0.47
1:B:300:VAL:O	1:B:420:ARG:NH2	2.48	0.47
1:B:3800:SER:OG	1:B:3801:CYS:N	2.47	0.47
1:B:4191:VAL:HB	1:B:4950:TRP:HH2	1.79	0.47
1:B:572:LEU:O	1:B:576:HIS:N	2.47	0.47
1:C:1184:ASP:OD2	1:C:1188:SER:OG	2.31	0.47
1:C:1086:ARG:HB2	1:C:1207:LEU:HB2	1.95	0.47
1:C:115:TYR:HB3	1:C:164:PRO:HD3	1.97	0.47
1:C:2737:LYS:HB3	1:C:2742:TRP:HB2	1.96	0.47
1:A:4757:ILE:HD13	1:D:4771:THR:OG1	2.14	0.47
1:D:4191:VAL:HB	1:D:4950:TRP:HH2	1.79	0.47
1:A:1707:ILE:HA	1:A:1711:LEU:HB2	1.97	0.47
1:A:2209:ARG:HG3	1:A:2251:ASN:HD21	1.79	0.47
1:B:2076:ILE:HG21	1:B:2081:LEU:HD22	1.97	0.47
1:B:2717:LYS:HB2	1:B:2792:ARG:HH22	1.79	0.47
1:B:374:TYR:HA	1:B:391:ALA:HA	1.96	0.47
1:C:2121:LEU:O	1:C:2125:GLY:N	2.47	0.47
1:C:2793:THR:OG1	1:C:2901:GLY:O	2.25	0.47
1:C:4752:LYS:HA	1:C:4755:ARG:HE	1.80	0.47
1:A:1086:ARG:HB2	1:A:1207:LEU:HB2	1.95	0.47
1:C:2076:ILE:HG21	1:C:2081:LEU:HD22	1.97	0.47
1:C:4771:THR:OG1	1:D:4757:ILE:HD13	2.14	0.47
1:D:335:LYS:NZ	1:D:398:HIS:O	2.44	0.47
1:D:125:TYR:CZ	1:D:417:ARG:HB3	2.50	0.47
1:D:718:VAL:HA	1:D:736:CYS:HB2	1.96	0.47
1:B:2209:ARG:HG3	1:B:2251:ASN:HD21	1.79	0.47
1:B:2424:LEU:HD23	1:B:2476:VAL:HG22	1.97	0.47
1:B:2737:LYS:HB3	1:B:2742:TRP:HB2	1.96	0.47
1:B:4207:ILE:HG22	1:B:4498:ARG:HE	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4174:ILE:HG21	1:B:4885:MET:HE2	1.96	0.47
1:C:4191:VAL:HA	1:C:4194:CYS:HB2	1.96	0.47
1:D:300:VAL:O	1:D:420:ARG:NH2	2.48	0.47
1:D:4732:LEU:O	1:D:4736:ASN:N	2.44	0.47
1:D:590:LYS:HB2	1:D:593:HIS:HD2	1.80	0.47
1:A:4207:ILE:HG22	1:A:4498:ARG:HE	1.80	0.47
1:C:125:TYR:CZ	1:C:417:ARG:HB3	2.50	0.47
1:B:2301:ASP:OD1	1:B:2304:ARG:NH2	2.48	0.47
1:B:3696:MET:O	1:B:3699:SER:OG	2.26	0.47
1:B:4130:PHE:O	1:B:4134:LEU:N	2.45	0.47
1:B:4752:LYS:HA	1:B:4755:ARG:HE	1.80	0.47
1:A:1172:THR:HG21	1:A:1190:LEU:HD13	1.97	0.46
1:A:2301:ASP:OD1	1:A:2304:ARG:NH2	2.48	0.46
1:A:2737:LYS:HB3	1:A:2742:TRP:HB2	1.96	0.46
1:A:300:VAL:O	1:A:420:ARG:NH2	2.48	0.46
1:A:298:ARG:HE	1:A:303:GLY:HA2	1.81	0.46
1:A:125:TYR:CZ	1:A:417:ARG:HB3	2.50	0.46
1:B:125:TYR:CZ	1:B:417:ARG:HB3	2.50	0.46
1:C:1833:ILE:HG22	1:C:1834:PHE:H	1.79	0.46
1:C:2424:LEU:HD23	1:C:2476:VAL:HG22	1.97	0.46
1:D:1172:THR:HG21	1:D:1190:LEU:HD13	1.97	0.46
1:A:1174:MET:SD	1:A:1236:TYR:OH	2.73	0.46
1:B:1445:TRP:H	1:B:1487:MET:HB2	1.81	0.46
1:B:590:LYS:HB2	1:B:593:HIS:HD2	1.80	0.46
1:C:1172:THR:HG21	1:C:1190:LEU:HD13	1.97	0.46
1:C:2209:ARG:HG3	1:C:2251:ASN:HD21	1.79	0.46
1:C:300:VAL:O	1:C:420:ARG:NH2	2.48	0.46
1:D:1833:ILE:HG22	1:D:1834:PHE:H	1.79	0.46
1:D:2301:ASP:OD1	1:D:2304:ARG:NH2	2.48	0.46
1:D:2737:LYS:HB3	1:D:2742:TRP:HB2	1.96	0.46
1:D:4565:SER:OG	1:D:4566:SER:N	2.49	0.46
1:A:2858:LYS:HG2	1:A:2872:LEU:HD13	1.96	0.46
1:A:4565:SER:OG	1:A:4566:SER:N	2.49	0.46
1:A:590:LYS:HB2	1:A:593:HIS:HD2	1.80	0.46
1:B:1172:THR:HG21	1:B:1190:LEU:HD13	1.97	0.46
1:B:1763:PHE:HB3	1:B:1781:GLU:HB3	1.98	0.46
1:B:3804:LEU:HD13	1:B:3910:ALA:HB2	1.96	0.46
1:B:4627:ILE:O	1:B:4631:TRP:N	2.48	0.46
1:B:657:PRO:HA	1:B:834:VAL:HA	1.97	0.46
1:C:1626:GLN:O	1:C:1687:TYR:OH	2.32	0.46
1:C:4191:VAL:HB	1:C:4950:TRP:HH2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4752:LYS:HA	1:D:4755:ARG:HE	1.80	0.46
1:A:4754:LEU:HD21	1:D:4774:LEU:HD13	1.95	0.46
1:A:1445:TRP:H	1:A:1487:MET:HB2	1.81	0.46
1:A:4752:LYS:HA	1:A:4755:ARG:HE	1.80	0.46
1:A:718:VAL:HA	1:A:736:CYS:HB2	1.96	0.46
1:B:1707:ILE:HA	1:B:1711:LEU:HB2	1.97	0.46
1:B:2121:LEU:O	1:B:2125:GLY:N	2.47	0.46
1:B:428:ARG:O	1:B:432:GLY:N	2.46	0.46
1:C:648:LEU:HD23	1:C:1684:GLN:HA	1.98	0.46
1:A:648:LEU:HD23	1:A:1684:GLN:HA	1.98	0.46
1:B:4201:MET:O	1:B:4205:ALA:N	2.49	0.46
1:B:648:LEU:HD23	1:B:1684:GLN:HA	1.98	0.46
1:B:718:VAL:HA	1:B:736:CYS:HB2	1.96	0.46
1:C:180:ASP:HB3	1:C:211:LEU:HD22	1.97	0.46
1:C:3804:LEU:HD13	1:C:3910:ALA:HB2	1.96	0.46
1:D:2858:LYS:HG2	1:D:2872:LEU:HD13	1.96	0.46
1:A:1763:PHE:HB3	1:A:1781:GLU:HB3	1.98	0.46
1:A:2326:ILE:HA	1:A:2326:ILE:HD13	1.83	0.46
1:A:2424:LEU:HD23	1:A:2476:VAL:HG22	1.97	0.46
1:A:4191:VAL:HB	1:A:4950:TRP:HH2	1.79	0.46
1:B:852:GLY:HA2	1:B:853:PRO:HA	1.69	0.46
1:D:2424:LEU:HD23	1:D:2476:VAL:HG22	1.97	0.46
1:A:4174:ILE:HG21	1:A:4885:MET:HE2	1.97	0.46
1:A:657:PRO:HA	1:A:834:VAL:HA	1.97	0.46
1:B:2858:LYS:HG2	1:B:2872:LEU:HD13	1.96	0.46
1:B:436:LEU:HD13	1:B:518:ALA:HA	1.98	0.46
1:C:1174:MET:SD	1:C:1236:TYR:OH	2.73	0.46
1:C:2301:ASP:OD1	1:C:2304:ARG:NH2	2.48	0.46
1:C:298:ARG:HA	1:C:305:TYR:HA	1.97	0.46
1:C:4632:ASP:OD1	1:C:4709:TRP:NE1	2.42	0.46
1:C:698:ALA:HB2	1:C:722:LEU:HD23	1.98	0.46
1:D:298:ARG:HA	1:D:305:TYR:HA	1.97	0.46
1:D:698:ALA:HB2	1:D:722:LEU:HD23	1.98	0.46
1:A:298:ARG:HA	1:A:305:TYR:HA	1.97	0.46
1:A:436:LEU:HD13	1:A:518:ALA:HA	1.98	0.46
1:B:180:ASP:HB3	1:B:211:LEU:HD22	1.97	0.46
1:C:1707:ILE:HA	1:C:1711:LEU:HB2	1.97	0.46
1:C:170:SER:OG	1:C:171:GLU:N	2.49	0.46
1:C:4627:ILE:O	1:C:4631:TRP:N	2.48	0.46
1:C:572:LEU:O	1:C:576:HIS:N	2.47	0.46
1:D:298:ARG:HE	1:D:303:GLY:HA2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4201:MET:O	1:D:4205:ALA:N	2.49	0.46
1:A:4875:ARG:HH11	1:D:4873:GLU:HA	1.68	0.46
1:D:657:PRO:HA	1:D:834:VAL:HA	1.97	0.46
1:B:1174:MET:SD	1:B:1236:TYR:OH	2.73	0.46
1:A:189:GLU:CG	1:B:2419:ARG:NH2	2.79	0.46
1:B:298:ARG:HA	1:B:305:TYR:HA	1.97	0.46
1:B:4565:SER:OG	1:B:4566:SER:N	2.49	0.46
1:B:189:GLU:CG	1:C:2419:ARG:NH2	2.79	0.46
1:C:2858:LYS:HG2	1:C:2872:LEU:HD13	1.96	0.46
1:D:1174:MET:SD	1:D:1236:TYR:OH	2.73	0.46
1:C:189:GLU:OE1	1:D:2419:ARG:CZ	2.64	0.46
1:D:537:LEU:HD11	1:D:551:PHE:HZ	1.81	0.46
1:A:695:VAL:O	1:A:725:TYR:N	2.49	0.46
1:B:537:LEU:HD11	1:B:551:PHE:HZ	1.81	0.46
1:C:288:HIS:ND1	1:C:349:MET:O	2.43	0.46
1:C:478:ARG:HE	1:C:485:ARG:HH22	1.64	0.46
1:D:648:LEU:HD23	1:D:1684:GLN:HA	1.98	0.46
1:D:1707:ILE:HA	1:D:1711:LEU:HB2	1.97	0.46
1:C:189:GLU:CG	1:D:2419:ARG:NH2	2.79	0.46
1:D:478:ARG:HE	1:D:485:ARG:HH22	1.64	0.46
1:A:537:LEU:HD11	1:A:551:PHE:HZ	1.81	0.45
1:C:298:ARG:HE	1:C:303:GLY:HA2	1.81	0.45
1:C:4565:SER:OG	1:C:4566:SER:N	2.49	0.45
1:D:4207:ILE:HG22	1:D:4498:ARG:HE	1.80	0.45
1:D:428:ARG:O	1:D:432:GLY:N	2.46	0.45
1:D:4627:ILE:O	1:D:4631:TRP:N	2.48	0.45
1:A:170:SER:OG	1:A:171:GLU:N	2.49	0.45
1:B:237:LEU:N	1:B:404:ASN:O	2.49	0.45
1:B:4869:ASP:O	1:B:4873:GLU:N	2.49	0.45
1:C:237:LEU:N	1:C:404:ASN:O	2.49	0.45
1:C:646:THR:OG1	1:C:1684:GLN:NE2	2.49	0.45
1:C:657:PRO:HA	1:C:834:VAL:HA	1.97	0.45
1:D:1763:PHE:HB3	1:D:1781:GLU:HB3	1.98	0.45
1:A:2419:ARG:CZ	1:D:189:GLU:OE1	2.64	0.45
1:A:848:ARG:HB2	1:A:1603:PHE:HZ	1.81	0.45
1:A:180:ASP:HB3	1:A:211:LEU:HD22	1.97	0.45
1:C:1445:TRP:H	1:C:1487:MET:HB2	1.81	0.45
1:C:1763:PHE:HB3	1:C:1781:GLU:HB3	1.98	0.45
1:D:848:ARG:HB2	1:D:1603:PHE:HZ	1.81	0.45
1:A:646:THR:OG1	1:A:1684:GLN:NE2	2.49	0.45
1:A:698:ALA:HB2	1:A:722:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLU:OE1	1:C:2419:ARG:CZ	2.64	0.45
1:B:698:ALA:HB2	1:B:722:LEU:HD23	1.98	0.45
1:C:4207:ILE:HG22	1:C:4498:ARG:HE	1.80	0.45
1:A:2419:ARG:NH2	1:D:189:GLU:CG	2.79	0.45
1:D:180:ASP:HB3	1:D:211:LEU:HD22	1.97	0.45
1:D:4869:ASP:O	1:D:4873:GLU:N	2.49	0.45
1:A:189:GLU:OE1	1:B:2419:ARG:CZ	2.64	0.45
1:A:4201:MET:O	1:A:4205:ALA:N	2.49	0.45
1:B:298:ARG:HE	1:B:303:GLY:HA2	1.81	0.45
1:C:4013:MET:O	1:C:4017:PHE:N	2.46	0.45
1:D:3859:LEU:HD22	1:D:3871:ILE:HG21	1.98	0.45
1:D:843:GLU:HA	1:D:848:ARG:HG2	1.98	0.45
1:A:227:TYR:CE1	1:A:355:LYS:HG2	2.47	0.45
1:A:4588:ILE:HG22	1:A:4723:LEU:HD23	1.99	0.45
1:B:1602:GLN:HB3	1:B:1604:LEU:HD12	1.99	0.45
1:B:4142:SER:HB3	1:B:4940:TYR:CE1	2.52	0.45
1:D:436:LEU:HD13	1:D:518:ALA:HA	1.98	0.45
1:D:4588:ILE:HG22	1:D:4723:LEU:HD23	1.99	0.45
1:D:766:ILE:HB	1:D:779:PHE:HB2	1.99	0.45
1:A:4142:SER:HB3	1:A:4940:TYR:CE1	2.52	0.45
1:A:478:ARG:HE	1:A:485:ARG:HH22	1.64	0.45
1:B:478:ARG:HE	1:B:485:ARG:HH22	1.64	0.45
1:C:1220:ASP:O	1:C:1223:THR:N	2.35	0.45
1:C:4201:MET:O	1:C:4205:ALA:N	2.49	0.45
1:C:4142:SER:HB3	1:C:4940:TYR:CE1	2.52	0.45
1:C:537:LEU:HD11	1:C:551:PHE:HZ	1.81	0.45
1:C:766:ILE:HB	1:C:779:PHE:HB2	1.99	0.45
1:D:1445:TRP:H	1:D:1487:MET:HB2	1.81	0.45
1:D:3800:SER:OG	1:D:3801:CYS:N	2.47	0.45
1:A:843:GLU:HA	1:A:848:ARG:HG2	1.98	0.45
1:B:1934:VAL:O	1:B:1938:GLN:N	2.43	0.45
1:C:419:ILE:HG12	1:C:489:PHE:CE1	2.52	0.45
1:C:4588:ILE:HG22	1:C:4723:LEU:HD23	1.99	0.45
1:D:289:ILE:HG22	1:D:354:ILE:HD12	1.99	0.45
1:A:2525:VAL:HG13	1:A:2528:LEU:HD12	1.99	0.45
1:B:695:VAL:O	1:B:725:TYR:N	2.49	0.45
1:C:3743:GLN:NE2	1:C:3781:TYR:OH	2.43	0.45
1:C:3952:PHE:HB3	1:C:3976:GLN:HE22	1.82	0.45
1:D:3737:ALA:O	1:D:3740:MET:HG2	2.17	0.45
1:A:3952:PHE:HB3	1:A:3976:GLN:HE22	1.82	0.45
1:B:308:LEU:HD22	1:B:370:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3737:ALA:O	1:B:3740:MET:HG2	2.17	0.45
1:C:4203:LEU:O	1:C:4207:ILE:HG12	2.17	0.45
1:C:428:ARG:O	1:C:432:GLY:N	2.46	0.45
1:C:436:LEU:HD13	1:C:518:ALA:HA	1.98	0.45
1:A:766:ILE:HB	1:A:779:PHE:HB2	1.99	0.44
1:B:4036:TYR:HE2	1:B:4048:ASP:HB3	1.82	0.44
1:B:419:ILE:HG12	1:B:489:PHE:CE1	2.52	0.44
1:C:143:LEU:CD2	1:D:2426:SER:HB3	2.47	0.44
1:C:1602:GLN:HB3	1:C:1604:LEU:HD12	1.99	0.44
1:C:4747:ILE:HG13	1:C:4754:LEU:HD22	1.99	0.44
1:C:843:GLU:HA	1:C:848:ARG:HG2	1.98	0.44
1:D:4844:ARG:HH12	1:D:4848:ASP:HB2	1.83	0.44
1:D:419:ILE:HG12	1:D:489:PHE:CE1	2.52	0.44
1:D:745:ASN:ND2	1:D:773:GLN:OE1	2.48	0.44
1:A:1626:GLN:O	1:A:1687:TYR:OH	2.32	0.44
1:A:4627:ILE:O	1:A:4631:TRP:N	2.48	0.44
1:A:4844:ARG:HH12	1:A:4848:ASP:HB2	1.83	0.44
1:A:4869:ASP:O	1:A:4873:GLU:N	2.49	0.44
1:A:419:ILE:HG12	1:A:489:PHE:CE1	2.52	0.44
1:B:848:ARG:HB2	1:B:1603:PHE:HZ	1.81	0.44
1:B:4747:ILE:HG13	1:B:4754:LEU:HD22	1.99	0.44
1:B:4845:ILE:O	1:B:4849:ILE:N	2.44	0.44
1:B:4844:ARG:HH12	1:B:4848:ASP:HB2	1.83	0.44
1:C:3737:ALA:O	1:C:3740:MET:HG2	2.17	0.44
1:D:1170:GLU:O	1:D:1172:THR:N	2.50	0.44
1:D:2121:LEU:O	1:D:2125:GLY:N	2.47	0.44
1:D:4203:LEU:O	1:D:4207:ILE:HG12	2.17	0.44
1:D:4632:ASP:OD1	1:D:4709:TRP:NE1	2.42	0.44
1:A:308:LEU:HD22	1:A:370:LEU:HD12	1.98	0.44
1:A:3859:LEU:HD22	1:A:3871:ILE:HG21	1.98	0.44
1:B:1799:VAL:O	1:B:1803:SER:N	2.46	0.44
1:B:2525:VAL:HG13	1:B:2528:LEU:HD12	1.99	0.44
1:B:3859:LEU:HD22	1:B:3871:ILE:HG21	1.98	0.44
1:B:3925:ILE:HG21	1:B:3925:ILE:HD13	1.70	0.44
1:B:4013:MET:O	1:B:4017:PHE:N	2.46	0.44
1:B:4588:ILE:HG22	1:B:4723:LEU:HD23	1.99	0.44
1:B:766:ILE:HB	1:B:779:PHE:HB2	1.99	0.44
1:C:1087:ILE:HG23	1:C:1128:LEU:HD12	2.00	0.44
1:C:289:ILE:HG22	1:C:354:ILE:HD12	1.99	0.44
1:C:695:VAL:O	1:C:725:TYR:N	2.49	0.44
1:D:466:PRO:HB3	1:D:478:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4747:ILE:HG13	1:A:4754:LEU:HD22	1.99	0.44
1:A:745:ASN:ND2	1:A:773:GLN:OE1	2.48	0.44
1:B:4203:LEU:O	1:B:4207:ILE:HG12	2.17	0.44
1:B:466:PRO:HB3	1:B:478:ARG:HG2	1.99	0.44
1:D:308:LEU:HD22	1:D:370:LEU:HD12	1.98	0.44
1:D:695:VAL:O	1:D:725:TYR:N	2.49	0.44
1:A:2390:MET:HG3	1:A:2465:HIS:CE1	2.53	0.44
1:A:3767:LEU:O	1:A:3770:GLY:N	2.51	0.44
1:A:4203:LEU:O	1:A:4207:ILE:HG12	2.17	0.44
1:B:646:THR:OG1	1:B:1684:GLN:NE2	2.49	0.44
1:C:848:ARG:HB2	1:C:1603:PHE:HZ	1.81	0.44
1:C:2390:MET:HG3	1:C:2465:HIS:CE1	2.53	0.44
1:C:4130:PHE:O	1:C:4134:LEU:N	2.45	0.44
1:D:1011:ARG:HB3	1:D:1032:LEU:HD21	2.00	0.44
1:D:1934:VAL:O	1:D:1938:GLN:N	2.43	0.44
1:D:4747:ILE:HG13	1:D:4754:LEU:HD22	1.99	0.44
1:A:1136:ALA:HB3	1:A:1145:TRP:HB2	2.00	0.44
1:A:1602:GLN:HB3	1:A:1604:LEU:HD12	1.99	0.44
1:A:2121:LEU:O	1:A:2125:GLY:N	2.47	0.44
1:A:2832:VAL:O	1:A:2895:LYS:NZ	2.45	0.44
1:A:466:PRO:HB3	1:A:478:ARG:HG2	1.99	0.44
1:B:843:GLU:HA	1:B:848:ARG:HG2	1.98	0.44
1:C:2525:VAL:HG13	1:C:2528:LEU:HD12	1.99	0.44
1:C:299:HIS:NE2	1:C:301:THR:OG1	2.46	0.44
1:C:308:LEU:HD22	1:C:370:LEU:HD12	1.98	0.44
1:D:1087:ILE:HG23	1:D:1128:LEU:HD12	2.00	0.44
1:D:2390:MET:HG3	1:D:2465:HIS:CE1	2.53	0.44
1:D:3952:PHE:HB3	1:D:3976:GLN:HE22	1.82	0.44
1:D:237:LEU:N	1:D:404:ASN:O	2.49	0.44
1:D:4142:SER:HB3	1:D:4940:TYR:CE1	2.52	0.44
1:A:1664:VAL:HG12	1:A:1672:VAL:HG11	2.00	0.44
1:A:1799:VAL:O	1:A:1803:SER:N	2.46	0.44
1:A:4867:ILE:HG23	1:A:4867:ILE:HD12	1.80	0.44
1:B:1092:LYS:H	1:B:1250:TRP:HZ3	1.66	0.44
1:B:123:HIS:CD2	1:B:126:SER:H	2.34	0.44
1:B:4632:ASP:OD1	1:B:4709:TRP:NE1	2.42	0.44
1:B:655:MET:HG2	1:B:836:HIS:HA	2.00	0.44
1:C:123:HIS:CD2	1:C:126:SER:H	2.34	0.44
1:C:4732:LEU:O	1:C:4736:ASN:N	2.44	0.44
1:C:655:MET:HG2	1:C:836:HIS:HA	2.00	0.44
1:B:1626:GLN:O	1:B:1687:TYR:OH	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:TYR:O	1:B:201:LEU:N	2.51	0.44
1:B:2390:MET:HG3	1:B:2465:HIS:CE1	2.53	0.44
1:B:2732:LYS:HA	1:B:2732:LYS:HD2	1.82	0.44
1:B:4500:PHE:HA	1:B:4503:MET:HB2	2.00	0.44
1:B:4732:LEU:O	1:B:4736:ASN:N	2.44	0.44
1:C:4500:PHE:HA	1:C:4503:MET:HB2	2.00	0.44
1:D:1664:VAL:HG12	1:D:1672:VAL:HG11	2.00	0.44
1:D:1720:MET:HE2	1:D:2128:ARG:HD2	2.00	0.44
1:D:4036:TYR:HE2	1:D:4048:ASP:HB3	1.82	0.44
1:A:289:ILE:HG22	1:A:354:ILE:HD12	1.99	0.44
1:A:655:MET:HG2	1:A:836:HIS:HA	2.00	0.44
1:B:4610:LYS:O	1:B:4615:GLY:N	2.51	0.44
1:D:196:TYR:O	1:D:201:LEU:N	2.51	0.44
1:D:3767:LEU:O	1:D:3770:GLY:N	2.51	0.44
1:A:1449:ASP:OD1	1:A:1449:ASP:N	2.51	0.43
1:A:196:TYR:O	1:A:201:LEU:N	2.51	0.43
1:A:4610:LYS:O	1:A:4615:GLY:N	2.51	0.43
1:A:4178:VAL:HG11	1:A:4881:VAL:HA	1.99	0.43
1:B:3743:GLN:NE2	1:B:3781:TYR:OH	2.43	0.43
1:B:4739:PHE:HA	1:B:4739:PHE:HD1	1.76	0.43
1:C:1011:ARG:HB3	1:C:1032:LEU:HD21	2.00	0.43
1:D:4610:LYS:O	1:D:4615:GLY:N	2.51	0.43
1:D:646:THR:OG1	1:D:1684:GLN:NE2	2.49	0.43
1:D:655:MET:HG2	1:D:836:HIS:HA	2.00	0.43
1:A:2426:SER:HB3	1:D:143:LEU:CD2	2.47	0.43
1:A:908:ARG:HA	1:A:916:PRO:HD3	2.00	0.43
1:B:289:ILE:HG22	1:B:354:ILE:HD12	1.99	0.43
1:B:288:HIS:ND1	1:B:349:MET:O	2.43	0.43
1:B:227:TYR:CE1	1:B:355:LYS:HG2	2.47	0.43
1:C:3859:LEU:HD22	1:C:3871:ILE:HG21	1.98	0.43
1:C:4759:SER:O	1:C:4763:HIS:ND1	2.30	0.43
1:C:4869:ASP:O	1:C:4873:GLU:N	2.49	0.43
1:C:4763:HIS:CE1	1:C:4870:ALA:HB1	2.53	0.43
1:C:758:CYS:SG	1:C:759:LEU:N	2.91	0.43
1:D:1602:GLN:HB3	1:D:1604:LEU:HD12	1.99	0.43
1:D:170:SER:OG	1:D:171:GLU:N	2.49	0.43
1:D:2525:VAL:HG13	1:D:2528:LEU:HD12	1.99	0.43
1:D:4763:HIS:CE1	1:D:4870:ALA:HB1	2.53	0.43
1:D:758:CYS:SG	1:D:759:LEU:N	2.91	0.43
1:D:908:ARG:HA	1:D:916:PRO:HD3	2.00	0.43
1:A:143:LEU:CD2	1:B:2426:SER:HB3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1720:MET:HE2	1:A:2128:ARG:HD2	2.00	0.43
1:A:4763:HIS:CE1	1:A:4870:ALA:HB1	2.53	0.43
1:B:1664:VAL:HG12	1:B:1672:VAL:HG11	2.00	0.43
1:A:189:GLU:HB2	1:B:2419:ARG:HH22	1.84	0.43
1:B:908:ARG:HA	1:B:916:PRO:HD3	2.00	0.43
1:C:466:PRO:HB3	1:C:478:ARG:HG2	1.99	0.43
1:C:4178:VAL:HG11	1:C:4881:VAL:HA	1.99	0.43
1:A:2419:ARG:HH22	1:D:189:GLU:HB2	1.84	0.43
1:A:1092:LYS:H	1:A:1250:TRP:HZ3	1.66	0.43
1:A:1654:HIS:O	1:A:1657:THR:OG1	2.26	0.43
1:A:4036:TYR:HE2	1:A:4048:ASP:HB3	1.82	0.43
1:A:4523:VAL:HG22	1:D:4808:ASP:OD2	2.19	0.43
1:A:4514:ILE:HG21	1:A:4740:PHE:CE2	2.52	0.43
1:A:462:TYR:O	1:A:485:ARG:NH1	2.51	0.43
1:A:758:CYS:SG	1:A:759:LEU:N	2.91	0.43
1:B:170:SER:OG	1:B:171:GLU:N	2.49	0.43
1:B:189:GLU:HB2	1:C:2419:ARG:HH22	1.84	0.43
1:C:1090:ALA:HB3	1:C:1203:PRO:HD2	2.00	0.43
1:C:462:TYR:O	1:C:485:ARG:NH1	2.51	0.43
1:D:1136:ALA:HB3	1:D:1145:TRP:HB2	2.00	0.43
1:A:3737:ALA:O	1:A:3740:MET:HG2	2.17	0.43
1:A:237:LEU:N	1:A:404:ASN:O	2.49	0.43
1:A:4791:ARG:HD2	1:A:4808:ASP:HB2	2.00	0.43
1:A:4924:MET:O	1:A:4928:ASN:HB2	2.18	0.43
1:B:1449:ASP:N	1:B:1449:ASP:OD1	2.51	0.43
1:B:4763:HIS:CE1	1:B:4870:ALA:HB1	2.53	0.43
1:B:4809:ASP:O	1:B:4813:CYS:N	2.39	0.43
1:B:758:CYS:SG	1:B:759:LEU:N	2.91	0.43
1:B:745:ASN:ND2	1:B:773:GLN:OE1	2.48	0.43
1:C:4036:TYR:HE2	1:C:4048:ASP:HB3	1.82	0.43
1:D:1220:ASP:O	1:D:1223:THR:N	2.35	0.43
1:C:189:GLU:HB2	1:D:2419:ARG:HH22	1.84	0.43
1:A:1165:MET:HB2	1:A:1174:MET:HB2	2.01	0.43
1:A:2440:ALA:HB2	1:A:2466:LYS:HD2	2.01	0.43
1:A:335:LYS:NZ	1:A:398:HIS:O	2.44	0.43
1:A:4500:PHE:HA	1:A:4503:MET:HB2	2.00	0.43
1:A:4808:ASP:OD2	1:B:4523:VAL:HG22	2.19	0.43
1:B:1011:ARG:HB3	1:B:1032:LEU:HD21	2.00	0.43
1:B:1087:ILE:HG23	1:B:1128:LEU:HD12	2.00	0.43
1:C:1092:LYS:H	1:C:1250:TRP:HZ3	1.66	0.43
1:C:4739:PHE:HA	1:C:4739:PHE:HD1	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4844:ARG:HH12	1:C:4848:ASP:HB2	1.83	0.43
1:C:604:HIS:HA	1:C:1588:VAL:HB	2.01	0.43
1:C:691:THR:HB	1:C:796:ALA:HB2	2.01	0.43
1:C:832:LEU:O	1:C:1614:ARG:NH1	2.51	0.43
1:D:1719:LEU:HD21	1:D:1830:ILE:HD13	2.01	0.43
1:D:691:THR:HB	1:D:796:ALA:HB2	2.01	0.43
1:A:1011:ARG:HB3	1:A:1032:LEU:HD21	2.00	0.43
1:A:532:SER:HA	1:A:535:GLU:HB3	2.01	0.43
1:B:1136:ALA:HB3	1:B:1145:TRP:HB2	2.00	0.43
1:B:1790:LYS:O	1:B:1794:MET:N	2.44	0.43
1:B:3952:PHE:HB3	1:B:3976:GLN:HE22	1.82	0.43
1:B:4178:VAL:HG11	1:B:4881:VAL:HA	1.99	0.43
1:C:1719:LEU:HD21	1:C:1830:ILE:HD13	2.01	0.43
1:C:196:TYR:O	1:C:201:LEU:N	2.51	0.43
1:C:2832:VAL:O	1:C:2895:LYS:NZ	2.45	0.43
1:C:4610:LYS:O	1:C:4615:GLY:N	2.51	0.43
1:C:4791:ARG:HD2	1:C:4808:ASP:HB2	2.00	0.43
1:C:4845:ILE:O	1:C:4849:ILE:N	2.44	0.43
1:D:4725:TRP:O	1:D:4729:MET:HG2	2.19	0.43
1:A:1090:ALA:HB3	1:A:1203:PRO:HD2	2.00	0.43
1:A:1719:LEU:HD21	1:A:1830:ILE:HD13	2.01	0.43
1:B:1090:ALA:HB3	1:B:1203:PRO:HD2	2.00	0.43
1:C:1091:GLU:HB3	1:C:1094:TYR:HD2	1.84	0.43
1:C:1449:ASP:OD1	1:C:1449:ASP:N	2.51	0.43
1:C:1664:VAL:HG12	1:C:1672:VAL:HG11	2.00	0.43
1:C:1733:THR:HG22	1:C:1755:THR:HB	2.00	0.43
1:C:2102:ALA:O	1:C:2106:THR:N	2.47	0.43
1:C:4514:ILE:HG21	1:C:4740:PHE:CE2	2.52	0.43
1:C:4571:PRO:O	1:C:4575:ILE:N	2.49	0.43
1:C:745:ASN:ND2	1:C:773:GLN:OE1	2.48	0.43
1:D:1165:MET:HB2	1:D:1174:MET:HB2	2.01	0.43
1:D:4178:VAL:HG11	1:D:4881:VAL:HA	1.99	0.43
1:D:4791:ARG:HD2	1:D:4808:ASP:HB2	2.00	0.43
1:D:462:TYR:O	1:D:485:ARG:NH1	2.51	0.43
1:A:1170:GLU:O	1:A:1172:THR:N	2.50	0.43
1:A:1733:THR:HG22	1:A:1755:THR:HB	2.00	0.43
1:A:4725:TRP:O	1:A:4729:MET:HG2	2.19	0.43
1:A:629:GLN:OE1	1:A:1669:ASN:ND2	2.52	0.43
1:B:4808:ASP:OD2	1:C:4523:VAL:HG22	2.19	0.43
1:C:1119:ARG:NH2	1:C:1196:ASP:O	2.48	0.43
1:C:1799:VAL:O	1:C:1803:SER:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3800:SER:OG	1:C:3801:CYS:N	2.47	0.43
1:A:1087:ILE:HG23	1:A:1128:LEU:HD12	2.00	0.43
1:A:832:LEU:O	1:A:1614:ARG:NH1	2.51	0.43
1:A:4809:ASP:O	1:A:4813:CYS:N	2.39	0.43
1:B:1172:THR:HG22	1:B:1193:LYS:HG3	2.01	0.43
1:B:1719:LEU:HD21	1:B:1830:ILE:HD13	2.01	0.43
1:B:3767:LEU:O	1:B:3770:GLY:N	2.51	0.43
1:B:4791:ARG:HD2	1:B:4808:ASP:HB2	2.00	0.43
1:B:629:GLN:OE1	1:B:1669:ASN:ND2	2.52	0.43
1:C:1032:LEU:HD23	1:C:1032:LEU:HA	1.82	0.43
1:C:1790:LYS:O	1:C:1794:MET:N	2.44	0.43
1:C:2196:ASN:OD1	1:C:2199:ARG:NH1	2.52	0.43
1:C:411:GLU:HA	1:C:414:ARG:HB2	2.01	0.43
1:C:4924:MET:O	1:C:4928:ASN:HB2	2.18	0.43
1:D:1090:ALA:HB3	1:D:1203:PRO:HD2	2.00	0.43
1:D:1733:THR:HG22	1:D:1755:THR:HB	2.00	0.43
1:D:2196:ASN:OD1	1:D:2199:ARG:NH1	2.52	0.43
1:D:4130:PHE:O	1:D:4134:LEU:N	2.45	0.43
1:D:4500:PHE:HA	1:D:4503:MET:HB2	2.00	0.43
1:D:4514:ILE:HG21	1:D:4740:PHE:CE2	2.52	0.43
1:D:4867:ILE:HD12	1:D:4867:ILE:HG23	1.80	0.43
1:D:4924:MET:O	1:D:4928:ASN:HB2	2.18	0.43
1:A:691:THR:HB	1:A:796:ALA:HB2	2.01	0.42
1:B:832:LEU:O	1:B:1614:ARG:NH1	2.51	0.42
1:B:2102:ALA:O	1:B:2106:THR:N	2.47	0.42
1:B:258:ARG:HA	1:B:316:LEU:HB2	2.01	0.42
1:B:3919:ASN:O	1:B:3922:THR:OG1	2.35	0.42
1:B:565:LEU:HD11	1:B:603:LYS:HG2	2.01	0.42
1:C:258:ARG:HA	1:C:316:LEU:HB2	2.01	0.42
1:C:565:LEU:HD11	1:C:603:LYS:HG2	2.01	0.42
1:D:2834:LEU:HG	1:D:2895:LYS:HZ3	1.84	0.42
1:A:1156:TRP:HB2	1:A:1160:ASP:HB2	2.01	0.42
1:B:1091:GLU:HB3	1:B:1094:TYR:HD2	1.84	0.42
1:B:4514:ILE:HG21	1:B:4740:PHE:CE2	2.52	0.42
1:B:462:TYR:O	1:B:485:ARG:NH1	2.51	0.42
1:B:604:HIS:HA	1:B:1588:VAL:HB	2.01	0.42
1:B:703:TYR:CZ	1:B:722:LEU:HD21	2.54	0.42
1:C:1136:ALA:HB3	1:C:1145:TRP:HB2	2.00	0.42
1:C:4808:ASP:OD2	1:D:4523:VAL:HG22	2.19	0.42
1:C:908:ARG:HA	1:C:916:PRO:HD3	2.00	0.42
1:D:604:HIS:HA	1:D:1588:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:GLN:OE1	1:D:1669:ASN:ND2	2.52	0.42
1:A:1172:THR:HG22	1:A:1193:LYS:HG3	2.01	0.42
1:A:4161:TRP:CD1	1:A:4201:MET:HE1	2.53	0.42
1:B:1165:MET:HB2	1:B:1174:MET:HB2	2.01	0.42
1:B:1119:ARG:NH2	1:B:1196:ASP:O	2.48	0.42
1:B:694:ARG:N	1:B:793:SER:O	2.45	0.42
1:C:703:TYR:CZ	1:C:722:LEU:HD21	2.54	0.42
1:D:1449:ASP:N	1:D:1449:ASP:OD1	2.51	0.42
1:D:3696:MET:O	1:D:3699:SER:OG	2.26	0.42
1:D:4161:TRP:CD1	1:D:4201:MET:HE1	2.53	0.42
1:D:532:SER:HA	1:D:535:GLU:HB3	2.01	0.42
1:A:355:LYS:HE3	1:A:355:LYS:HB3	1.94	0.42
1:A:585:ALA:HA	1:A:588:ILE:HD12	2.02	0.42
1:B:1733:THR:HG22	1:B:1755:THR:HB	2.00	0.42
1:B:4166:VAL:O	1:B:4170:LYS:N	2.52	0.42
1:B:613:VAL:O	1:B:617:LEU:N	2.46	0.42
1:C:3759:THR:O	1:C:3763:GLY:N	2.51	0.42
1:C:4725:TRP:O	1:C:4729:MET:HG2	2.19	0.42
1:C:629:GLN:OE1	1:C:1669:ASN:ND2	2.52	0.42
1:D:1092:LYS:H	1:D:1250:TRP:HZ3	1.66	0.42
1:C:189:GLU:HG3	1:D:2419:ARG:NH2	2.35	0.42
1:D:585:ALA:HA	1:D:588:ILE:HD12	2.02	0.42
1:B:1570:LEU:O	1:B:1573:SER:OG	2.36	0.42
1:B:4924:MET:O	1:B:4928:ASN:HB2	2.18	0.42
1:C:243:GLU:OE2	1:C:389:ARG:NH1	2.53	0.42
1:C:4636:ILE:HG22	1:C:4671:LEU:HD22	2.02	0.42
1:C:565:LEU:HA	1:C:568:SER:HB2	2.02	0.42
1:D:1029:ASN:HA	1:D:1030:PRO:HD3	1.82	0.42
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.84	0.42
1:D:123:HIS:CD2	1:D:126:SER:H	2.34	0.42
1:D:832:LEU:O	1:D:1614:ARG:NH1	2.51	0.42
1:D:116:GLY:N	1:D:162:ILE:O	2.45	0.42
1:D:1682:GLU:HA	1:D:1685:LEU:HD13	2.02	0.42
1:A:2419:ARG:NH2	1:D:189:GLU:HG3	2.35	0.42
1:D:243:GLU:OE2	1:D:389:ARG:NH1	2.53	0.42
1:D:572:LEU:O	1:D:576:HIS:N	2.47	0.42
1:A:190:ARG:HG2	1:A:207:PHE:CE1	2.55	0.42
1:A:2196:ASN:OD1	1:A:2199:ARG:NH1	2.52	0.42
1:B:1170:GLU:O	1:B:1172:THR:N	2.50	0.42
1:B:4725:TRP:O	1:B:4729:MET:HG2	2.19	0.42
1:C:1692:LYS:HA	1:C:1810:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3921:LEU:HD23	1:C:3921:LEU:HA	1.84	0.42
1:D:852:GLY:HA3	1:D:1086:ARG:HG3	2.01	0.42
1:D:1799:VAL:O	1:D:1803:SER:N	2.46	0.42
1:D:2326:ILE:HD13	1:D:2326:ILE:HA	1.83	0.42
1:A:123:HIS:CD2	1:A:126:SER:H	2.34	0.42
1:A:1730:THR:O	1:A:1733:THR:OG1	2.31	0.42
1:A:565:LEU:HA	1:A:568:SER:HB2	2.02	0.42
1:B:2440:ALA:HB2	1:B:2466:LYS:HD2	2.01	0.42
1:B:2834:LEU:HG	1:B:2895:LYS:HZ3	1.84	0.42
1:B:532:SER:HA	1:B:535:GLU:HB3	2.01	0.42
1:B:691:THR:HB	1:B:796:ALA:HB2	2.01	0.42
1:C:2440:ALA:HB2	1:C:2466:LYS:HD2	2.01	0.42
1:C:3767:LEU:O	1:C:3770:GLY:N	2.51	0.42
1:C:3925:ILE:HD13	1:C:3925:ILE:HG21	1.70	0.42
1:C:585:ALA:HA	1:C:588:ILE:HD12	2.02	0.42
1:D:1172:THR:HG22	1:D:1193:LYS:HG3	2.01	0.42
1:D:2440:ALA:HB2	1:D:2466:LYS:HD2	2.01	0.42
1:D:3759:THR:O	1:D:3763:GLY:N	2.51	0.42
1:D:3797:LEU:HD13	1:D:3840:LEU:HD11	2.02	0.42
1:D:3914:ALA:HB3	1:D:3975:LEU:HD11	2.02	0.42
1:D:565:LEU:HA	1:D:568:SER:HB2	2.02	0.42
1:A:189:GLU:HG3	1:B:2419:ARG:NH2	2.35	0.42
1:A:258:ARG:HA	1:A:316:LEU:HB2	2.01	0.42
1:A:4636:ILE:HG22	1:A:4671:LEU:HD22	2.02	0.42
1:B:1091:GLU:HA	1:B:1250:TRP:CZ3	2.55	0.42
1:B:1692:LYS:HA	1:B:1810:VAL:HG13	2.02	0.42
1:B:2326:ILE:HA	1:B:2326:ILE:HD13	1.83	0.42
1:C:776:GLN:HG2	1:C:1472:GLU:HA	2.01	0.42
1:D:190:ARG:HG2	1:D:207:PHE:CE1	2.55	0.42
1:D:258:ARG:HA	1:D:316:LEU:HB2	2.01	0.42
1:D:4636:ILE:HG22	1:D:4671:LEU:HD22	2.02	0.42
1:A:1682:GLU:HA	1:A:1685:LEU:HD13	2.02	0.42
1:A:2102:ALA:O	1:A:2106:THR:N	2.47	0.42
1:A:4931:GLU:OE2	1:A:4942:TRP:NE1	2.53	0.42
1:A:604:HIS:HA	1:A:1588:VAL:HB	2.01	0.42
1:B:243:GLU:OE2	1:B:389:ARG:NH1	2.53	0.42
1:B:4621:GLN:HE22	1:B:4633:ARG:HH12	1.68	0.42
1:B:565:LEU:HA	1:B:568:SER:HB2	2.02	0.42
1:C:1172:THR:HG22	1:C:1193:LYS:HG3	2.01	0.42
1:C:1090:ALA:HA	1:C:1249:MET:HG2	2.02	0.42
1:C:3797:LEU:HD13	1:C:3840:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:GLU:HA	1:D:414:ARG:HB2	2.01	0.42
1:D:4515:ASN:HD22	1:D:4518:LEU:HB2	1.85	0.42
1:D:674:TYR:OH	1:D:676:GLU:OE2	2.27	0.42
1:D:852:GLY:HA2	1:D:853:PRO:HA	1.69	0.42
1:A:1091:GLU:HA	1:A:1250:TRP:CZ3	2.55	0.42
1:A:4621:GLN:HE22	1:A:4633:ARG:HH12	1.68	0.42
1:A:4739:PHE:HD1	1:A:4739:PHE:HA	1.76	0.42
1:A:565:LEU:HD11	1:A:603:LYS:HG2	2.01	0.42
1:A:852:GLY:HA3	1:A:1086:ARG:HG3	2.01	0.42
1:B:1682:GLU:HA	1:B:1685:LEU:HD13	2.02	0.42
1:B:2196:ASN:OD1	1:B:2199:ARG:NH1	2.52	0.42
1:B:2858:LYS:HG3	1:B:2872:LEU:HD22	2.02	0.42
1:B:4636:ILE:HG22	1:B:4671:LEU:HD22	2.02	0.42
1:B:614:LEU:HD23	1:B:617:LEU:HD12	2.01	0.42
1:C:1156:TRP:HB2	1:C:1160:ASP:HB2	2.01	0.42
1:C:1165:MET:HB2	1:C:1174:MET:HB2	2.01	0.42
1:C:3914:ALA:HB3	1:C:3975:LEU:HD11	2.02	0.42
1:C:3919:ASN:O	1:C:3922:THR:OG1	2.35	0.42
1:C:534:TYR:O	1:C:538:ALA:N	2.51	0.42
1:C:796:ALA:HB3	1:C:798:ILE:HG13	2.02	0.42
1:D:2421:ARG:HA	1:D:2424:LEU:HB2	2.01	0.42
1:D:796:ALA:HB3	1:D:798:ILE:HG13	2.02	0.42
1:A:1029:ASN:HA	1:A:1030:PRO:HD3	1.82	0.41
1:A:3743:GLN:NE2	1:A:3781:TYR:OH	2.43	0.41
1:B:190:ARG:HG2	1:B:207:PHE:CE1	2.55	0.41
1:B:712:GLU:OE2	1:B:1636:ASN:ND2	2.46	0.41
1:B:189:GLU:HG3	1:C:2419:ARG:NH2	2.35	0.41
1:B:4852:PHE:CG	1:C:4823:ARG:HG2	2.55	0.41
1:C:4931:GLU:OE2	1:C:4942:TRP:NE1	2.53	0.41
1:D:1156:TRP:HB2	1:D:1160:ASP:HB2	2.01	0.41
1:D:565:LEU:HD11	1:D:603:LYS:HG2	2.01	0.41
1:D:614:LEU:HD23	1:D:617:LEU:HD12	2.01	0.41
1:A:4515:ASN:HD22	1:A:4518:LEU:HB2	1.85	0.41
1:A:703:TYR:CZ	1:A:722:LEU:HD21	2.54	0.41
1:B:776:GLN:HG2	1:B:1472:GLU:HA	2.01	0.41
1:B:2421:ARG:HA	1:B:2424:LEU:HB2	2.01	0.41
1:B:3911:ILE:HD13	1:B:3911:ILE:HA	1.91	0.41
1:B:585:ALA:HA	1:B:588:ILE:HD12	2.02	0.41
1:C:1682:GLU:HA	1:C:1685:LEU:HD13	2.02	0.41
1:D:1090:ALA:HA	1:D:1249:MET:HG2	2.02	0.41
1:D:1146:HIS:HB2	1:D:1192:PHE:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1119:ARG:NH2	1:D:1196:ASP:O	2.48	0.41
1:D:182:ILE:HD12	1:D:209:GLN:HB3	2.02	0.41
1:D:4739:PHE:HD1	1:D:4739:PHE:HA	1.76	0.41
1:C:4852:PHE:CG	1:D:4823:ARG:HG2	2.55	0.41
1:D:703:TYR:CZ	1:D:722:LEU:HD21	2.54	0.41
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.84	0.41
1:A:243:GLU:OE2	1:A:389:ARG:NH1	2.53	0.41
1:A:411:GLU:HA	1:A:414:ARG:HB2	2.01	0.41
1:A:725:TYR:OH	1:A:775:VAL:HG11	2.21	0.41
1:B:833:LYS:HA	1:B:1614:ARG:HH12	1.86	0.41
1:C:1905:LEU:HD23	1:C:2081:LEU:HA	2.03	0.41
1:B:143:LEU:CD2	1:C:2426:SER:HB3	2.47	0.41
1:C:2858:LYS:HG3	1:C:2872:LEU:HD22	2.02	0.41
1:C:836:HIS:HB2	1:C:839:GLU:HG2	2.03	0.41
1:C:852:GLY:HA3	1:C:1086:ARG:HG3	2.01	0.41
1:D:1692:LYS:HA	1:D:1810:VAL:HG13	2.02	0.41
1:A:1146:HIS:HB2	1:A:1192:PHE:HE1	1.85	0.41
1:A:1256:PRO:HB3	1:A:1597:SER:HA	2.02	0.41
1:A:3914:ALA:HB3	1:A:3975:LEU:HD11	2.02	0.41
1:A:796:ALA:HB3	1:A:798:ILE:HG13	2.02	0.41
1:B:2160:PRO:HB3	1:B:2207:ILE:HD12	2.02	0.41
1:B:796:ALA:HB3	1:B:798:ILE:HG13	2.02	0.41
1:B:836:HIS:HB2	1:B:839:GLU:HG2	2.03	0.41
1:C:1256:PRO:HB3	1:C:1597:SER:HA	2.02	0.41
1:C:1934:VAL:O	1:C:1938:GLN:N	2.43	0.41
1:C:2884:ALA:HA	1:C:2887:ARG:HB3	2.03	0.41
1:C:3779:LEU:HD11	1:C:3783:LYS:HE2	2.03	0.41
1:C:532:SER:HA	1:C:535:GLU:HB3	2.01	0.41
1:D:244:CYS:SG	1:D:245:LEU:N	2.93	0.41
1:A:4823:ARG:HG2	1:D:4852:PHE:CG	2.55	0.41
1:A:1090:ALA:HA	1:A:1249:MET:HG2	2.02	0.41
1:A:833:LYS:HA	1:A:1614:ARG:HH12	1.86	0.41
1:A:2421:ARG:HA	1:A:2424:LEU:HB2	2.01	0.41
1:A:2858:LYS:HG3	1:A:2872:LEU:HD22	2.02	0.41
1:A:3800:SER:OG	1:A:3801:CYS:N	2.47	0.41
1:A:614:LEU:HD23	1:A:617:LEU:HD12	2.01	0.41
1:B:852:GLY:HA3	1:B:1086:ARG:HG3	2.01	0.41
1:B:1137:PHE:HD1	1:B:1144:ARG:HB3	1.86	0.41
1:B:1090:ALA:HA	1:B:1249:MET:HG2	2.02	0.41
1:B:1905:LEU:HD23	1:B:2081:LEU:HA	2.03	0.41
1:B:2127:ILE:HD12	1:B:2127:ILE:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2541:HIS:O	1:B:2545:LEU:N	2.49	0.41
1:C:244:CYS:SG	1:C:245:LEU:N	2.93	0.41
1:C:4161:TRP:CD1	1:C:4201:MET:HE1	2.53	0.41
1:C:653:SER:OG	1:C:794:PHE:O	2.31	0.41
1:D:3743:GLN:NE2	1:D:3781:TYR:OH	2.43	0.41
1:D:725:TYR:OH	1:D:775:VAL:HG11	2.21	0.41
1:D:833:LYS:HA	1:D:1614:ARG:HH12	1.86	0.41
1:A:1905:LEU:HD23	1:A:2081:LEU:HA	2.03	0.41
1:A:2732:LYS:HA	1:A:2732:LYS:HD2	1.82	0.41
1:A:3925:ILE:HG21	1:A:3925:ILE:HD13	1.70	0.41
1:A:4045:SER:HA	1:A:4078:THR:HG22	2.03	0.41
1:B:1156:TRP:HB2	1:B:1160:ASP:HB2	2.01	0.41
1:B:2884:ALA:HA	1:B:2887:ARG:HB3	2.03	0.41
1:C:182:ILE:HD12	1:C:209:GLN:HB3	2.02	0.41
1:C:3743:GLN:O	1:C:3746:SER:OG	2.32	0.41
1:D:1091:GLU:HA	1:D:1250:TRP:CZ3	2.55	0.41
1:D:288:HIS:ND1	1:D:349:MET:O	2.43	0.41
1:D:4621:GLN:HE22	1:D:4633:ARG:HH12	1.68	0.41
1:A:1137:PHE:HD1	1:A:1144:ARG:HB3	1.86	0.41
1:A:1692:LYS:HA	1:A:1810:VAL:HG13	2.02	0.41
1:A:2154:LYS:HA	1:A:2154:LYS:HD3	1.90	0.41
1:A:244:CYS:SG	1:A:245:LEU:N	2.93	0.41
1:A:3797:LEU:HD13	1:A:3840:LEU:HD11	2.02	0.41
1:B:3921:LEU:HA	1:B:3921:LEU:HD23	1.84	0.41
1:C:1132:GLU:HG2	1:C:1133:ARG:HG3	2.03	0.41
1:C:1170:GLU:O	1:C:1172:THR:N	2.50	0.41
1:C:2463:PRO:HD3	1:C:2516:ALA:HB2	2.02	0.41
1:C:614:LEU:HD23	1:C:617:LEU:HD12	2.01	0.41
1:D:3779:LEU:HD11	1:D:3783:LYS:HE2	2.03	0.41
1:D:3996:ILE:H	1:D:3996:ILE:HG22	1.64	0.41
1:D:534:TYR:CZ	1:D:571:ILE:HG13	2.56	0.41
1:D:613:VAL:O	1:D:617:LEU:N	2.46	0.41
1:A:182:ILE:HD12	1:A:209:GLN:HB3	2.02	0.41
1:A:534:TYR:CZ	1:A:571:ILE:HG13	2.56	0.41
1:A:650:ASN:HA	1:A:1626:GLN:HA	2.03	0.41
1:A:836:HIS:HB2	1:A:839:GLU:HG2	2.03	0.41
1:A:935:MET:O	1:A:939:THR:OG1	2.36	0.41
1:B:3914:ALA:HB3	1:B:3975:LEU:HD11	2.02	0.41
1:A:4852:PHE:CG	1:B:4823:ARG:HG2	2.55	0.41
1:B:534:TYR:CZ	1:B:571:ILE:HG13	2.56	0.41
1:C:1029:ASN:HA	1:C:1030:PRO:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1137:PHE:HD1	1:C:1144:ARG:HB3	1.86	0.41
1:C:2421:ARG:HA	1:C:2424:LEU:HB2	2.01	0.41
1:C:299:HIS:N	1:C:304:LYS:O	2.54	0.41
1:C:4872:GLY:C	1:D:4875:ARG:CZ	2.89	0.41
1:C:4894:ILE:HD12	1:C:4961:LYS:HE3	2.03	0.41
1:D:1256:PRO:HB3	1:D:1597:SER:HA	2.02	0.41
1:D:776:GLN:HG2	1:D:1472:GLU:HA	2.01	0.41
1:D:4045:SER:HA	1:D:4078:THR:HG22	2.03	0.41
1:D:836:HIS:HB2	1:D:839:GLU:HG2	2.03	0.41
1:A:881:ILE:HG21	1:A:1062:TYR:CZ	2.56	0.41
1:A:551:PHE:HA	1:A:551:PHE:HD1	1.74	0.41
1:A:776:GLN:HG2	1:A:1472:GLU:HA	2.01	0.41
1:B:1146:HIS:HB2	1:B:1192:PHE:HE1	1.85	0.41
1:B:1699:ARG:HH22	1:B:1821:LEU:HD11	1.86	0.41
1:B:182:ILE:HD12	1:B:209:GLN:HB3	2.02	0.41
1:B:3779:LEU:HD11	1:B:3783:LYS:HE2	2.03	0.41
1:B:4022:LEU:HD23	1:B:4022:LEU:HA	1.85	0.41
1:B:4872:GLY:C	1:C:4875:ARG:CZ	2.89	0.41
1:C:1091:GLU:HA	1:C:1250:TRP:CZ3	2.55	0.41
1:C:706:TYR:CD1	1:C:1253:LYS:HD2	2.56	0.41
1:C:190:ARG:HG2	1:C:207:PHE:CE1	2.55	0.41
1:C:4621:GLN:HE22	1:C:4633:ARG:HH12	1.68	0.41
1:C:534:TYR:CZ	1:C:571:ILE:HG13	2.56	0.41
1:D:1652:LYS:HB3	1:D:1652:LYS:HE2	1.90	0.41
1:D:1716:THR:HA	1:D:1719:LEU:HD12	2.03	0.41
1:D:1905:LEU:HD23	1:D:2081:LEU:HA	2.03	0.41
1:D:650:ASN:HA	1:D:1626:GLN:HA	2.03	0.41
1:A:2160:PRO:HB3	1:A:2207:ILE:HD12	2.02	0.41
1:B:1132:GLU:HG2	1:B:1133:ARG:HG3	2.03	0.41
1:B:244:CYS:SG	1:B:245:LEU:N	2.93	0.41
1:B:2829:MET:HE1	1:B:2896:PHE:HB2	2.03	0.41
1:B:411:GLU:HA	1:B:414:ARG:HB2	2.01	0.41
1:B:4161:TRP:CD1	1:B:4201:MET:HE1	2.53	0.41
1:B:725:TYR:OH	1:B:775:VAL:HG11	2.21	0.41
1:C:650:ASN:HA	1:C:1626:GLN:HA	2.03	0.41
1:C:3911:ILE:HA	1:C:3911:ILE:HD13	1.91	0.41
1:C:4515:ASN:HD22	1:C:4518:LEU:HB2	1.85	0.41
1:D:881:ILE:HG21	1:D:1062:TYR:CZ	2.56	0.41
1:D:1132:GLU:HG2	1:D:1133:ARG:HG3	2.03	0.41
1:D:2160:PRO:HB3	1:D:2207:ILE:HD12	2.02	0.41
1:D:4853:PHE:HA	1:D:4857:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ALA:HA	1:A:161:THR:HA	2.03	0.41
1:A:1255:LEU:HA	1:A:1256:PRO:HD3	1.92	0.41
1:A:1716:THR:HA	1:A:1719:LEU:HD12	2.03	0.41
1:A:2463:PRO:HD3	1:A:2516:ALA:HB2	2.02	0.41
1:A:4823:ARG:HA	1:D:4852:PHE:CE1	2.53	0.41
1:A:681:HIS:HA	1:A:751:THR:HG22	2.03	0.41
1:A:852:GLY:HA2	1:A:853:PRO:HA	1.69	0.41
1:B:1505:LEU:H	1:B:1523:ASN:HA	1.86	0.41
1:B:2463:PRO:HD3	1:B:2516:ALA:HB2	2.02	0.41
1:C:1177:LEU:HA	1:C:1177:LEU:HD12	1.92	0.41
1:C:833:LYS:HA	1:C:1614:ARG:HH12	1.86	0.41
1:C:217:ILE:HG23	1:C:285:SER:HB3	2.03	0.41
1:C:3808:ALA:HA	1:C:3811:ARG:HD2	2.03	0.41
1:C:4045:SER:HA	1:C:4078:THR:HG22	2.03	0.41
1:C:506:HIS:HB2	1:C:561:ARG:NH1	2.36	0.41
1:C:64:ILE:HG12	1:C:417:ARG:HH21	1.86	0.41
1:D:2884:ALA:HA	1:D:2887:ARG:HB3	2.03	0.41
1:A:1132:GLU:HG2	1:A:1133:ARG:HG3	2.03	0.40
1:A:1783:PRO:HB3	1:A:1786:ILE:HD12	2.02	0.40
1:B:3797:LEU:HD13	1:B:3840:LEU:HD11	2.02	0.40
1:B:4045:SER:HA	1:B:4078:THR:HG22	2.03	0.40
1:B:4515:ASN:HD22	1:B:4518:LEU:HB2	1.85	0.40
1:B:534:TYR:O	1:B:538:ALA:N	2.51	0.40
1:B:681:HIS:HA	1:B:751:THR:HG22	2.03	0.40
1:C:3642:ILE:HD12	1:C:3642:ILE:HG23	1.91	0.40
1:D:1137:PHE:HD1	1:D:1144:ARG:HB3	1.86	0.40
1:D:217:ILE:HG23	1:D:285:SER:HB3	2.03	0.40
1:D:2858:LYS:HG3	1:D:2872:LEU:HD22	2.02	0.40
1:D:4640:SER:HB3	1:D:4643:ASN:ND2	2.37	0.40
1:A:4875:ARG:CZ	1:D:4872:GLY:C	2.89	0.40
1:D:4931:GLU:OE2	1:D:4942:TRP:NE1	2.53	0.40
1:A:1699:ARG:HH22	1:A:1821:LEU:HD11	1.86	0.40
1:A:2270:LEU:HD21	1:A:2299:TYR:HB2	2.04	0.40
1:A:4166:VAL:O	1:A:4170:LYS:N	2.52	0.40
1:A:731:HIS:HE1	1:A:738:ALA:HB1	1.87	0.40
1:B:1032:LEU:HD23	1:B:1032:LEU:HA	1.82	0.40
1:B:706:TYR:CD1	1:B:1253:LYS:HD2	2.56	0.40
1:B:3808:ALA:HA	1:B:3811:ARG:HD2	2.03	0.40
1:B:4591:TYR:CE1	1:B:4595:LYS:HB2	2.57	0.40
1:B:4722:TYR:OH	1:B:4745:LEU:O	2.40	0.40
1:B:4770:LEU:HA	1:B:4770:LEU:HD23	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4853:PHE:HA	1:B:4857:VAL:HB	2.03	0.40
1:B:64:ILE:H	1:B:64:ILE:HG13	1.79	0.40
1:A:116:GLY:N	1:A:162:ILE:O	2.45	0.40
1:A:2069:ARG:HD3	1:A:2069:ARG:HA	1.92	0.40
1:A:3779:LEU:HD11	1:A:3783:LYS:HE2	2.03	0.40
1:A:534:TYR:O	1:A:538:ALA:N	2.51	0.40
1:B:2270:LEU:HD21	1:B:2299:TYR:HB2	2.04	0.40
1:B:217:ILE:HG23	1:B:285:SER:HB3	2.03	0.40
1:B:415:THR:O	1:B:419:ILE:HG13	2.22	0.40
1:B:4873:GLU:HA	1:C:4875:ARG:HH11	1.68	0.40
1:C:3777:LYS:HE3	1:C:3777:LYS:HB2	1.94	0.40
1:C:4640:SER:HB3	1:C:4643:ASN:ND2	2.37	0.40
1:C:725:TYR:OH	1:C:775:VAL:HG11	2.21	0.40
1:C:681:HIS:HA	1:C:751:THR:HG22	2.03	0.40
1:D:2775:PRO:HB2	1:D:2889:LYS:NZ	2.36	0.40
1:D:506:HIS:HB2	1:D:561:ARG:NH1	2.36	0.40
1:A:2834:LEU:HG	1:A:2895:LYS:HZ3	1.87	0.40
1:A:628:ASN:O	1:A:632:ILE:HG12	2.22	0.40
1:B:1256:PRO:HB3	1:B:1597:SER:HA	2.02	0.40
1:B:1716:THR:HA	1:B:1719:LEU:HD12	2.03	0.40
1:B:1729:MET:HG2	1:B:2110:ASN:HA	2.03	0.40
1:B:2775:PRO:HB2	1:B:2889:LYS:NZ	2.36	0.40
1:B:3747:ALA:O	1:B:3749:LYS:HD2	2.22	0.40
1:A:4852:PHE:CE1	1:B:4823:ARG:HA	2.53	0.40
1:B:551:PHE:HD1	1:B:551:PHE:HA	1.74	0.40
1:B:650:ASN:HA	1:B:1626:GLN:HA	2.03	0.40
1:C:881:ILE:HG21	1:C:1062:TYR:CZ	2.56	0.40
1:C:1146:HIS:HB2	1:C:1192:PHE:HE1	1.85	0.40
1:C:1783:PRO:HB3	1:C:1786:ILE:HD12	2.02	0.40
1:C:2270:LEU:HD21	1:C:2299:TYR:HB2	2.04	0.40
1:C:3886:ILE:HG23	1:C:3886:ILE:HD12	1.92	0.40
1:D:706:TYR:CD1	1:D:1253:LYS:HD2	2.56	0.40
1:D:3756:VAL:O	1:D:3759:THR:OG1	2.31	0.40
1:D:628:ASN:O	1:D:632:ILE:HG12	2.22	0.40
1:D:731:HIS:HE1	1:D:738:ALA:HB1	1.87	0.40
1:D:694:ARG:N	1:D:793:SER:O	2.45	0.40
1:A:3747:ALA:O	1:A:3749:LYS:HD2	2.22	0.40
1:A:3808:ALA:HA	1:A:3811:ARG:HD2	2.03	0.40
1:A:3919:ASN:O	1:A:3922:THR:OG1	2.35	0.40
1:A:3921:LEU:HD23	1:A:3921:LEU:HA	1.84	0.40
1:A:3988:GLU:HB2	1:A:4937:GLN:NE2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4640:SER:HB3	1:A:4643:ASN:ND2	2.37	0.40
1:A:4804:ASP:N	1:A:4804:ASP:OD1	2.54	0.40
1:A:506:HIS:HB2	1:A:561:ARG:NH1	2.36	0.40
1:B:116:GLY:N	1:B:162:ILE:O	2.45	0.40
1:B:2788:TRP:HH2	1:B:2844:MET:HB2	1.87	0.40
1:B:3993:ASN:HD22	1:B:4110:MET:HG3	1.87	0.40
1:B:628:ASN:O	1:B:632:ILE:HG12	2.22	0.40
1:B:64:ILE:HG12	1:B:417:ARG:HH21	1.86	0.40
1:B:894:VAL:HG11	1:B:976:TYR:HD2	1.87	0.40
1:C:1255:LEU:HA	1:C:1256:PRO:HD3	1.92	0.40
1:C:118:ALA:HA	1:C:161:THR:HA	2.03	0.40
1:C:49:LEU:HD21	1:C:203:VAL:HG23	2.04	0.40
1:C:2160:PRO:HB3	1:C:2207:ILE:HD12	2.02	0.40
1:B:189:GLU:CD	1:C:2419:ARG:CZ	2.90	0.40
1:C:3993:ASN:HD22	1:C:4110:MET:HG3	1.87	0.40
1:C:4722:TYR:OH	1:C:4745:LEU:O	2.40	0.40
1:C:894:VAL:HG11	1:C:976:TYR:HD2	1.87	0.40
1:D:1783:PRO:HB3	1:D:1786:ILE:HD12	2.02	0.40
1:D:3808:ALA:HA	1:D:3811:ARG:HD2	2.03	0.40
1:D:4894:ILE:HD12	1:D:4961:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
1	B	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
1	C	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
1	D	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
All	All	13156/19872 (66%)	11932 (91%)	1140 (9%)	84 (1%)	34	74

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4071	ALA
1	B	4071	ALA
1	C	4071	ALA
1	D	4071	ALA
1	A	730	LEU
1	A	1580	PRO
1	A	3802	SER
1	A	4164	PRO
1	A	4916	LEU
1	B	730	LEU
1	B	1580	PRO
1	B	3802	SER
1	B	4164	PRO
1	B	4916	LEU
1	C	730	LEU
1	C	1580	PRO
1	C	3802	SER
1	C	4164	PRO
1	C	4916	LEU
1	D	730	LEU
1	D	1580	PRO
1	D	3802	SER
1	D	4164	PRO
1	D	4916	LEU
1	A	1581	GLN
1	A	1809	PRO
1	A	2075	VAL
1	A	3805	ASP
1	A	4030	SER
1	A	4646	TRP
1	B	1581	GLN
1	B	1809	PRO
1	B	2075	VAL
1	B	3805	ASP
1	B	4030	SER
1	B	4646	TRP
1	C	1581	GLN
1	C	1809	PRO
1	C	2075	VAL
1	C	3805	ASP
1	C	4030	SER
1	C	4646	TRP

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Mol	Chain	Res	Type
1	D	1581	GLN
1	D	1809	PRO
1	D	2075	VAL
1	D	3805	ASP
1	D	4030	SER
1	D	4646	TRP
1	A	819	TYR
1	A	980	PRO
1	A	3804	LEU
1	B	819	TYR
1	B	980	PRO
1	B	3804	LEU
1	C	819	TYR
1	C	980	PRO
1	C	3804	LEU
1	D	819	TYR
1	D	980	PRO
1	D	3804	LEU
1	A	792	VAL
1	B	792	VAL
1	C	792	VAL
1	D	792	VAL
1	A	853	PRO
1	A	1848	PRO
1	B	853	PRO
1	B	1848	PRO
1	C	853	PRO
1	C	1848	PRO
1	D	853	PRO
1	D	1848	PRO
1	A	1476	VAL
1	A	2329	PRO
1	A	4163	LYS
1	B	1476	VAL
1	B	2329	PRO
1	B	4163	LYS
1	C	1476	VAL
1	C	2329	PRO
1	C	4163	LYS
1	D	1476	VAL
1	D	2329	PRO
1	D	4163	LYS

### 5.3.2 Protein sidechains ⓘ

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	2659/4355 (61%)	2628 (99%)	31 (1%)	78	90
1	B	2658/4355 (61%)	2627 (99%)	31 (1%)	78	90
1	C	2659/4355 (61%)	2627 (99%)	32 (1%)	78	90
1	D	2660/4355 (61%)	2628 (99%)	32 (1%)	78	90
All	All	10636/17420 (61%)	10510 (99%)	126 (1%)	79	90

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	84	ASN
1	A	298	ARG
1	A	420	ARG
1	A	439	LYS
1	A	527	LYS
1	A	531	ASN
1	A	628	ASN
1	A	658	ASN
1	A	841	LYS
1	A	854	THR
1	A	925	PRO
1	A	990	PRO
1	A	1054	VAL
1	A	1089	ARG
1	A	1761	MET
1	A	2211	ASN
1	A	3722	LYS
1	A	3813	ASN
1	A	3906	ASN
1	A	4131	GLN
1	A	4136	ARG
1	A	4170	LYS
1	A	4171	ARG

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Mol	Chain	Res	Type
1	A	4179	ASN
1	A	4499	ASN
1	A	4515	ASN
1	A	4652	ARG
1	A	4781	LEU
1	A	4875	ARG
1	A	4879	GLU
1	B	44	ASN
1	B	84	ASN
1	B	298	ARG
1	B	420	ARG
1	B	439	LYS
1	B	527	LYS
1	B	531	ASN
1	B	628	ASN
1	B	658	ASN
1	B	841	LYS
1	B	854	THR
1	B	925	PRO
1	B	990	PRO
1	B	1054	VAL
1	B	1089	ARG
1	B	1761	MET
1	B	2211	ASN
1	B	3722	LYS
1	B	3813	ASN
1	B	3906	ASN
1	B	4131	GLN
1	B	4136	ARG
1	B	4170	LYS
1	B	4171	ARG
1	B	4179	ASN
1	B	4499	ASN
1	B	4515	ASN
1	B	4652	ARG
1	B	4781	LEU
1	B	4875	ARG
1	B	4879	GLU
1	C	44	ASN
1	C	84	ASN
1	C	298	ARG
1	C	420	ARG

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Mol	Chain	Res	Type
1	C	439	LYS
1	C	527	LYS
1	C	531	ASN
1	C	628	ASN
1	C	658	ASN
1	C	841	LYS
1	C	854	THR
1	C	925	PRO
1	C	950	VAL
1	C	990	PRO
1	C	1054	VAL
1	C	1089	ARG
1	C	1761	MET
1	C	2211	ASN
1	C	3722	LYS
1	C	3813	ASN
1	C	3906	ASN
1	C	4131	GLN
1	C	4136	ARG
1	C	4170	LYS
1	C	4171	ARG
1	C	4179	ASN
1	C	4499	ASN
1	C	4515	ASN
1	C	4652	ARG
1	C	4781	LEU
1	C	4875	ARG
1	C	4879	GLU
1	D	44	ASN
1	D	84	ASN
1	D	298	ARG
1	D	420	ARG
1	D	439	LYS
1	D	527	LYS
1	D	531	ASN
1	D	628	ASN
1	D	658	ASN
1	D	841	LYS
1	D	854	THR
1	D	925	PRO
1	D	950	VAL
1	D	990	PRO

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Mol	Chain	Res	Type
1	D	1054	VAL
1	D	1089	ARG
1	D	1761	MET
1	D	2211	ASN
1	D	3722	LYS
1	D	3813	ASN
1	D	3906	ASN
1	D	4131	GLN
1	D	4136	ARG
1	D	4170	LYS
1	D	4171	ARG
1	D	4179	ASN
1	D	4499	ASN
1	D	4515	ASN
1	D	4652	ARG
1	D	4781	LEU
1	D	4875	ARG
1	D	4879	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	84	ASN
1	A	123	HIS
1	A	293	GLN
1	A	364	GLN
1	A	375	GLN
1	A	476	GLN
1	A	531	ASN
1	A	593	HIS
1	A	604	HIS
1	A	628	ASN
1	A	1267	HIS
1	A	1294	ASN
1	A	1602	GLN
1	A	1631	HIS
1	A	1684	GLN
1	A	1722	ASN
1	A	1835	HIS
1	A	2090	HIS
1	A	2212	GLN

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Mol	Chain	Res	Type
1	A	2225	ASN
1	A	2251	ASN
1	A	2310	ASN
1	A	3856	GLN
1	A	3906	ASN
1	A	3916	GLN
1	A	3926	GLN
1	A	3950	HIS
1	A	3956	GLN
1	A	3961	GLN
1	A	3976	GLN
1	A	3993	ASN
1	A	4179	ASN
1	A	4499	ASN
1	A	4515	ASN
1	A	4621	GLN
1	A	4914	HIS
1	A	4962	GLN
1	B	23	GLN
1	B	44	ASN
1	B	84	ASN
1	B	123	HIS
1	B	293	GLN
1	B	364	GLN
1	B	375	GLN
1	B	476	GLN
1	B	531	ASN
1	B	593	HIS
1	B	604	HIS
1	B	628	ASN
1	B	1267	HIS
1	B	1294	ASN
1	B	1440	ASN
1	B	1602	GLN
1	B	1631	HIS
1	B	1684	GLN
1	B	1722	ASN
1	B	1835	HIS
1	B	2090	HIS
1	B	2212	GLN
1	B	2225	ASN
1	B	2251	ASN

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Mol	Chain	Res	Type
1	B	2310	ASN
1	B	2730	HIS
1	B	3856	GLN
1	B	3906	ASN
1	B	3916	GLN
1	B	3926	GLN
1	B	3956	GLN
1	B	3961	GLN
1	B	3976	GLN
1	B	3993	ASN
1	B	4179	ASN
1	B	4499	ASN
1	B	4515	ASN
1	B	4621	GLN
1	B	4914	HIS
1	B	4962	GLN
1	C	23	GLN
1	C	44	ASN
1	C	84	ASN
1	C	123	HIS
1	C	293	GLN
1	C	364	GLN
1	C	375	GLN
1	C	476	GLN
1	C	531	ASN
1	C	593	HIS
1	C	604	HIS
1	C	628	ASN
1	C	1267	HIS
1	C	1294	ASN
1	C	1440	ASN
1	C	1602	GLN
1	C	1631	HIS
1	C	1684	GLN
1	C	1691	ASN
1	C	1722	ASN
1	C	1835	HIS
1	C	2090	HIS
1	C	2212	GLN
1	C	2225	ASN
1	C	2251	ASN
1	C	2310	ASN

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Mol	Chain	Res	Type
1	C	2730	HIS
1	C	3856	GLN
1	C	3906	ASN
1	C	3916	GLN
1	C	3926	GLN
1	C	3956	GLN
1	C	3961	GLN
1	C	3976	GLN
1	C	3993	ASN
1	C	4179	ASN
1	C	4499	ASN
1	C	4515	ASN
1	C	4621	GLN
1	C	4914	HIS
1	C	4962	GLN
1	D	44	ASN
1	D	84	ASN
1	D	123	HIS
1	D	293	GLN
1	D	364	GLN
1	D	375	GLN
1	D	476	GLN
1	D	531	ASN
1	D	593	HIS
1	D	604	HIS
1	D	628	ASN
1	D	1267	HIS
1	D	1294	ASN
1	D	1602	GLN
1	D	1631	HIS
1	D	1684	GLN
1	D	1722	ASN
1	D	1835	HIS
1	D	2090	HIS
1	D	2212	GLN
1	D	2225	ASN
1	D	2251	ASN
1	D	2730	HIS
1	D	3856	GLN
1	D	3906	ASN
1	D	3916	GLN
1	D	3926	GLN

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Mol	Chain	Res	Type
1	D	3956	GLN
1	D	3961	GLN
1	D	3976	GLN
1	D	3993	ASN
1	D	4179	ASN
1	D	4499	ASN
1	D	4515	ASN
1	D	4621	GLN
1	D	4914	HIS
1	D	4962	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.