



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:22 am BST

PDB ID : 1TWC  
Title : RNA polymerase II complexed with GTP  
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.  
Deposited on : 2004-06-30  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

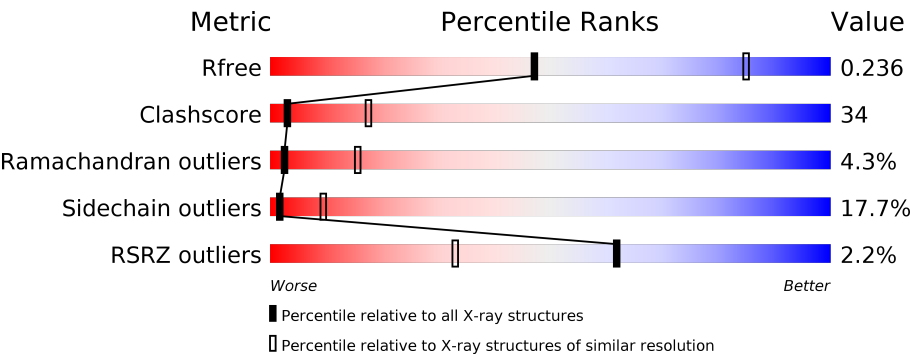
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	<div><div></div><div><div></div><div>21%</div><div>32%</div><div>19%</div><div>6%</div><div>22%</div></div></div>
2	B	1224	<div><div>3%</div><div><div></div><div>22%</div><div>39%</div><div>21%</div><div>7%</div><div>11%</div></div></div>
3	C	318	<div><div></div><div><div></div><div>18%</div><div>36%</div><div>22%</div><div>7%</div><div>16%</div></div></div>
4	E	215	<div><div>2%</div><div><div></div><div>20%</div><div>39%</div><div>31%</div><div>11%</div></div></div>
5	F	155	<div><div></div><div><div></div><div>13%</div><div>22%</div><div>15%</div><div>46%</div></div></div>
6	H	146	<div><div>3%</div><div><div></div><div>8%</div><div>31%</div><div>29%</div><div>23%</div><div>9%</div></div></div>

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Mol	Chain	Length	Quality of chain
7	I	122	
8	J	70	
9	K	120	
10	L	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	GTP	B	3008	X	-	-	-

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 27772 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1351	Total	C	N	O	S	0	0	0
			10625	6704	1844	2019	58			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1091	Total	C	N	O	S	0	0	0
			8690	5511	1516	1610	53			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1760	1116	310	322	12			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	83	Total	C	N	O	S	0	0	0
			670	428	114	125	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	121	Total	C	N	O	S	0	0	0
			990	610	181	188	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	64	Total	C	N	O	S	0	0	0
			525	334	92	93	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	J	1	Total	Zn	0	0
			1	1		
11	B	1	Total	Zn	0	0
			1	1		
11	I	2	Total	Zn	0	0
			2	2		
11	C	1	Total	Zn	0	0
			1	1		
11	A	2	Total	Zn	0	0
			2	2		

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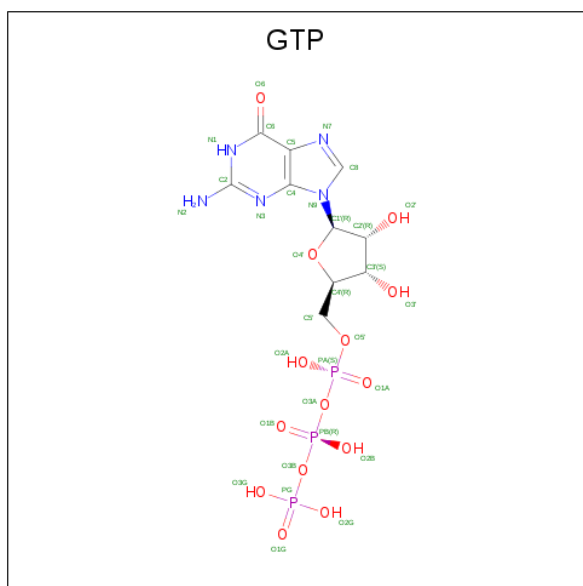
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	1	Total	Zn	0	0
			1	1		

- Molecule 12 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	Mn	0	0
			2	2		

- Molecule 13 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	11	Total	O	0	0
			11	11		
14	B	11	Total	O	0	0
			11	11		
14	F	1	Total	O	0	0
			1	1		

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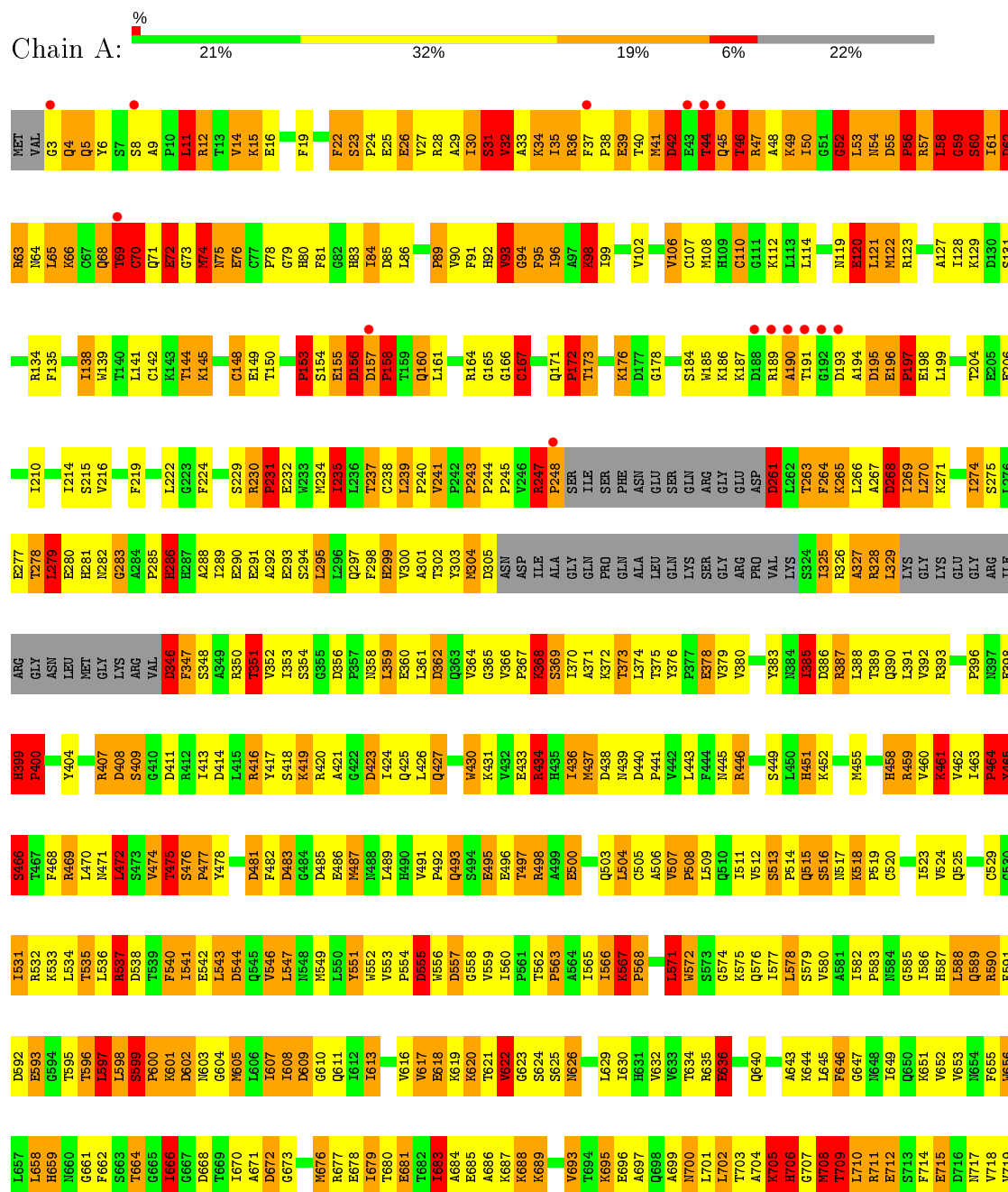
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	L	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

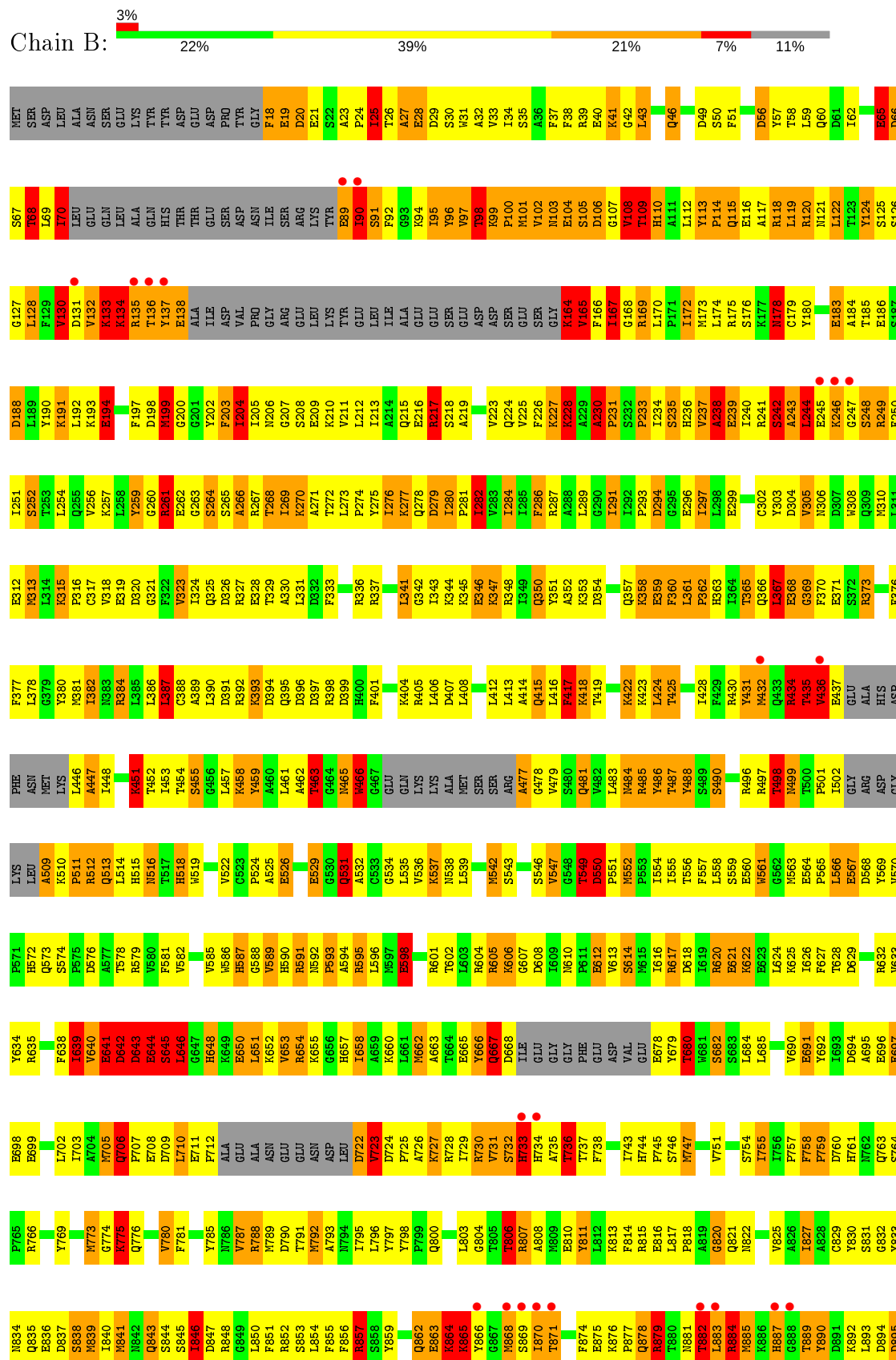
- Molecule 1: DNA-directed RNA polymerase II largest subunit

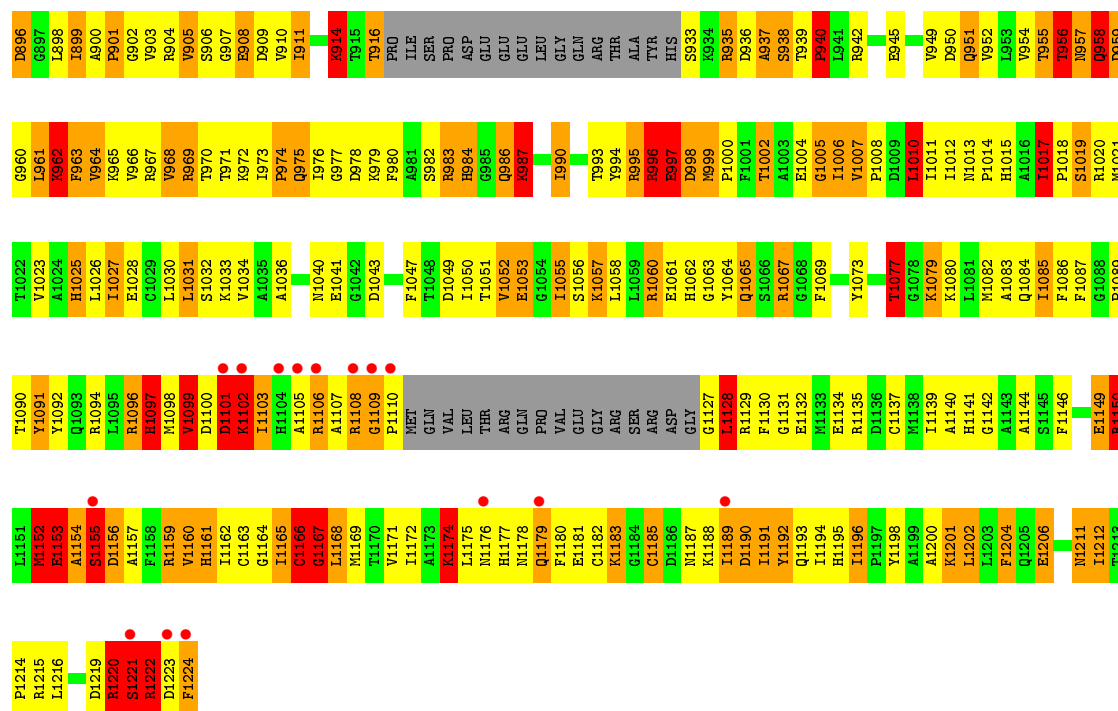




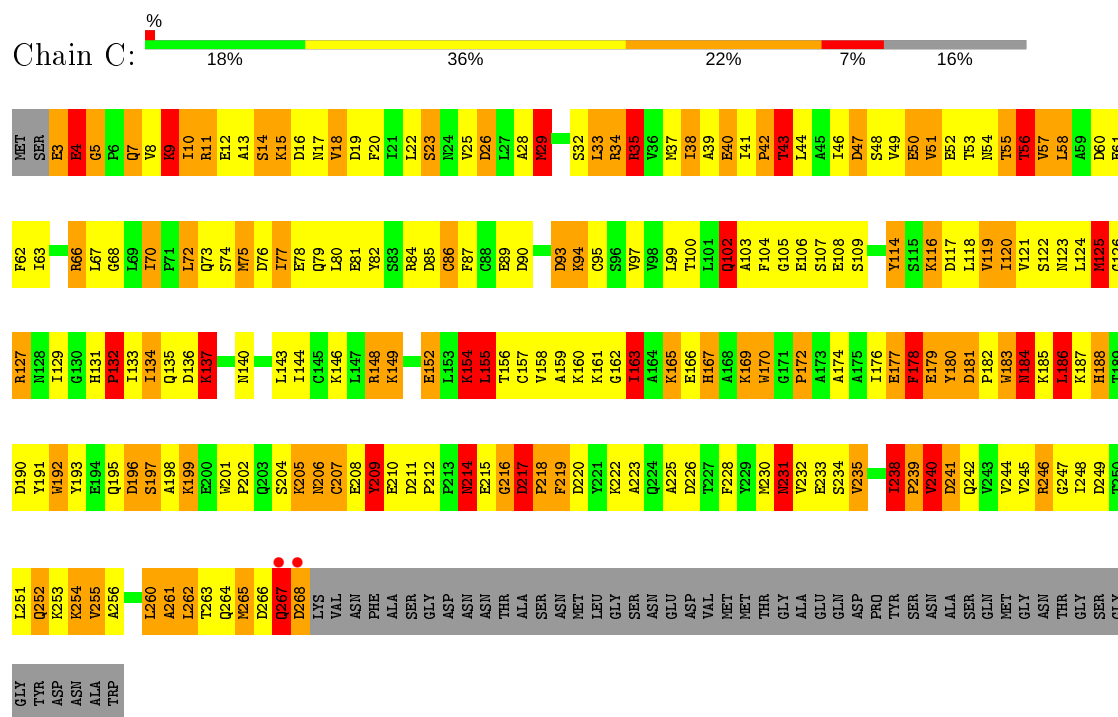


- Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

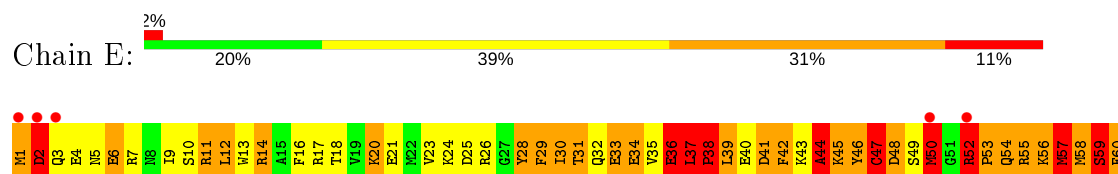




• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

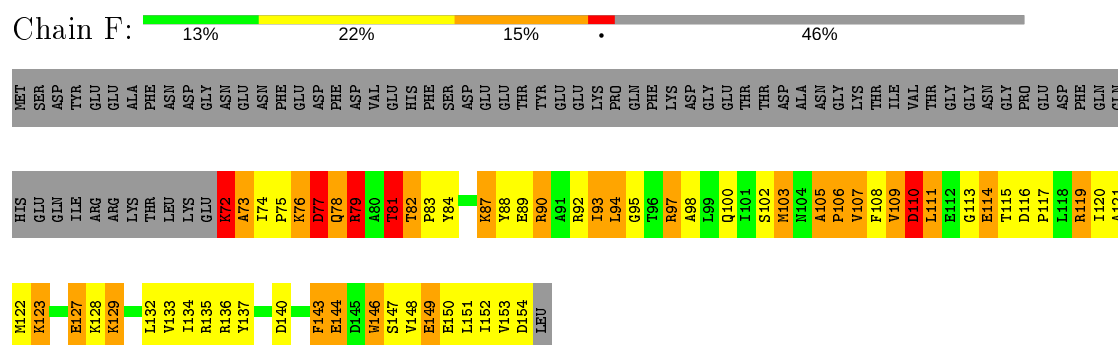


• Molecule 4: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

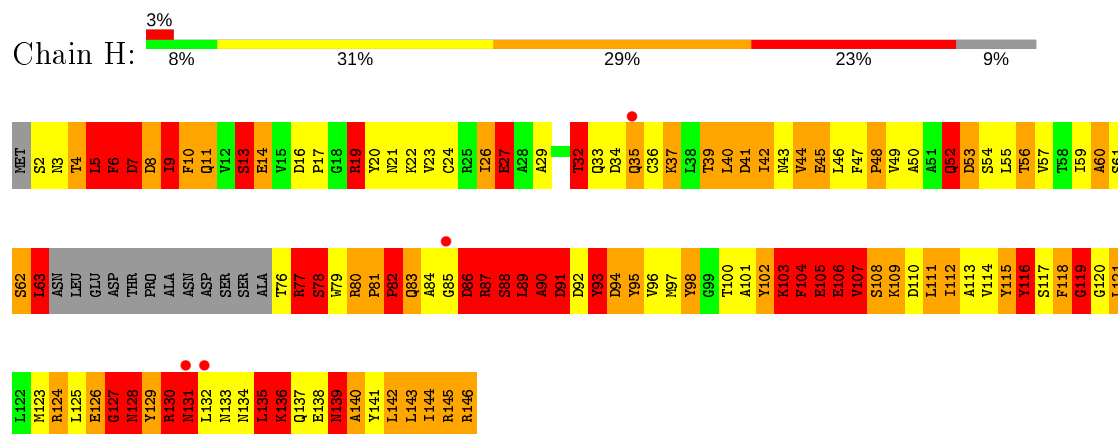




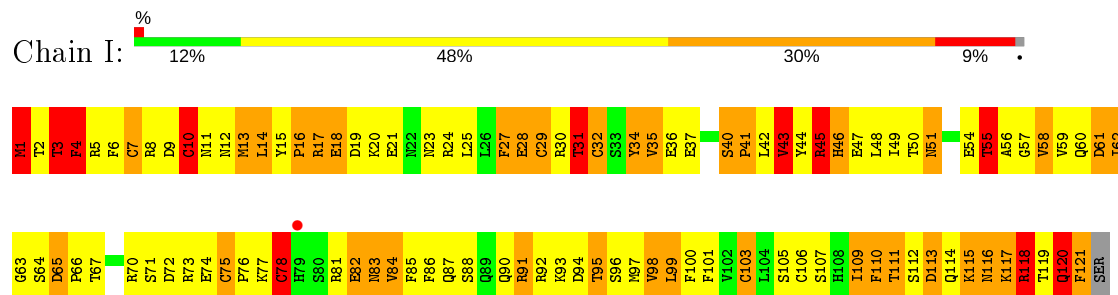
- Molecule 5: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



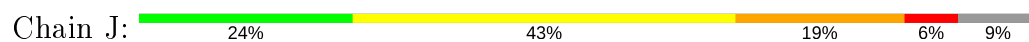
- Molecule 6: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

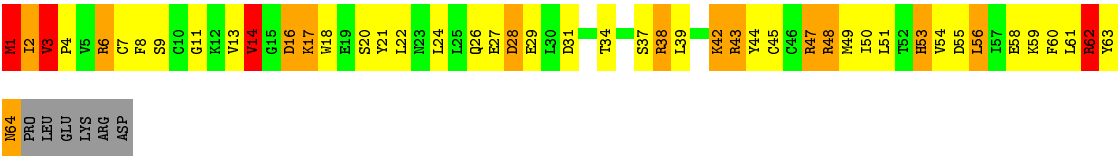


- Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

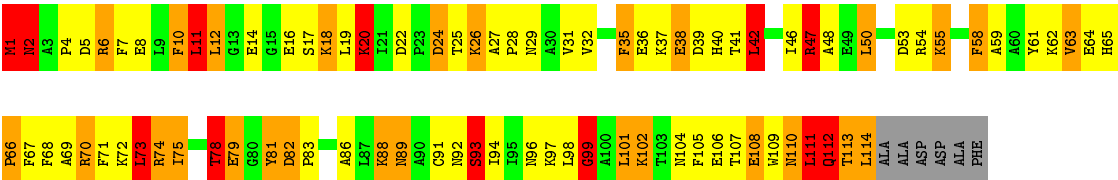
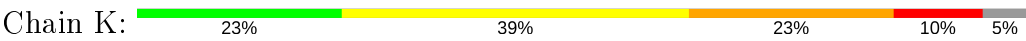


- Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

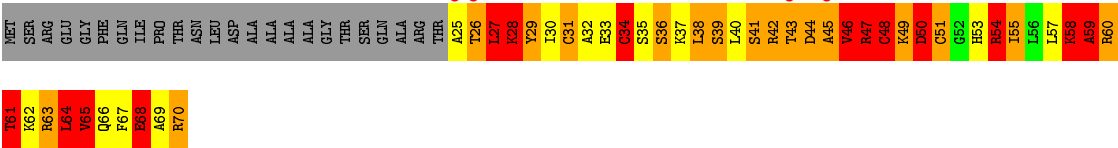




- Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.23Å 223.61Å 374.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 39.76 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 91.6 (39.76-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.234 , 0.255 0.198 , 0.236	Depositor DCC
$R_{free}$ test set	3424 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.3	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 55.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	27772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	3.17	1078/10811 (10.0%)	2.44	610/14626 (4.2%)
2	B	3.28	922/8860 (10.4%)	2.47	497/11945 (4.2%)
3	C	3.33	245/2133 (11.5%)	2.58	122/2891 (4.2%)
4	E	3.29	172/1796 (9.6%)	2.31	92/2416 (3.8%)
5	F	2.94	59/682 (8.7%)	2.24	31/922 (3.4%)
6	H	3.24	126/1086 (11.6%)	2.37	58/1470 (3.9%)
7	I	3.57	138/1009 (13.7%)	2.46	75/1357 (5.5%)
8	J	2.92	47/533 (8.8%)	2.82	46/715 (6.4%)
9	K	3.18	100/937 (10.7%)	2.62	58/1265 (4.6%)
10	L	3.58	46/366 (12.6%)	2.81	36/485 (7.4%)
All	All	3.24	2933/28213 (10.4%)	2.46	1625/38092 (4.3%)

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	28
2	B	0	32
3	C	0	13
4	E	1	7
6	H	0	13
7	I	0	3
9	K	0	2
10	L	0	4
All	All	1	102

All (2933) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	771	GLU	CD-OE2	27.21	1.55	1.25
2	B	552	MET	CG-SD	25.82	2.48	1.81
1	A	728	LYS	CD-CE	23.14	2.09	1.51
10	L	68	GLU	CG-CD	22.53	1.85	1.51
1	A	1005	GLU	CD-OE1	21.89	1.49	1.25
1	A	496	GLU	CD-OE1	20.92	1.48	1.25
3	C	165	LYS	CE-NZ	20.84	2.01	1.49
2	B	1150	ARG	CZ-NH1	20.35	1.59	1.33
4	E	162	ARG	CG-CD	19.89	2.01	1.51
2	B	529	GLU	CD-OE2	19.69	1.47	1.25
2	B	194	GLU	CD-OE1	19.69	1.47	1.25
1	A	1277	GLU	CD-OE2	18.98	1.46	1.25
1	A	618	GLU	CD-OE2	18.85	1.46	1.25
3	C	154	LYS	CD-CE	18.81	1.98	1.51
6	H	19	ARG	CG-CD	18.75	1.98	1.51
3	C	166	GLU	CD-OE2	18.74	1.46	1.25
1	A	1015	VAL	CB-CG2	-18.32	1.14	1.52
2	B	299	GLU	CD-OE1	18.25	1.45	1.25
2	B	641	GLU	CG-CD	18.22	1.79	1.51
7	I	28	GLU	CD-OE2	17.97	1.45	1.25
1	A	16	GLU	CD-OE1	17.84	1.45	1.25
2	B	1150	ARG	CZ-NH2	17.75	1.56	1.33
1	A	466	SER	CB-OG	-17.74	1.19	1.42
7	I	10	CYS	CB-SG	-17.56	1.52	1.82
4	E	162	ARG	NE-CZ	17.53	1.55	1.33
1	A	938	LYS	CD-CE	17.52	1.95	1.51
2	B	945	GLU	CD-OE1	17.36	1.44	1.25
9	K	108	GLU	CD-OE2	17.29	1.44	1.25
2	B	963	PHE	CE1-CZ	17.12	1.69	1.37
2	B	346	GLU	CG-CD	17.05	1.77	1.51
3	C	50	GLU	CG-CD	17.00	1.77	1.51
1	A	801	GLU	CD-OE1	16.93	1.44	1.25
1	A	1135	ARG	CZ-NH2	16.91	1.55	1.33
1	A	1232	ASN	CB-CG	16.88	1.89	1.51
1	A	801	GLU	CD-OE2	16.77	1.44	1.25
2	B	1154	ALA	CA-CB	16.70	1.87	1.52
1	A	346	ASP	CB-CG	16.61	1.86	1.51
1	A	1280	GLU	CD-OE2	16.52	1.43	1.25
4	E	50	MET	SD-CE	16.51	2.70	1.77
1	A	1349	TYR	CG-CD2	-16.50	1.17	1.39
2	B	239	GLU	CD-OE2	16.45	1.43	1.25
7	I	37	GLU	CD-OE1	16.34	1.43	1.25
2	B	598	GLU	CG-CD	16.27	1.76	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	68	GLU	CD-OE1	16.26	1.43	1.25
2	B	650	GLU	CD-OE2	16.21	1.43	1.25
2	B	531	GLN	CG-CD	16.18	1.88	1.51
2	B	275	TYR	CE2-CZ	-16.08	1.17	1.38
1	A	795	GLU	CG-CD	16.08	1.76	1.51
7	I	55	THR	CB-CG2	15.96	2.05	1.52
7	I	17	ARG	CG-CD	15.94	1.91	1.51
1	A	1196	GLU	CD-OE1	15.93	1.43	1.25
1	A	16	GLU	CD-OE2	15.82	1.43	1.25
1	A	734	GLU	CD-OE2	15.79	1.43	1.25
2	B	477	ALA	CA-CB	15.76	1.85	1.52
1	A	496	GLU	CD-OE2	15.71	1.43	1.25
1	A	751	SER	CB-OG	15.49	1.62	1.42
6	H	45	GLU	CD-OE1	15.41	1.42	1.25
2	B	459	TYR	CG-CD2	15.39	1.59	1.39
6	H	139	ASN	CB-CG	15.30	1.86	1.51
1	A	724	GLU	CD-OE1	15.19	1.42	1.25
2	B	509	ALA	CA-CB	15.19	1.84	1.52
1	A	1119	TYR	CE2-CZ	-15.19	1.18	1.38
2	B	211	VAL	CB-CG1	-15.19	1.21	1.52
2	B	1019	SER	CB-OG	-15.12	1.22	1.42
2	B	620	ARG	CZ-NH2	15.01	1.52	1.33
1	A	681	GLU	CD-OE2	14.92	1.42	1.25
4	E	137	GLU	CD-OE1	14.91	1.42	1.25
1	A	734	GLU	CD-OE1	14.85	1.42	1.25
1	A	695	LYS	CD-CE	14.76	1.88	1.51
1	A	941	LYS	CD-CE	14.70	1.88	1.51
2	B	346	GLU	CD-OE1	14.67	1.41	1.25
2	B	96	TYR	CG-CD1	14.64	1.58	1.39
2	B	564	GLU	CD-OE1	14.58	1.41	1.25
1	A	498	ARG	NE-CZ	-14.54	1.14	1.33
2	B	529	GLU	CD-OE1	14.39	1.41	1.25
4	E	180	ARG	CG-CD	14.39	1.88	1.51
1	A	620	LYS	CE-NZ	14.37	1.84	1.49
2	B	723	VAL	CA-CB	14.37	1.84	1.54
1	A	931	GLU	CG-CD	14.36	1.73	1.51
1	A	934	LYS	CD-CE	14.36	1.87	1.51
4	E	20	LYS	CE-NZ	14.33	1.84	1.49
2	B	723	VAL	CB-CG1	14.30	1.82	1.52
1	A	653	VAL	CB-CG2	-14.26	1.23	1.52
1	A	931	GLU	CD-OE2	14.24	1.41	1.25
4	E	131	THR	CB-CG2	14.21	1.99	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	34	GLU	CD-OE2	14.20	1.41	1.25
1	A	775	ILE	CG1-CD1	14.15	2.48	1.50
1	A	620	LYS	CD-CE	14.13	1.86	1.51
2	B	870	ILE	CA-CB	14.11	1.87	1.54
1	A	705	LYS	CB-CG	14.05	1.90	1.52
1	A	618	GLU	CD-OE1	14.00	1.41	1.25
4	E	152	LYS	CD-CE	13.98	1.86	1.51
2	B	758	PHE	CE2-CZ	-13.95	1.10	1.37
1	A	1417	GLU	CD-OE1	13.85	1.40	1.25
2	B	552	MET	SD-CE	13.79	2.55	1.77
2	B	764	SER	CB-OG	-13.77	1.24	1.42
10	L	26	THR	CA-CB	13.76	1.89	1.53
1	A	1417	GLU	CD-OE2	13.75	1.40	1.25
2	B	885	MET	SD-CE	13.71	2.54	1.77
1	A	290	GLU	CD-OE2	13.66	1.40	1.25
2	B	239	GLU	CG-CD	13.65	1.72	1.51
1	A	681	GLU	CD-OE1	13.65	1.40	1.25
4	E	66	GLU	CD-OE2	13.63	1.40	1.25
1	A	895	LYS	CD-CE	13.60	1.85	1.51
1	A	795	GLU	CD-OE2	13.50	1.40	1.25
1	A	1225	PHE	CD1-CE1	13.43	1.66	1.39
2	B	347	LYS	CG-CD	13.41	1.98	1.52
1	A	1277	GLU	CG-CD	13.33	1.72	1.51
1	A	836	TYR	CG-CD2	13.33	1.56	1.39
9	K	81	TYR	CD2-CE2	-13.31	1.19	1.39
3	C	23	SER	CB-OG	13.23	1.59	1.42
2	B	736	THR	CB-CG2	13.22	1.96	1.52
1	A	995	GLU	CD-OE2	13.22	1.40	1.25
1	A	1162	VAL	CB-CG1	13.22	1.80	1.52
1	A	724	GLU	CG-CD	13.20	1.71	1.51
1	A	446	ARG	CZ-NH1	13.20	1.50	1.33
2	B	194	GLU	CD-OE2	13.13	1.40	1.25
3	C	78	GLU	CD-OE2	13.14	1.40	1.25
1	A	1204	ASP	CB-CG	13.09	1.79	1.51
2	B	1206	GLU	CD-OE1	13.09	1.40	1.25
3	C	104	PHE	CD2-CE2	13.04	1.65	1.39
1	A	1415	SER	CB-OG	-13.01	1.25	1.42
1	A	1214	GLU	CD-OE1	12.98	1.40	1.25
2	B	987	LYS	CE-NZ	12.95	1.81	1.49
1	A	1372	VAL	CB-CG1	-12.93	1.25	1.52
2	B	1132	GLU	CD-OE1	12.92	1.39	1.25
1	A	1234	GLU	CD-OE1	12.89	1.39	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	653	VAL	CB-CG2	-12.88	1.25	1.52
3	C	197	SER	CB-OG	12.87	1.58	1.42
1	A	555	ASP	CB-CG	12.86	1.78	1.51
1	A	1074	GLU	CD-OE2	12.85	1.39	1.25
9	K	32	VAL	CB-CG2	-12.83	1.25	1.52
1	A	264	PHE	CB-CG	12.83	1.73	1.51
7	I	32	CYS	CB-SG	-12.82	1.60	1.82
2	B	838	SER	CB-OG	-12.79	1.25	1.42
6	H	141	TYR	CE1-CZ	-12.78	1.22	1.38
4	E	72	PHE	CE2-CZ	12.72	1.61	1.37
2	B	833	TYR	CE1-CZ	-12.70	1.22	1.38
4	E	162	ARG	CB-CG	12.70	1.86	1.52
2	B	1007	VAL	CB-CG1	-12.69	1.26	1.52
2	B	305	VAL	CB-CG1	12.68	1.79	1.52
2	B	226	PHE	CE2-CZ	12.66	1.61	1.37
3	C	12	GLU	CD-OE2	12.65	1.39	1.25
7	I	28	GLU	CD-OE1	12.65	1.39	1.25
3	C	177	GLU	CD-OE2	12.62	1.39	1.25
1	A	1290	LYS	CE-NZ	12.61	1.80	1.49
2	B	621	GLU	CD-OE2	12.60	1.39	1.25
7	I	1	MET	CG-SD	12.59	2.13	1.81
2	B	962	LYS	CD-CE	12.58	1.82	1.51
2	B	164	LYS	CD-CE	12.56	1.82	1.51
1	A	1411	GLU	CG-CD	12.56	1.70	1.51
2	B	319	GLU	CG-CD	12.55	1.70	1.51
4	E	106	GLN	CG-CD	12.53	1.79	1.51
4	E	57	MET	SD-CE	12.49	2.47	1.77
4	E	121	MET	CG-SD	12.48	2.13	1.81
2	B	459	TYR	CE2-CZ	12.47	1.54	1.38
2	B	371	GLU	CD-OE1	12.44	1.39	1.25
7	I	45	ARG	CG-CD	12.38	1.82	1.51
1	A	601	LYS	CD-CE	12.35	1.82	1.51
2	B	1101	ASP	CB-CG	12.35	1.77	1.51
1	A	291	GLU	CG-CD	12.35	1.70	1.51
1	A	1154	TYR	CE2-CZ	12.34	1.54	1.38
4	E	192	ARG	NE-CZ	12.25	1.49	1.33
1	A	585	GLY	C-O	12.22	1.43	1.23
1	A	1285	MET	SD-CE	12.22	2.46	1.77
1	A	487	MET	SD-CE	-12.20	1.09	1.77
4	E	201	LYS	CG-CD	12.19	1.93	1.52
2	B	785	TYR	CE1-CZ	-12.11	1.22	1.38
1	A	544	ASP	CB-CG	12.11	1.77	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	239	GLU	CD-OE1	12.04	1.38	1.25
2	B	328	GLU	CD-OE1	12.02	1.38	1.25
4	E	41	ASP	CB-CG	12.02	1.76	1.51
9	K	61	TYR	CE1-CZ	-12.01	1.23	1.38
3	C	192	TRP	CE3-CZ3	-11.98	1.18	1.38
1	A	830	LYS	CD-CE	11.96	1.81	1.51
1	A	1417	GLU	CG-CD	11.90	1.69	1.51
1	A	1230	GLU	CD-OE1	11.88	1.38	1.25
1	A	728	LYS	CG-CD	11.87	1.92	1.52
2	B	598	GLU	CD-OE2	11.87	1.38	1.25
2	B	706	GLN	CB-CG	11.87	1.84	1.52
2	B	968	VAL	CB-CG2	-11.85	1.27	1.52
2	B	296	GLU	CD-OE1	11.82	1.38	1.25
2	B	115	GLN	CG-CD	11.80	1.78	1.51
2	B	1097	HIS	CA-CB	11.78	1.79	1.53
1	A	481	ASP	CB-CG	11.76	1.76	1.51
3	C	50	GLU	CD-OE2	11.76	1.38	1.25
1	A	1187	GLN	CB-CG	11.75	1.84	1.52
1	A	1110	ASN	CB-CG	11.75	1.78	1.51
1	A	423	ASP	CB-CG	11.73	1.76	1.51
1	A	677	ARG	NE-CZ	11.71	1.48	1.33
2	B	230	ALA	CA-CB	11.68	1.76	1.52
2	B	31	TRP	CZ3-CH2	-11.67	1.21	1.40
2	B	1041	GLU	CD-OE1	11.65	1.38	1.25
3	C	97	VAL	C-O	-11.63	1.01	1.23
2	B	1041	GLU	CD-OE2	11.60	1.38	1.25
1	A	879	GLU	CD-OE1	11.59	1.38	1.25
9	K	61	TYR	CG-CD2	-11.54	1.24	1.39
6	H	104	PHE	CA-C	11.50	1.82	1.52
2	B	792	MET	SD-CE	11.50	2.42	1.77
6	H	19	ARG	NE-CZ	11.49	1.48	1.33
1	A	1419	ASP	CB-CG	11.48	1.75	1.51
1	A	464	PRO	C-O	-11.47	1.00	1.23
3	C	180	TYR	CG-CD1	-11.44	1.24	1.39
3	C	116	LYS	CD-CE	11.42	1.79	1.51
1	A	593	GLU	C-O	11.41	1.45	1.23
1	A	496	GLU	CG-CD	11.39	1.69	1.51
1	A	681	GLU	CG-CD	11.39	1.69	1.51
2	B	303	TYR	CG-CD2	-11.38	1.24	1.39
1	A	833	GLU	CG-CD	11.38	1.69	1.51
1	A	404	TYR	CG-CD1	-11.36	1.24	1.39
1	A	945	GLU	CD-OE2	11.36	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	719	VAL	CB-CG1	-11.30	1.29	1.52
4	E	66	GLU	CD-OE1	11.29	1.38	1.25
2	B	975	GLN	CD-NE2	11.26	1.61	1.32
2	B	594	ALA	CA-CB	-11.26	1.28	1.52
1	A	948	VAL	CB-CG1	-11.25	1.29	1.52
1	A	507	VAL	CB-CG2	-11.24	1.29	1.52
9	K	61	TYR	CE2-CZ	-11.24	1.24	1.38
3	C	40	GLU	CD-OE2	11.23	1.38	1.25
1	A	1035	TYR	CE2-CZ	-11.23	1.24	1.38
7	I	84	VAL	CB-CG1	-11.23	1.29	1.52
2	B	690	VAL	CB-CG1	-11.21	1.29	1.52
2	B	415	GLN	CB-CG	11.19	1.82	1.52
2	B	31	TRP	CD2-CE2	-11.18	1.27	1.41
1	A	37	PHE	CD1-CE1	11.16	1.61	1.39
1	A	821	ARG	CD-NE	-11.12	1.27	1.46
7	I	82	GLU	CG-CD	11.11	1.68	1.51
2	B	436	VAL	CA-CB	11.10	1.78	1.54
1	A	914	GLU	CD-OE1	11.09	1.37	1.25
8	J	42	LYS	CD-CE	11.09	1.78	1.51
3	C	15	LYS	CG-CD	11.08	1.90	1.52
2	B	96	TYR	CE1-CZ	11.08	1.52	1.38
3	C	3	GLU	CD-OE1	11.06	1.37	1.25
3	C	87	PHE	CD2-CE2	11.06	1.61	1.39
1	A	1291	VAL	CB-CG1	-11.03	1.29	1.52
2	B	235	SER	CB-OG	-11.02	1.27	1.42
2	B	370	PHE	CD1-CE1	11.00	1.61	1.39
4	E	34	GLU	CD-OE1	11.00	1.37	1.25
9	K	63	VAL	CB-CG1	-10.99	1.29	1.52
1	A	720	ARG	CG-CD	10.98	1.79	1.51
1	A	1171	GLN	CG-CD	10.97	1.76	1.51
2	B	660	LYS	CD-CE	-10.97	1.23	1.51
1	A	291	GLU	CD-OE1	10.95	1.37	1.25
4	E	211	TYR	CE1-CZ	-10.93	1.24	1.38
1	A	1112	LYS	CB-CG	10.92	1.82	1.52
4	E	26	ARG	CB-CG	-10.89	1.23	1.52
1	A	1222	ASN	CB-CG	10.89	1.76	1.51
3	C	12	GLU	CD-OE1	10.89	1.37	1.25
2	B	226	PHE	CD1-CE1	10.88	1.61	1.39
1	A	37	PHE	CG-CD2	10.86	1.55	1.38
2	B	96	TYR	CE2-CZ	10.86	1.52	1.38
3	C	208	GLU	CD-OE2	10.86	1.37	1.25
1	A	961	ARG	CZ-NH2	10.85	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1259	MET	CG-SD	10.85	2.09	1.81
1	A	677	ARG	CZ-NH2	10.84	1.47	1.33
2	B	959	ASP	CB-CG	10.83	1.74	1.51
2	B	18	PHE	CB-CG	10.80	1.69	1.51
2	B	137	TYR	CG-CD1	10.78	1.53	1.39
2	B	434	ARG	CG-CD	10.76	1.78	1.51
3	C	191	TYR	CB-CG	10.76	1.67	1.51
7	I	72	ASP	CB-CG	10.76	1.74	1.51
9	K	7	PHE	CB-CG	-10.74	1.33	1.51
2	B	775	LYS	CB-CG	10.72	1.81	1.52
1	A	1103	GLU	CD-OE2	10.72	1.37	1.25
2	B	986	GLN	CG-CD	10.72	1.75	1.51
1	A	290	GLU	CD-OE1	10.69	1.37	1.25
6	H	77	ARG	CB-CG	10.69	1.81	1.52
2	B	328	GLU	CD-OE2	10.66	1.37	1.25
2	B	1153	GLU	CD-OE2	10.62	1.37	1.25
1	A	708	MET	SD-CE	10.62	2.37	1.77
2	B	137	TYR	CB-CG	10.62	1.67	1.51
2	B	705	MET	SD-CE	-10.61	1.18	1.77
4	E	162	ARG	CZ-NH1	10.60	1.46	1.33
1	A	1102	LYS	CD-CE	10.59	1.77	1.51
1	A	1316	VAL	CB-CG2	-10.59	1.30	1.52
3	C	40	GLU	CD-OE1	10.58	1.37	1.25
1	A	1350	LYS	CE-NZ	10.57	1.75	1.49
4	E	98	ILE	CA-CB	10.54	1.79	1.54
2	B	191	LYS	CB-CG	10.53	1.80	1.52
1	A	714	PHE	CD2-CE2	-10.52	1.18	1.39
3	C	220	ASP	CB-CG	10.52	1.73	1.51
1	A	518	LYS	CD-CE	10.51	1.77	1.51
5	F	127	GLU	CD-OE1	10.49	1.37	1.25
2	B	519	TRP	CD2-CE2	-10.49	1.28	1.41
1	A	1064	VAL	CB-CG1	-10.48	1.30	1.52
1	A	1277	GLU	CD-OE1	10.48	1.37	1.25
2	B	531	GLN	CD-OE1	10.47	1.47	1.24
2	B	895	ASP	CB-CG	10.46	1.73	1.51
1	A	724	GLU	CD-OE2	10.45	1.37	1.25
6	H	129	TYR	CE1-CZ	10.45	1.52	1.38
1	A	1135	ARG	CG-CD	10.44	1.78	1.51
1	A	830	LYS	CG-CD	10.44	1.88	1.52
1	A	1446	ASP	CB-CG	10.43	1.73	1.51
2	B	962	LYS	CG-CD	10.43	1.87	1.52
7	I	92	ARG	C-O	10.42	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	734	GLU	CG-CD	10.41	1.67	1.51
1	A	843	LYS	CG-CD	10.41	1.87	1.52
3	C	122	SER	CB-OG	10.41	1.55	1.42
1	A	1280	GLU	CG-CD	10.41	1.67	1.51
2	B	1219	ASP	CB-CG	10.39	1.73	1.51
2	B	101	MET	SD-CE	10.37	2.35	1.77
2	B	31	TRP	CG-CD1	-10.36	1.22	1.36
2	B	951	GLN	CG-CD	10.36	1.74	1.51
1	A	995	GLU	CD-OE1	10.35	1.37	1.25
6	H	52	GLN	CG-CD	10.35	1.74	1.51
2	B	486	TYR	CG-CD1	10.32	1.52	1.39
2	B	999	MET	SD-CE	-10.31	1.20	1.77
3	C	3	GLU	CD-OE2	10.30	1.36	1.25
7	I	83	ASN	CB-CG	-10.28	1.27	1.51
1	A	839	ARG	NE-CZ	10.27	1.46	1.33
3	C	50	GLU	CD-OE1	10.27	1.36	1.25
3	C	199	LYS	CD-CE	10.27	1.76	1.51
1	A	1130	GLN	CG-CD	10.26	1.74	1.51
2	B	853	SER	CB-OG	10.26	1.55	1.42
8	J	29	GLU	CD-OE1	10.25	1.36	1.25
2	B	169	ARG	NE-CZ	10.25	1.46	1.33
4	E	72	PHE	CG-CD1	10.24	1.54	1.38
9	K	1	MET	SD-CE	10.24	2.35	1.77
1	A	836	TYR	CZ-OH	10.23	1.55	1.37
1	A	1014	ALA	CA-CB	-10.23	1.30	1.52
2	B	963	PHE	CB-CG	-10.22	1.33	1.51
1	A	5	GLN	CB-CG	10.21	1.80	1.52
5	F	72	LYS	CD-CE	10.20	1.76	1.51
1	A	347	PHE	N-CA	10.20	1.66	1.46
1	A	987	VAL	CB-CG1	-10.19	1.31	1.52
2	B	620	ARG	CG-CD	10.19	1.77	1.51
1	A	1214	GLU	C-O	10.18	1.42	1.23
2	B	529	GLU	CG-CD	10.15	1.67	1.51
2	B	57	TYR	CE2-CZ	-10.15	1.25	1.38
2	B	958	GLN	CG-CD	10.14	1.74	1.51
2	B	643	ASP	CB-CG	10.14	1.73	1.51
1	A	945	GLU	CD-OE1	10.13	1.36	1.25
1	A	1132	LYS	CE-NZ	10.13	1.74	1.49
1	A	678	GLU	CD-OE2	10.12	1.36	1.25
2	B	347	LYS	CD-CE	10.12	1.76	1.51
7	I	84	VAL	CB-CG2	-10.10	1.31	1.52
6	H	126	GLU	CD-OE1	10.10	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	274	ILE	CA-CB	10.10	1.78	1.54
2	B	183	GLU	CD-OE1	10.10	1.36	1.25
2	B	665	GLU	CG-CD	10.09	1.67	1.51
2	B	50	SER	CB-OG	-10.08	1.29	1.42
1	A	1298	TYR	CD2-CE2	-10.07	1.24	1.39
7	I	47	GLU	CG-CD	10.06	1.67	1.51
7	I	47	GLU	CD-OE2	10.06	1.36	1.25
9	K	111	LEU	C-O	10.04	1.42	1.23
1	A	1109	LYS	CB-CG	10.01	1.79	1.52
4	E	161	LYS	CD-CE	10.01	1.76	1.51
2	B	1069	PHE	CE2-CZ	-10.00	1.18	1.37
2	B	781	PHE	CB-CG	-9.99	1.34	1.51
5	F	103	MET	SD-CE	9.98	2.33	1.77
1	A	777	PHE	CD1-CE1	9.98	1.59	1.39
2	B	963	PHE	CD2-CE2	9.98	1.59	1.39
1	A	1035	TYR	CG-CD1	-9.98	1.26	1.39
6	H	45	GLU	CD-OE2	9.98	1.36	1.25
2	B	519	TRP	CB-CG	9.97	1.68	1.50
1	A	792	TYR	CD2-CE2	-9.97	1.24	1.39
1	A	843	LYS	CD-CE	9.96	1.76	1.51
1	A	1336	MET	C-O	-9.96	1.04	1.23
3	C	89	GLU	C-O	9.94	1.42	1.23
1	A	1055	ARG	CG-CD	9.93	1.76	1.51
1	A	1337	GLU	CG-CD	9.93	1.66	1.51
1	A	1419	ASP	CG-OD1	9.93	1.48	1.25
1	A	376	TYR	CD1-CE1	-9.91	1.24	1.39
1	A	1261	LYS	CD-CE	9.91	1.76	1.51
1	A	1362	TYR	CG-CD2	-9.90	1.26	1.39
1	A	525	GLN	CG-CD	9.90	1.73	1.51
2	B	320	ASP	CB-CG	9.88	1.72	1.51
6	H	131	ASN	CB-CG	9.88	1.73	1.51
1	A	846	GLU	CD-OE1	9.86	1.36	1.25
2	B	1134	GLU	CD-OE1	9.87	1.36	1.25
1	A	542	GLU	CD-OE1	9.85	1.36	1.25
3	C	209	TYR	CD2-CE2	9.85	1.54	1.39
10	L	29	TYR	CE1-CZ	-9.85	1.25	1.38
1	A	1074	GLU	CG-CD	9.82	1.66	1.51
2	B	370	PHE	CE2-CZ	9.82	1.56	1.37
1	A	792	TYR	CE1-CZ	-9.82	1.25	1.38
1	A	1223	ASP	CB-CG	9.80	1.72	1.51
1	A	481	ASP	CA-CB	-9.80	1.32	1.53
2	B	641	GLU	CD-OE1	9.79	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1301	GLU	CD-OE1	9.76	1.36	1.25
1	A	580	VAL	CB-CG2	-9.75	1.32	1.52
7	I	91	ARG	CA-C	-9.73	1.27	1.52
1	A	1445	ILE	CB-CG2	9.72	1.82	1.52
2	B	237	VAL	CB-CG1	-9.72	1.32	1.52
2	B	105	SER	CA-CB	9.71	1.67	1.52
4	E	54	GLN	CB-CG	9.70	1.78	1.52
8	J	3	VAL	CA-CB	-9.69	1.34	1.54
1	A	552	TRP	CG-CD1	-9.69	1.23	1.36
3	C	166	GLU	CD-OE1	9.69	1.36	1.25
10	L	54	ARG	CG-CD	9.69	1.76	1.51
3	C	180	TYR	CD2-CE2	9.67	1.53	1.39
5	F	154	ASP	CB-CG	9.67	1.72	1.51
4	E	40	GLU	CD-OE1	9.66	1.36	1.25
3	C	57	VAL	CB-CG2	-9.65	1.32	1.52
2	B	370	PHE	CD2-CE2	9.64	1.58	1.39
1	A	684	ALA	CA-CB	9.64	1.72	1.52
2	B	665	GLU	CD-OE2	9.63	1.36	1.25
4	E	133	GLU	CD-OE1	9.63	1.36	1.25
1	A	1230	GLU	CD-OE2	9.62	1.36	1.25
2	B	126	SER	CA-CB	-9.61	1.38	1.52
2	B	434	ARG	CB-CG	9.61	1.78	1.52
1	A	520	CYS	CB-SG	-9.61	1.66	1.82
2	B	486	TYR	CE1-CZ	9.61	1.51	1.38
2	B	607	GLY	C-O	-9.61	1.08	1.23
3	C	66	ARG	CZ-NH1	-9.61	1.20	1.33
1	A	610	GLY	C-O	9.59	1.39	1.23
2	B	1155	SER	CA-CB	9.58	1.67	1.52
1	A	597	LEU	CG-CD1	9.58	1.87	1.51
10	L	48	CYS	CB-SG	-9.58	1.66	1.82
1	A	1003	LYS	CB-CG	9.57	1.78	1.52
2	B	994	TYR	CD1-CE1	-9.57	1.25	1.39
6	H	9	ILE	CA-CB	9.56	1.76	1.54
6	H	118	PHE	CD2-CE2	9.56	1.58	1.39
2	B	315	LYS	CE-NZ	9.56	1.73	1.49
1	A	1232	ASN	C-O	9.54	1.41	1.23
2	B	662	MET	SD-CE	9.54	2.31	1.77
10	L	28	LYS	CA-C	9.53	1.77	1.52
9	K	2	ASN	C-O	9.52	1.41	1.23
9	K	36	GLU	CD-OE1	9.52	1.36	1.25
2	B	202	TYR	CE1-CZ	-9.52	1.26	1.38
1	A	398	GLU	CG-CD	9.51	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	17	SER	C-O	-9.51	1.05	1.23
2	B	1102	LYS	CB-CG	9.51	1.78	1.52
1	A	931	GLU	CD-OE1	9.50	1.36	1.25
3	C	102	GLN	CB-CG	9.48	1.78	1.52
7	I	82	GLU	CD-OE1	9.48	1.36	1.25
1	A	66	LYS	CB-CG	9.47	1.78	1.52
2	B	27	ALA	CA-CB	-9.46	1.32	1.52
2	B	41	LYS	CE-NZ	9.46	1.72	1.49
2	B	497	ARG	CZ-NH1	9.46	1.45	1.33
2	B	57	TYR	CE1-CZ	-9.45	1.26	1.38
2	B	983	ARG	CD-NE	-9.45	1.30	1.46
7	I	107	SER	CB-OG	-9.45	1.29	1.42
4	E	46	TYR	CD2-CE2	9.45	1.53	1.39
1	A	37	PHE	CE1-CZ	9.44	1.55	1.37
3	C	209	TYR	CE2-CZ	9.43	1.50	1.38
1	A	729	ALA	CA-CB	-9.42	1.32	1.52
1	A	1287	TYR	CG-CD1	9.42	1.51	1.39
2	B	833	TYR	CG-CD2	-9.42	1.26	1.39
2	B	399	ASP	CB-CG	9.41	1.71	1.51
2	B	1091	TYR	CE1-CZ	-9.41	1.26	1.38
2	B	706	GLN	CG-CD	9.40	1.72	1.51
10	L	45	ALA	CA-CB	9.40	1.72	1.52
1	A	1214	GLU	CG-CD	9.38	1.66	1.51
5	F	129	LYS	CE-NZ	9.38	1.72	1.49
1	A	840	ARG	CG-CD	9.38	1.75	1.51
2	B	479	VAL	CB-CG1	-9.37	1.33	1.52
9	K	111	LEU	CG-CD1	9.37	1.86	1.51
1	A	551	TYR	CE1-CZ	-9.36	1.26	1.38
4	E	13	TRP	CG-CD1	9.36	1.49	1.36
2	B	106	ASP	CB-CG	9.36	1.71	1.51
1	A	1297	GLU	CD-OE1	-9.35	1.15	1.25
4	E	191	LYS	CE-NZ	9.35	1.72	1.49
1	A	1111	MET	CG-SD	9.34	2.05	1.81
10	L	48	CYS	CA-C	9.34	1.77	1.52
8	J	58	GLU	CG-CD	9.34	1.66	1.51
1	A	1187	GLN	CG-CD	9.32	1.72	1.51
2	B	697	GLU	CD-OE2	9.28	1.35	1.25
5	F	146	TRP	CB-CG	-9.28	1.33	1.50
2	B	531	GLN	CB-CG	9.28	1.77	1.52
2	B	666	TYR	CE1-CZ	9.28	1.50	1.38
1	A	1438	THR	CB-CG2	-9.27	1.21	1.52
2	B	999	MET	CG-SD	9.27	2.05	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1291	VAL	CB-CG2	9.26	1.72	1.52
7	I	100	PHE	CE1-CZ	-9.26	1.19	1.37
2	B	766	ARG	NE-CZ	9.25	1.45	1.33
1	A	985	ASP	CG-OD2	9.25	1.46	1.25
2	B	216	GLU	CD-OE2	9.23	1.35	1.25
1	A	237	THR	CB-CG2	9.23	1.82	1.52
1	A	478	TYR	CD2-CE2	-9.23	1.25	1.39
2	B	216	GLU	CD-OE1	9.23	1.35	1.25
6	H	20	TYR	CE2-CZ	-9.23	1.26	1.38
2	B	448	ILE	N-CA	9.22	1.64	1.46
3	C	114	TYR	CE2-CZ	-9.22	1.26	1.38
1	A	44	THR	CA-CB	9.21	1.77	1.53
1	A	1129	GLU	CG-CD	9.21	1.65	1.51
2	B	249	ARG	NE-CZ	9.20	1.45	1.33
1	A	46	THR	CA-CB	9.19	1.77	1.53
2	B	30	SER	CB-OG	-9.18	1.30	1.42
2	B	797	TYR	CE1-CZ	-9.18	1.26	1.38
10	L	50	ASP	CB-CG	9.18	1.71	1.51
2	B	319	GLU	CD-OE1	9.17	1.35	1.25
2	B	459	TYR	CD1-CE1	9.17	1.53	1.39
2	B	581	PHE	CG-CD1	-9.16	1.25	1.38
2	B	359	GLU	CD-OE1	9.16	1.35	1.25
3	C	89	GLU	CD-OE2	9.16	1.35	1.25
1	A	16	GLU	CG-CD	9.15	1.65	1.51
2	B	124	TYR	CE1-CZ	-9.15	1.26	1.38
1	A	1302	PRO	CB-CG	9.15	1.95	1.50
1	A	1405	THR	CA-CB	9.15	1.77	1.53
1	A	91	PHE	CG-CD1	-9.14	1.25	1.38
2	B	1149	GLU	CD-OE1	9.14	1.35	1.25
3	C	170	TRP	CZ3-CH2	-9.14	1.25	1.40
4	E	67	GLU	CD-OE1	9.12	1.35	1.25
1	A	1214	GLU	CD-OE2	9.12	1.35	1.25
2	B	226	PHE	CG-CD2	9.11	1.52	1.38
1	A	37	PHE	CD2-CE2	9.11	1.57	1.39
1	A	1286	LYS	CB-CG	9.11	1.77	1.52
1	A	497	THR	CB-CG2	-9.10	1.22	1.52
1	A	678	GLU	CG-CD	9.10	1.65	1.51
10	L	62	LYS	CD-CE	9.09	1.74	1.51
2	B	975	GLN	CB-CG	-9.09	1.28	1.52
1	A	932	GLU	CD-OE2	9.05	1.35	1.25
3	C	195	GLN	CG-CD	9.05	1.71	1.51
2	B	65	GLU	CG-CD	9.05	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	7	GLN	CB-CG	9.04	1.76	1.52
1	A	771	GLU	CD-OE1	9.04	1.35	1.25
1	A	787	PHE	CD1-CE1	9.04	1.57	1.39
2	B	1156	ASP	CB-CG	9.03	1.70	1.51
1	A	676	MET	CG-SD	9.03	2.04	1.81
1	A	1342	GLU	CD-OE1	9.02	1.35	1.25
2	B	875	GLU	CG-CD	9.02	1.65	1.51
1	A	662	PHE	CE1-CZ	-9.02	1.20	1.37
1	A	626	ASN	CG-ND2	9.01	1.55	1.32
1	A	373	THR	CB-CG2	-9.01	1.22	1.52
1	A	787	PHE	CG-CD1	-9.00	1.25	1.38
2	B	296	GLU	CG-CD	9.00	1.65	1.51
2	B	96	TYR	CG-CD2	9.00	1.50	1.39
1	A	1005	GLU	CG-CD	8.98	1.65	1.51
1	A	971	PHE	CE2-CZ	-8.97	1.20	1.37
1	A	1337	GLU	CD-OE1	8.96	1.35	1.25
7	I	43	VAL	CB-CG1	-8.95	1.34	1.52
1	A	1093	LYS	CB-CG	8.95	1.76	1.52
2	B	373	ARG	CZ-NH1	8.95	1.44	1.33
4	E	59	SER	CB-OG	8.95	1.53	1.42
4	E	66	GLU	CG-CD	8.94	1.65	1.51
1	A	777	PHE	CD2-CE2	8.94	1.57	1.39
2	B	418	LYS	CD-CE	8.93	1.73	1.51
1	A	61	ILE	CA-CB	8.92	1.75	1.54
2	B	1057	LYS	CD-CE	8.92	1.73	1.51
3	C	154	LYS	CG-CD	8.92	1.82	1.52
2	B	723	VAL	CB-CG2	8.91	1.71	1.52
1	A	672	ASP	CB-CG	-8.90	1.33	1.51
9	K	61	TYR	C-O	-8.90	1.06	1.23
1	A	1305	VAL	CB-CG1	-8.89	1.34	1.52
1	A	478	TYR	CD1-CE1	-8.88	1.26	1.39
1	A	1239	ARG	CG-CD	8.87	1.74	1.51
2	B	246	LYS	CA-C	8.87	1.76	1.52
3	C	125	MET	SD-CE	8.85	2.27	1.77
6	H	121	LEU	C-O	8.85	1.40	1.23
7	I	75	CYS	CB-SG	-8.85	1.67	1.82
2	B	296	GLU	CD-OE2	8.85	1.35	1.25
6	H	95	TYR	CD2-CE2	8.85	1.52	1.39
6	H	129	TYR	CG-CD2	8.84	1.50	1.39
1	A	833	GLU	CD-OE1	8.84	1.35	1.25
3	C	28	ALA	C-O	8.84	1.40	1.23
6	H	98	TYR	CE1-CZ	-8.84	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1315	GLU	CD-OE2	8.83	1.35	1.25
1	A	1149	ALA	CA-CB	-8.82	1.33	1.52
1	A	1078	GLN	CG-CD	8.82	1.71	1.51
2	B	275	TYR	CG-CD1	-8.81	1.27	1.39
7	I	36	GLU	CG-CD	8.81	1.65	1.51
6	H	41	ASP	CB-CG	8.81	1.70	1.51
2	B	137	TYR	CE1-CZ	8.79	1.50	1.38
2	B	103	ASN	CB-CG	8.79	1.71	1.51
2	B	1164	GLY	C-O	8.79	1.37	1.23
8	J	48	ARG	CZ-NH1	-8.79	1.21	1.33
2	B	21	GLU	CD-OE2	8.78	1.35	1.25
4	E	152	LYS	CG-CD	8.78	1.82	1.52
7	I	98	VAL	CB-CG2	-8.78	1.34	1.52
2	B	245	GLU	CG-CD	8.77	1.65	1.51
3	C	66	ARG	NE-CZ	-8.77	1.21	1.33
5	F	93	ILE	C-O	-8.77	1.06	1.23
1	A	1426	GLU	CD-OE2	8.75	1.35	1.25
3	C	9	LYS	CG-CD	8.74	1.82	1.52
2	B	958	GLN	CB-CG	8.73	1.76	1.52
3	C	18	VAL	CB-CG2	-8.73	1.34	1.52
3	C	177	GLU	CG-CD	8.73	1.65	1.51
4	E	196	VAL	CB-CG1	-8.73	1.34	1.52
2	B	184	ALA	CA-CB	-8.73	1.34	1.52
2	B	595	ARG	NE-CZ	8.72	1.44	1.33
2	B	708	GLU	CD-OE2	8.72	1.35	1.25
1	A	1121	GLU	CD-OE1	8.72	1.35	1.25
1	A	1132	LYS	CD-CE	8.71	1.73	1.51
4	E	90	VAL	CB-CG1	8.71	1.71	1.52
2	B	595	ARG	CG-CD	8.71	1.73	1.51
3	C	159	ALA	C-O	-8.69	1.06	1.23
2	B	1221	SER	CA-CB	8.69	1.66	1.52
4	E	155	ARG	NE-CZ	8.69	1.44	1.33
2	B	815	ARG	CZ-NH2	8.69	1.44	1.33
2	B	115	GLN	CB-CG	8.68	1.75	1.52
2	B	485	ARG	NE-CZ	-8.68	1.21	1.33
2	B	1132	GLU	CG-CD	8.67	1.65	1.51
1	A	673	GLY	C-O	-8.66	1.09	1.23
2	B	217	ARG	CZ-NH1	-8.66	1.21	1.33
1	A	1215	ARG	CB-CG	8.65	1.75	1.52
2	B	626	ILE	C-O	-8.65	1.06	1.23
7	I	28	GLU	CG-CD	8.65	1.65	1.51
1	A	549	MET	SD-CE	-8.64	1.29	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	478	GLY	N-CA	8.64	1.59	1.46
1	A	398	GLU	CD-OE2	8.64	1.35	1.25
1	A	941	LYS	CE-NZ	8.63	1.70	1.49
3	C	198	ALA	CA-CB	-8.63	1.34	1.52
1	A	673	GLY	CA-C	-8.63	1.38	1.51
2	B	542	MET	SD-CE	-8.62	1.29	1.77
1	A	1080	THR	CA-CB	8.61	1.75	1.53
1	A	1132	LYS	CB-CG	8.61	1.75	1.52
7	I	20	LYS	CD-CE	8.61	1.72	1.51
1	A	1337	GLU	CD-OE2	8.60	1.35	1.25
3	C	196	ASP	CB-CG	8.60	1.69	1.51
3	C	178	PHE	CG-CD2	-8.60	1.25	1.38
4	E	33	GLU	CD-OE1	8.59	1.35	1.25
2	B	118	ARG	CZ-NH1	-8.59	1.21	1.33
7	I	35	VAL	CB-CG2	-8.59	1.34	1.52
2	B	376	PHE	CE2-CZ	-8.59	1.21	1.37
2	B	250	PHE	CE1-CZ	8.58	1.53	1.37
1	A	728	LYS	CE-NZ	8.57	1.70	1.49
3	C	134	ILE	CA-CB	-8.57	1.35	1.54
2	B	266	ALA	CA-CB	8.57	1.70	1.52
2	B	186	GLU	CD-OE2	8.56	1.35	1.25
2	B	219	ALA	CA-CB	8.56	1.70	1.52
2	B	330	ALA	CA-CB	-8.55	1.34	1.52
2	B	459	TYR	CD2-CE2	8.55	1.52	1.39
1	A	1411	GLU	CD-OE1	8.55	1.35	1.25
3	C	180	TYR	CD1-CE1	8.55	1.52	1.39
1	A	1159	ARG	NE-CZ	8.53	1.44	1.33
1	A	553	VAL	CB-CG1	-8.53	1.34	1.52
1	A	1355	VAL	CA-CB	-8.53	1.36	1.54
2	B	138	GLU	CD-OE2	-8.53	1.16	1.25
1	A	304	MET	SD-CE	8.53	2.25	1.77
1	A	893	PHE	CG-CD1	-8.53	1.25	1.38
2	B	488	TYR	CE1-CZ	-8.53	1.27	1.38
2	B	592	ASN	CG-OD1	8.52	1.42	1.24
2	B	28	GLU	CG-CD	8.52	1.64	1.51
2	B	1135	ARG	NE-CZ	-8.52	1.22	1.33
9	K	105	PHE	CD1-CE1	-8.51	1.22	1.39
3	C	108	GLU	CG-CD	8.51	1.64	1.51
2	B	389	ALA	CA-CB	-8.51	1.34	1.52
1	A	498	ARG	CZ-NH2	-8.50	1.22	1.33
7	I	11	ASN	CG-OD1	-8.50	1.05	1.24
1	A	589	GLN	CG-CD	8.49	1.70	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1359	ASP	CB-CG	8.49	1.69	1.51
2	B	641	GLU	CD-OE2	8.49	1.34	1.25
3	C	75	MET	SD-CE	8.49	2.25	1.77
1	A	481	ASP	CG-OD2	8.48	1.44	1.25
2	B	569	TYR	CG-CD2	-8.48	1.28	1.39
2	B	797	TYR	CD1-CE1	8.48	1.52	1.39
9	K	79	GLU	CG-CD	8.48	1.64	1.51
2	B	1092	TYR	CG-CD1	-8.48	1.28	1.39
1	A	1280	GLU	CD-OE1	8.48	1.34	1.25
3	C	51	VAL	CB-CG1	-8.48	1.35	1.52
1	A	421	ALA	CA-CB	-8.47	1.34	1.52
1	A	688	LYS	CD-CE	8.47	1.72	1.51
1	A	1234	GLU	CG-CD	8.47	1.64	1.51
1	A	404	TYR	CE2-CZ	-8.45	1.27	1.38
2	B	531	GLN	CD-NE2	8.44	1.53	1.32
1	A	69	THR	CA-C	8.43	1.74	1.52
3	C	106	GLU	CD-OE1	8.43	1.34	1.25
6	H	126	GLU	CG-CD	8.43	1.64	1.51
7	I	34	TYR	CG-CD2	-8.43	1.28	1.39
2	B	883	LEU	CA-CB	8.43	1.73	1.53
3	C	135	GLN	CG-CD	8.43	1.70	1.51
2	B	462	ALA	CA-CB	-8.43	1.34	1.52
1	A	1103	GLU	CD-OE1	8.42	1.34	1.25
9	K	22	ASP	CB-CG	8.42	1.69	1.51
8	J	48	ARG	CZ-NH2	-8.41	1.22	1.33
2	B	319	GLU	CD-OE2	8.40	1.34	1.25
1	A	836	TYR	CE2-CZ	8.40	1.49	1.38
2	B	622	LYS	CE-NZ	8.40	1.70	1.49
1	A	977	LYS	CB-CG	8.39	1.75	1.52
4	E	20	LYS	CD-CE	8.39	1.72	1.51
2	B	227	LYS	CE-NZ	8.38	1.70	1.49
2	B	108	VAL	CB-CG2	8.38	1.70	1.52
10	L	25	ALA	CA-CB	8.38	1.70	1.52
2	B	668	ASP	CB-CG	8.38	1.69	1.51
9	K	47	ARG	CZ-NH1	8.38	1.44	1.33
1	A	1349	TYR	CE1-CZ	-8.38	1.27	1.38
2	B	1215	ARG	CG-CD	8.37	1.72	1.51
3	C	143	LEU	C-O	-8.37	1.07	1.23
1	A	1280	GLU	C-O	-8.37	1.07	1.23
1	A	1422	ARG	NE-CZ	8.37	1.44	1.33
4	E	28	TYR	CE2-CZ	-8.37	1.27	1.38
2	B	485	ARG	CG-CD	-8.36	1.31	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	VAL	CB-CG1	-8.36	1.35	1.52
4	E	42	PHE	CD1-CE1	8.36	1.55	1.39
1	A	74	MET	CB-CG	8.36	1.78	1.51
2	B	797	TYR	CG-CD1	-8.35	1.28	1.39
1	A	49	LYS	CD-CE	8.35	1.72	1.51
1	A	1351	GLU	CD-OE2	8.35	1.34	1.25
1	A	551	TYR	CD2-CE2	-8.34	1.26	1.39
2	B	769	TYR	CE1-CZ	-8.34	1.27	1.38
1	A	1132	LYS	CG-CD	8.33	1.80	1.52
2	B	271	ALA	CA-CB	-8.33	1.34	1.52
3	C	84	ARG	C-O	-8.32	1.07	1.23
1	A	277	GLU	CD-OE2	8.31	1.34	1.25
1	A	1363	VAL	CB-CG1	8.31	1.70	1.52
1	A	897	TYR	CG-CD2	-8.31	1.28	1.39
5	F	137	TYR	CD2-CE2	-8.31	1.26	1.39
4	E	4	GLU	CD-OE1	-8.30	1.16	1.25
2	B	246	LYS	N-CA	8.30	1.62	1.46
7	I	91	ARG	C-O	-8.29	1.07	1.23
1	A	1269	GLU	CD-OE1	8.28	1.34	1.25
7	I	120	GLN	CB-CG	8.28	1.74	1.52
9	K	54	ARG	NE-CZ	8.27	1.43	1.33
2	B	459	TYR	CE1-CZ	8.27	1.49	1.38
1	A	1235	LYS	CD-CE	8.27	1.72	1.51
2	B	458	LYS	C-O	-8.27	1.07	1.23
3	C	137	LYS	CD-CE	8.26	1.72	1.51
3	C	9	LYS	CD-CE	8.26	1.71	1.51
2	B	994	TYR	CG-CD2	-8.26	1.28	1.39
3	C	225	ALA	CA-CB	-8.26	1.35	1.52
2	B	209	GLU	CD-OE2	-8.26	1.16	1.25
2	B	1061	GLU	CD-OE1	8.25	1.34	1.25
1	A	419	LYS	C-O	-8.24	1.07	1.23
2	B	404	LYS	CE-NZ	-8.24	1.28	1.49
1	A	376	TYR	CG-CD1	-8.24	1.28	1.39
2	B	908	GLU	CB-CG	8.24	1.67	1.52
3	C	78	GLU	C-O	-8.23	1.07	1.23
1	A	697	ALA	CA-CB	-8.22	1.35	1.52
1	A	712	GLU	CD-OE2	8.22	1.34	1.25
2	B	641	GLU	CB-CG	8.22	1.67	1.52
2	B	874	PHE	CD2-CE2	-8.22	1.22	1.39
7	I	93	LYS	CD-CE	8.22	1.71	1.51
1	A	1157	ASP	CB-CG	8.21	1.69	1.51
1	A	1281	ARG	NE-CZ	8.20	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	731	VAL	CB-CG2	8.20	1.70	1.52
1	A	1345	ARG	NE-CZ	-8.19	1.22	1.33
1	A	1196	GLU	CD-OE2	8.19	1.34	1.25
1	A	567	LYS	CD-CE	8.18	1.71	1.51
3	C	20	PHE	CB-CG	-8.18	1.37	1.51
1	A	1119	TYR	CG-CD1	-8.18	1.28	1.39
1	A	1235	LYS	CE-NZ	8.18	1.69	1.49
2	B	204	ILE	CA-CB	-8.18	1.36	1.54
4	E	131	THR	CA-CB	8.17	1.74	1.53
4	E	211	TYR	CE2-CZ	-8.17	1.27	1.38
3	C	34	ARG	CD-NE	-8.16	1.32	1.46
1	A	868	TYR	CE2-CZ	-8.15	1.27	1.38
6	H	88	SER	CA-CB	8.15	1.65	1.52
2	B	183	GLU	CG-CD	8.15	1.64	1.51
7	I	101	PHE	CB-CG	-8.14	1.37	1.51
1	A	359	LEU	CA-CB	-8.14	1.35	1.53
8	J	21	TYR	CA-CB	8.14	1.71	1.53
3	C	252	GLN	CB-CG	8.13	1.74	1.52
1	A	622	VAL	CA-CB	-8.12	1.37	1.54
3	C	15	LYS	CD-CE	8.12	1.71	1.51
1	A	875	ALA	CA-CB	-8.12	1.35	1.52
4	E	102	GLU	CG-CD	8.12	1.64	1.51
4	E	191	LYS	CD-CE	8.12	1.71	1.51
1	A	870	GLU	CD-OE2	8.11	1.34	1.25
2	B	245	GLU	CA-C	8.10	1.74	1.52
1	A	839	ARG	CG-CD	8.10	1.72	1.51
1	A	1381	LEU	C-O	-8.10	1.07	1.23
6	H	116	TYR	CG-CD1	8.10	1.49	1.39
3	C	106	GLU	CD-OE2	8.09	1.34	1.25
9	K	36	GLU	CA-CB	-8.09	1.36	1.53
1	A	386	ASP	CB-CG	8.08	1.68	1.51
1	A	1287	TYR	C-O	8.08	1.38	1.23
1	A	1362	TYR	CE2-CZ	8.07	1.49	1.38
7	I	42	LEU	C-O	-8.07	1.08	1.23
1	A	1109	LYS	CG-CD	8.07	1.79	1.52
9	K	64	GLU	CD-OE2	-8.06	1.16	1.25
1	A	685	GLU	CD-OE1	8.06	1.34	1.25
1	A	836	TYR	CG-CD1	8.06	1.49	1.39
6	H	105	GLU	CG-CD	8.06	1.64	1.51
2	B	1040	ASN	CB-CG	-8.05	1.32	1.51
4	E	50	MET	CG-SD	8.05	2.02	1.81
2	B	89	GLU	CA-C	8.05	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	699	GLU	CD-OE1	8.05	1.34	1.25
2	B	519	TRP	CZ3-CH2	-8.04	1.27	1.40
2	B	646	LEU	CG-CD2	8.04	1.81	1.51
8	J	48	ARG	CG-CD	-8.03	1.31	1.51
7	I	54	GLU	CD-OE2	8.03	1.34	1.25
4	E	93	MET	CG-SD	8.03	2.02	1.81
9	K	36	GLU	CD-OE2	8.03	1.34	1.25
2	B	191	LYS	CD-CE	8.03	1.71	1.51
8	J	6	ARG	CZ-NH1	-8.02	1.22	1.33
9	K	71	PHE	C-O	8.02	1.38	1.23
1	A	990	VAL	CA-CB	-8.01	1.38	1.54
1	A	1029	ARG	CB-CG	-8.01	1.30	1.52
3	C	87	PHE	CB-CG	-8.01	1.37	1.51
4	E	200	ARG	NE-CZ	-8.01	1.22	1.33
2	B	747	MET	SD-CE	-8.01	1.33	1.77
1	A	1109	LYS	CD-CE	8.00	1.71	1.51
2	B	337	ARG	CD-NE	-8.00	1.32	1.46
3	C	267	GLN	CA-C	8.00	1.73	1.52
1	A	1424	VAL	C-O	8.00	1.38	1.23
9	K	16	GLU	CG-CD	8.00	1.64	1.51
9	K	35	PHE	CE1-CZ	-7.99	1.22	1.37
1	A	1061	GLY	CA-C	7.99	1.64	1.51
1	A	1424	VAL	CB-CG1	-7.98	1.36	1.52
2	B	1171	VAL	C-O	7.96	1.38	1.23
1	A	468	PHE	CE2-CZ	-7.96	1.22	1.37
2	B	242	SER	CB-OG	7.96	1.52	1.42
4	E	36	GLU	C-O	-7.96	1.08	1.23
5	F	97	ARG	CB-CG	-7.95	1.31	1.52
4	E	103	LYS	CD-CE	7.95	1.71	1.51
2	B	262	GLU	CD-OE1	7.95	1.34	1.25
1	A	52	GLY	C-O	-7.95	1.10	1.23
2	B	855	PHE	CG-CD2	-7.95	1.26	1.38
7	I	34	TYR	CD2-CE2	7.94	1.51	1.39
1	A	69	THR	CA-CB	7.94	1.74	1.53
9	K	91	CYS	CB-SG	-7.94	1.68	1.82
1	A	714	PHE	CD1-CE1	-7.94	1.23	1.39
6	H	23	VAL	CA-CB	-7.94	1.38	1.54
2	B	1155	SER	N-CA	7.93	1.62	1.46
2	B	130	VAL	CB-CG2	-7.93	1.36	1.52
1	A	469	ARG	CD-NE	-7.93	1.32	1.46
2	B	32	ALA	CA-CB	7.93	1.69	1.52
2	B	1002	THR	CA-C	7.93	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	646	LEU	CG-CD1	7.92	1.81	1.51
1	A	1338	VAL	CB-CG2	-7.92	1.36	1.52
9	K	79	GLU	CD-OE1	7.92	1.34	1.25
4	E	37	LEU	CG-CD1	7.92	1.81	1.51
2	B	512	ARG	CZ-NH1	7.92	1.43	1.33
6	H	107	VAL	CA-CB	7.92	1.71	1.54
1	A	738	LYS	C-O	-7.92	1.08	1.23
9	K	20	LYS	CD-CE	7.91	1.71	1.51
2	B	589	VAL	CB-CG2	-7.91	1.36	1.52
1	A	1362	TYR	CE1-CZ	-7.91	1.28	1.38
2	B	337	ARG	NE-CZ	-7.90	1.22	1.33
3	C	97	VAL	CA-CB	-7.90	1.38	1.54
7	I	21	GLU	C-O	-7.90	1.08	1.23
2	B	259	TYR	CE1-CZ	-7.90	1.28	1.38
2	B	662	MET	C-O	-7.90	1.08	1.23
2	B	1053	GLU	CD-OE2	7.89	1.34	1.25
2	B	1086	PHE	CG-CD1	-7.89	1.26	1.38
4	E	102	GLU	CD-OE2	7.89	1.34	1.25
1	A	733	ALA	C-O	-7.89	1.08	1.23
1	A	558	GLY	C-O	-7.88	1.11	1.23
1	A	940	ARG	CD-NE	-7.88	1.33	1.46
1	A	1220	PHE	CG-CD1	-7.88	1.26	1.38
1	A	1336	MET	CG-SD	-7.88	1.60	1.81
2	B	184	ALA	C-O	-7.87	1.08	1.23
2	B	1101	ASP	CA-C	7.87	1.73	1.52
1	A	874	ASP	CG-OD2	7.86	1.43	1.25
2	B	19	GLU	CG-CD	7.85	1.63	1.51
3	C	84	ARG	NE-CZ	7.85	1.43	1.33
2	B	176	SER	CB-OG	-7.84	1.32	1.42
2	B	759	PRO	C-O	7.84	1.39	1.23
7	I	110	PHE	CD1-CE1	7.84	1.54	1.39
7	I	34	TYR	CE2-CZ	-7.84	1.28	1.38
1	A	1232	ASN	CG-OD1	7.84	1.41	1.24
2	B	227	LYS	CD-CE	7.83	1.70	1.51
2	B	346	GLU	CD-OE2	7.82	1.34	1.25
2	B	1097	HIS	CA-C	7.82	1.73	1.52
1	A	813	PHE	CE1-CZ	-7.82	1.22	1.37
2	B	250	PHE	CD2-CE2	7.82	1.54	1.39
1	A	478	TYR	CE1-CZ	-7.81	1.28	1.38
7	I	101	PHE	CD1-CE1	7.81	1.54	1.39
6	H	2	SER	CA-C	7.81	1.73	1.52
1	A	264	PHE	CG-CD2	7.81	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	671	ALA	CA-CB	-7.80	1.36	1.52
2	B	218	SER	C-O	-7.80	1.08	1.23
5	F	77	ASP	C-O	7.80	1.38	1.23
2	B	856	PHE	CE2-CZ	7.79	1.52	1.37
1	A	1350	LYS	CG-CD	7.79	1.78	1.52
2	B	652	LYS	CD-CE	7.79	1.70	1.51
2	B	843	GLN	CG-CD	-7.79	1.33	1.51
2	B	313	MET	SD-CE	-7.79	1.34	1.77
2	B	1154	ALA	CA-C	7.78	1.73	1.52
1	A	25	GLU	CG-CD	7.78	1.63	1.51
1	A	685	GLU	CG-CD	7.78	1.63	1.51
9	K	110	ASN	CB-CG	7.78	1.69	1.51
2	B	459	TYR	CG-CD1	7.78	1.49	1.39
6	H	95	TYR	CD1-CE1	7.78	1.51	1.39
2	B	612	GLU	CD-OE1	7.77	1.34	1.25
1	A	4	GLN	CB-CG	7.77	1.73	1.52
2	B	194	GLU	CG-CD	7.77	1.63	1.51
1	A	870	GLU	CD-OE1	7.77	1.34	1.25
1	A	1112	LYS	CD-CE	7.77	1.70	1.51
1	A	1288	ASP	CG-OD1	7.77	1.43	1.25
7	I	61	ASP	C-O	-7.77	1.08	1.23
3	C	172	PRO	CA-C	-7.76	1.37	1.52
2	B	250	PHE	CB-CG	7.76	1.64	1.51
1	A	1314	SER	CA-CB	-7.75	1.41	1.52
1	A	806	ARG	CZ-NH1	7.75	1.43	1.33
2	B	216	GLU	CG-CD	7.74	1.63	1.51
6	H	19	ARG	CD-NE	7.74	1.59	1.46
1	A	1044	TRP	CB-CG	-7.74	1.36	1.50
2	B	733	HIS	N-CA	7.74	1.61	1.46
4	E	1	MET	SD-CE	7.73	2.21	1.77
1	A	98	LYS	CD-CE	7.73	1.70	1.51
1	A	1074	GLU	CD-OE1	7.73	1.34	1.25
2	B	228	LYS	CB-CG	7.73	1.73	1.52
2	B	1102	LYS	N-CA	7.73	1.61	1.46
2	B	318	VAL	CB-CG2	-7.72	1.36	1.52
2	B	394	ASP	CB-CG	7.72	1.68	1.51
3	C	106	GLU	CG-CD	7.72	1.63	1.51
9	K	54	ARG	CG-CD	7.72	1.71	1.51
1	A	900	ASP	C-O	7.71	1.38	1.23
2	B	39	ARG	NE-CZ	7.71	1.43	1.33
1	A	71	GLN	CG-CD	7.71	1.68	1.51
1	A	1419	ASP	CG-OD2	7.70	1.43	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	15	TYR	CG-CD2	-7.70	1.29	1.39
1	A	747	VAL	CB-CG1	-7.69	1.36	1.52
6	H	3	ASN	CB-CG	7.69	1.68	1.51
1	A	792	TYR	CG-CD1	-7.69	1.29	1.39
3	C	117	ASP	C-O	7.69	1.38	1.23
4	E	207	ARG	CG-CD	7.68	1.71	1.51
1	A	933	TYR	CG-CD1	-7.68	1.29	1.39
2	B	188	ASP	C-O	7.68	1.38	1.23
1	A	1275	GLY	C-O	7.67	1.35	1.23
6	H	104	PHE	CE2-CZ	7.67	1.51	1.37
2	B	414	ALA	CA-CB	-7.67	1.36	1.52
2	B	371	GLU	CG-CD	7.67	1.63	1.51
9	K	16	GLU	CD-OE1	7.67	1.34	1.25
2	B	1092	TYR	CE1-CZ	-7.67	1.28	1.38
2	B	1100	ASP	CB-CG	7.66	1.67	1.51
1	A	896	ARG	CZ-NH1	7.66	1.43	1.33
1	A	897	TYR	CE1-CZ	-7.66	1.28	1.38
1	A	1045	VAL	CA-CB	-7.65	1.38	1.54
2	B	978	ASP	CB-CG	7.65	1.67	1.51
6	H	118	PHE	CG-CD1	7.64	1.50	1.38
1	A	1264	GLU	CD-OE1	-7.64	1.17	1.25
3	C	252	GLN	CD-OE1	7.64	1.40	1.24
6	H	102	TYR	CG-CD2	-7.64	1.29	1.39
1	A	1326	ARG	C-O	-7.64	1.08	1.23
6	H	104	PHE	CG-CD1	7.64	1.50	1.38
1	A	969	GLN	CG-CD	7.63	1.68	1.51
3	C	186	LEU	CA-C	7.63	1.72	1.52
4	E	179	GLN	CD-OE1	7.63	1.40	1.24
1	A	603	ASN	CB-CG	-7.63	1.33	1.51
1	A	774	ARG	CD-NE	-7.63	1.33	1.46
4	E	212	ARG	CZ-NH1	-7.63	1.23	1.33
10	L	37	LYS	C-O	-7.63	1.08	1.23
2	B	250	PHE	CG-CD2	7.63	1.50	1.38
1	A	1101	LEU	N-CA	-7.62	1.31	1.46
1	A	1129	GLU	CD-OE1	7.62	1.34	1.25
5	F	88	TYR	CD2-CE2	-7.62	1.27	1.39
4	E	65	THR	C-O	7.61	1.37	1.23
1	A	644	LYS	C-O	-7.61	1.08	1.23
4	E	45	LYS	CD-CE	7.60	1.70	1.51
3	C	163	ILE	CA-CB	-7.60	1.37	1.54
1	A	1422	ARG	CZ-NH1	7.60	1.43	1.33
2	B	1155	SER	CB-OG	7.60	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	27	GLU	CD-OE1	7.60	1.34	1.25
2	B	231	PRO	CA-C	7.59	1.68	1.52
2	B	848	ARG	NE-CZ	-7.59	1.23	1.33
2	B	986	GLN	CB-CG	7.59	1.73	1.52
2	B	240	ILE	C-O	-7.58	1.08	1.23
2	B	751	VAL	CB-CG1	-7.58	1.36	1.52
2	B	261	ARG	NE-CZ	7.58	1.43	1.33
1	A	1350	LYS	CD-CE	7.57	1.70	1.51
9	K	6	ARG	CB-CG	-7.57	1.32	1.52
1	A	933	TYR	CE2-CZ	-7.56	1.28	1.38
2	B	303	TYR	CD2-CE2	-7.56	1.28	1.39
3	C	50	GLU	CB-CG	7.56	1.66	1.52
5	F	100	GLN	CG-CD	7.56	1.68	1.51
5	F	143	PHE	C-O	-7.56	1.08	1.23
1	A	1105	LEU	C-O	-7.56	1.08	1.23
1	A	1358	SER	CB-OG	7.55	1.52	1.42
2	B	250	PHE	CD1-CE1	7.55	1.54	1.39
1	A	1383	SER	CA-CB	-7.55	1.41	1.52
4	E	71	LYS	N-CA	7.55	1.61	1.46
4	E	67	GLU	CD-OE2	7.55	1.33	1.25
1	A	364	VAL	CB-CG1	-7.54	1.37	1.52
2	B	33	VAL	CB-CG1	-7.54	1.37	1.52
2	B	245	GLU	CB-CG	7.54	1.66	1.52
2	B	810	GLU	CG-CD	7.54	1.63	1.51
1	A	908	LEU	C-O	-7.54	1.09	1.23
4	E	85	GLU	CD-OE2	7.54	1.33	1.25
9	K	81	TYR	CD1-CE1	-7.53	1.28	1.39
1	A	468	PHE	CG-CD1	-7.53	1.27	1.38
9	K	61	TYR	CD2-CE2	7.53	1.50	1.39
1	A	1144	LYS	CD-CE	7.52	1.70	1.51
2	B	1091	TYR	C-O	-7.52	1.09	1.23
1	A	366	VAL	C-N	-7.51	1.20	1.34
1	A	1307	GLU	CD-OE1	7.51	1.33	1.25
6	H	37	LYS	C-O	7.51	1.37	1.23
1	A	961	ARG	NE-CZ	7.51	1.42	1.33
1	A	451	HIS	CA-CB	-7.51	1.37	1.53
4	E	112	TYR	CD1-CE1	7.51	1.50	1.39
2	B	344	LYS	CD-CE	7.50	1.70	1.51
7	I	6	PHE	CE1-CZ	-7.50	1.23	1.37
1	A	939	ASP	CB-CG	7.49	1.67	1.51
2	B	870	ILE	N-CA	7.49	1.61	1.46
5	F	76	LYS	CD-CE	7.49	1.70	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	836	TYR	CE1-CZ	7.49	1.48	1.38
1	A	647	GLY	CA-C	7.49	1.63	1.51
2	B	811	TYR	CE2-CZ	-7.49	1.28	1.38
4	E	148	GLU	CD-OE2	7.49	1.33	1.25
2	B	608	ASP	C-O	-7.48	1.09	1.23
1	A	933	TYR	CE1-CZ	-7.48	1.28	1.38
4	E	129	PRO	CG-CD	7.48	1.75	1.50
3	C	114	TYR	CG-CD2	-7.47	1.29	1.39
1	A	879	GLU	CG-CD	7.47	1.63	1.51
2	B	957	ASN	CA-C	7.46	1.72	1.52
9	K	94	ILE	CA-CB	7.46	1.72	1.54
1	A	486	GLU	CD-OE2	-7.46	1.17	1.25
1	A	1290	LYS	CD-CE	7.46	1.69	1.51
8	J	37	SER	CA-CB	-7.45	1.41	1.52
9	K	26	LYS	CG-CD	7.45	1.77	1.52
10	L	43	THR	CB-CG2	7.45	1.76	1.52
1	A	1434	ALA	CA-CB	-7.45	1.36	1.52
3	C	94	LYS	CE-NZ	7.45	1.67	1.49
4	E	7	ARG	NE-CZ	7.45	1.42	1.33
2	B	1129	ARG	NE-CZ	7.44	1.42	1.33
2	B	1130	PHE	CE1-CZ	-7.44	1.23	1.37
1	A	1256	GLU	CG-CD	7.44	1.63	1.51
3	C	179	GLU	CD-OE1	-7.44	1.17	1.25
4	E	192	ARG	CZ-NH2	7.44	1.42	1.33
2	B	758	PHE	CG-CD2	-7.43	1.27	1.38
2	B	1080	LYS	CD-CE	7.43	1.69	1.51
2	B	567	GLU	CD-OE2	7.43	1.33	1.25
5	F	153	VAL	CB-CG2	-7.43	1.37	1.52
1	A	894	GLU	CG-CD	7.42	1.63	1.51
1	A	469	ARG	CZ-NH2	-7.42	1.23	1.33
2	B	547	VAL	CB-CG1	-7.42	1.37	1.52
1	A	293	GLU	CD-OE1	7.42	1.33	1.25
6	H	91	ASP	CA-C	7.42	1.72	1.52
9	K	86	ALA	CA-CB	-7.42	1.36	1.52
1	A	1121	GLU	CG-CD	7.42	1.63	1.51
2	B	41	LYS	CD-CE	7.42	1.69	1.51
2	B	612	GLU	CG-CD	7.41	1.63	1.51
7	I	58	VAL	CB-CG1	-7.41	1.37	1.52
1	A	1152	ILE	CA-CB	-7.41	1.37	1.54
4	E	192	ARG	CD-NE	7.40	1.59	1.46
5	F	123	LYS	CE-NZ	7.40	1.67	1.49
1	A	566	ILE	CB-CG2	7.40	1.75	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	55	THR	C-O	7.39	1.37	1.23
2	B	692	TYR	C-O	-7.39	1.09	1.23
2	B	377	PHE	CB-CG	-7.39	1.38	1.51
1	A	392	VAL	CA-CB	-7.38	1.39	1.54
2	B	327	ARG	CB-CG	-7.38	1.32	1.52
1	A	842	VAL	C-O	-7.38	1.09	1.23
1	A	1210	GLY	C-O	7.38	1.35	1.23
9	K	20	LYS	CG-CD	7.37	1.77	1.52
2	B	325	GLN	CB-CG	-7.37	1.32	1.52
7	I	30	ARG	CG-CD	7.37	1.70	1.51
2	B	1188	LYS	CD-CE	7.36	1.69	1.51
1	A	1027	ALA	C-O	7.36	1.37	1.23
7	I	56	ALA	C-O	-7.36	1.09	1.23
1	A	941	LYS	CB-CG	-7.35	1.32	1.52
10	L	26	THR	N-CA	7.35	1.61	1.46
1	A	1285	MET	CG-SD	7.34	2.00	1.81
2	B	194	GLU	CB-CG	7.34	1.66	1.52
2	B	360	PHE	CE2-CZ	-7.34	1.23	1.37
1	A	1420	ASP	CG-OD2	7.33	1.42	1.25
5	F	149	GLU	CG-CD	7.33	1.62	1.51
2	B	1083	ALA	CA-CB	-7.33	1.37	1.52
1	A	787	PHE	CB-CG	-7.33	1.38	1.51
3	C	122	SER	CA-CB	7.32	1.64	1.52
1	A	1227	ILE	C-O	-7.32	1.09	1.23
2	B	694	ASP	CB-CG	7.32	1.67	1.51
1	A	687	LYS	CE-NZ	7.31	1.67	1.49
2	B	38	PHE	CD2-CE2	-7.31	1.24	1.39
2	B	1036	ALA	CA-CB	7.31	1.67	1.52
3	C	161	LYS	CD-CE	-7.31	1.32	1.51
7	I	99	LEU	C-O	-7.31	1.09	1.23
1	A	644	LYS	CD-CE	7.31	1.69	1.51
1	A	1385	THR	CA-C	7.31	1.72	1.52
2	B	882	THR	N-CA	7.31	1.60	1.46
5	F	90	ARG	NE-CZ	-7.31	1.23	1.33
2	B	614	SER	CB-OG	-7.30	1.32	1.42
2	B	1052	VAL	CB-CG2	-7.30	1.37	1.52
3	C	154	LYS	CB-CG	7.30	1.72	1.52
1	A	788	SER	CA-CB	7.30	1.63	1.52
1	A	1298	TYR	CG-CD1	-7.30	1.29	1.39
1	A	1362	TYR	CB-CG	-7.30	1.40	1.51
4	E	194	GLU	CD-OE2	-7.30	1.17	1.25
1	A	705	LYS	CA-CB	7.29	1.70	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1138	ILE	C-O	7.29	1.37	1.23
3	C	183	TRP	CE2-CZ2	-7.29	1.27	1.39
1	A	677	ARG	CZ-NH1	7.29	1.42	1.33
2	B	1106	ARG	CA-C	7.29	1.72	1.52
6	H	93	TYR	CG-CD1	7.29	1.48	1.39
2	B	208	SER	CB-OG	-7.29	1.32	1.42
6	H	63	LEU	C-O	7.29	1.37	1.23
8	J	29	GLU	CD-OE2	7.29	1.33	1.25
1	A	268	ASP	CB-CG	7.28	1.67	1.51
1	A	1376	THR	CB-CG2	-7.28	1.28	1.52
1	A	1237	ILE	N-CA	-7.28	1.31	1.46
2	B	564	GLU	CD-OE2	7.28	1.33	1.25
1	A	352	VAL	CB-CG2	7.28	1.68	1.52
1	A	1191	TRP	CB-CG	-7.28	1.37	1.50
1	A	1299	VAL	CB-CG1	-7.28	1.37	1.52
2	B	593	PRO	CB-CG	7.28	1.86	1.50
6	H	104	PHE	CE1-CZ	7.27	1.51	1.37
9	K	55	LYS	CB-CG	7.27	1.72	1.52
1	A	1272	THR	CB-CG2	7.27	1.76	1.52
6	H	48	PRO	C-O	7.27	1.37	1.23
2	B	200	GLY	C-O	-7.27	1.12	1.23
1	A	509	LEU	C-O	-7.26	1.09	1.23
3	C	114	TYR	CD2-CE2	-7.26	1.28	1.39
6	H	2	SER	CA-CB	7.26	1.63	1.52
1	A	551	TYR	CE2-CZ	-7.26	1.29	1.38
1	A	1259	MET	SD-CE	7.26	2.18	1.77
1	A	811	GLN	N-CA	-7.25	1.31	1.46
2	B	70	ILE	CA-CB	7.25	1.71	1.54
2	B	391	ASP	C-O	-7.25	1.09	1.23
2	B	319	GLU	CB-CG	7.25	1.66	1.52
2	B	733	HIS	CA-C	7.25	1.71	1.52
1	A	756	ILE	CB-CG2	-7.25	1.30	1.52
3	C	70	ILE	N-CA	7.25	1.60	1.46
2	B	108	VAL	CA-CB	7.25	1.70	1.54
2	B	570	VAL	CB-CG1	-7.24	1.37	1.52
10	L	42	ARG	NE-CZ	7.24	1.42	1.33
1	A	506	ALA	C-O	-7.24	1.09	1.23
9	K	58	PHE	CB-CG	7.24	1.63	1.51
1	A	1092	LYS	CB-CG	7.24	1.72	1.52
4	E	172	GLU	CD-OE2	7.24	1.33	1.25
9	K	26	LYS	CD-CE	7.23	1.69	1.51
1	A	946	VAL	CA-CB	-7.23	1.39	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	711	GLU	CG-CD	7.23	1.62	1.51
2	B	967	ARG	N-CA	-7.23	1.31	1.46
1	A	437	MET	SD-CE	7.22	2.18	1.77
2	B	735	ALA	N-CA	7.22	1.60	1.46
1	A	973	ILE	CB-CG2	7.21	1.75	1.52
2	B	875	GLU	CD-OE1	7.21	1.33	1.25
1	A	1226	VAL	CB-CG1	-7.21	1.37	1.52
2	B	652	LYS	CE-NZ	7.20	1.67	1.49
4	E	1	MET	CG-SD	7.20	1.99	1.81
9	K	5	ASP	CG-OD2	7.20	1.42	1.25
2	B	901	PRO	C-O	-7.20	1.08	1.23
8	J	21	TYR	CB-CG	7.20	1.62	1.51
2	B	384	ARG	CB-CG	7.19	1.72	1.52
3	C	94	LYS	CB-CG	7.18	1.72	1.52
1	A	1154	TYR	CG-CD2	-7.18	1.29	1.39
2	B	572	HIS	C-O	-7.18	1.09	1.23
1	A	1120	LEU	C-O	-7.18	1.09	1.23
2	B	738	PHE	CG-CD1	-7.18	1.27	1.38
9	K	92	ASN	N-CA	7.18	1.60	1.46
3	C	191	TYR	CG-CD2	-7.18	1.29	1.39
6	H	124	ARG	CB-CG	-7.17	1.33	1.52
1	A	1038	THR	C-O	-7.17	1.09	1.23
4	E	26	ARG	CD-NE	7.17	1.58	1.46
4	E	52	ARG	C-O	7.17	1.36	1.23
1	A	571	LEU	CG-CD2	7.17	1.78	1.51
7	I	94	ASP	CB-CG	7.17	1.66	1.51
1	A	1019	CYS	CA-CB	-7.17	1.38	1.53
6	H	22	LYS	CE-NZ	7.17	1.67	1.49
2	B	855	PHE	CD2-CE2	7.17	1.53	1.39
1	A	763	ALA	CA-CB	-7.16	1.37	1.52
1	A	773	LYS	CB-CG	-7.16	1.33	1.52
1	A	888	GLY	CA-C	-7.16	1.40	1.51
1	A	1365	TYR	CD2-CE2	7.16	1.50	1.39
2	B	980	PHE	CG-CD1	-7.15	1.28	1.38
4	E	13	TRP	CB-CG	7.15	1.63	1.50
1	A	14	VAL	C-O	-7.15	1.09	1.23
2	B	39	ARG	C-O	-7.15	1.09	1.23
1	A	847	ASP	CG-OD1	7.15	1.41	1.25
2	B	498	THR	CA-CB	7.15	1.72	1.53
2	B	241	ARG	NE-CZ	7.14	1.42	1.33
3	C	253	LYS	C-O	7.14	1.36	1.23
3	C	17	ASN	C-O	-7.14	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	233	GLU	CD-OE1	7.13	1.33	1.25
1	A	905	ASP	N-CA	-7.13	1.32	1.46
1	A	346	ASP	CG-OD2	7.12	1.41	1.25
2	B	1061	GLU	CB-CG	7.12	1.65	1.52
4	E	28	TYR	CG-CD1	-7.12	1.29	1.39
1	A	1160	SER	CB-OG	7.12	1.51	1.42
1	A	1164	PRO	CG-CD	7.12	1.74	1.50
2	B	231	PRO	CB-CG	7.12	1.85	1.50
7	I	70	ARG	NE-CZ	-7.12	1.23	1.33
3	C	23	SER	CA-CB	7.11	1.63	1.52
9	K	26	LYS	CE-NZ	7.11	1.66	1.49
1	A	767	GLN	CA-CB	-7.11	1.38	1.53
2	B	1137	CYS	CB-SG	-7.11	1.70	1.82
2	B	466	TRP	CA-C	7.11	1.71	1.52
2	B	19	GLU	N-CA	7.11	1.60	1.46
1	A	1229	SER	C-O	7.11	1.36	1.23
1	A	1094	VAL	CB-CG2	7.10	1.67	1.52
2	B	119	LEU	CA-CB	-7.10	1.37	1.53
10	L	68	GLU	CD-OE2	7.10	1.33	1.25
1	A	500	GLU	CD-OE2	7.10	1.33	1.25
2	B	346	GLU	CB-CG	7.09	1.65	1.52
1	A	780	VAL	C-O	7.09	1.36	1.23
2	B	557	PHE	CG-CD2	7.09	1.49	1.38
1	A	1268	LEU	N-CA	-7.08	1.32	1.46
1	A	500	GLU	CD-OE1	7.08	1.33	1.25
2	B	99	LYS	CD-CE	7.08	1.69	1.51
2	B	567	GLU	C-O	-7.08	1.09	1.23
1	A	25	GLU	CD-OE1	7.07	1.33	1.25
2	B	249	ARG	C-O	7.07	1.36	1.23
1	A	1359	ASP	N-CA	7.07	1.60	1.46
2	B	116	GLU	CG-CD	7.07	1.62	1.51
6	H	45	GLU	CG-CD	7.07	1.62	1.51
2	B	698	GLU	CD-OE1	-7.07	1.17	1.25
7	I	1	MET	CB-CG	7.07	1.74	1.51
5	F	114	GLU	CD-OE1	7.07	1.33	1.25
2	B	1020	ARG	CZ-NH2	-7.06	1.23	1.33
2	B	18	PHE	CG-CD2	7.06	1.49	1.38
3	C	179	GLU	C-O	-7.06	1.09	1.23
4	E	78	LEU	N-CA	-7.06	1.32	1.46
1	A	1382	THR	C-O	7.06	1.36	1.23
1	A	693	VAL	CA-CB	-7.05	1.40	1.54
1	A	360	GLU	CG-CD	7.05	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	243	ALA	CA-CB	7.05	1.67	1.52
2	B	882	THR	CA-CB	7.05	1.71	1.53
3	C	49	VAL	CB-CG2	-7.05	1.38	1.52
5	F	146	TRP	CG-CD1	-7.05	1.26	1.36
1	A	1164	PRO	CA-C	7.05	1.67	1.52
1	A	1315	GLU	CG-CD	7.04	1.62	1.51
2	B	56	ASP	C-O	-7.04	1.09	1.23
4	E	179	GLN	CG-CD	-7.04	1.34	1.51
2	B	1092	TYR	CE2-CZ	-7.03	1.29	1.38
5	F	98	ALA	C-O	-7.03	1.09	1.23
1	A	1151	GLU	CG-CD	7.03	1.62	1.51
3	C	256	ALA	CA-CB	-7.03	1.37	1.52
7	I	3	THR	CB-CG2	7.02	1.75	1.52
1	A	390	GLN	C-O	7.02	1.36	1.23
1	A	264	PHE	CE1-CZ	7.02	1.50	1.37
2	B	422	LYS	CB-CG	7.02	1.71	1.52
1	A	420	ARG	CB-CG	-7.02	1.33	1.52
7	I	56	ALA	CA-CB	-7.01	1.37	1.52
8	J	18	TRP	CE2-CZ2	-7.01	1.27	1.39
2	B	903	VAL	CB-CG1	-7.01	1.38	1.52
1	A	1187	GLN	C-O	7.00	1.36	1.23
2	B	118	ARG	CG-CD	7.00	1.69	1.51
6	H	13	SER	CA-CB	7.00	1.63	1.52
6	H	11	GLN	CA-C	-7.00	1.34	1.52
1	A	735	VAL	CB-CG2	7.00	1.67	1.52
1	A	1264	GLU	CD-OE2	-6.99	1.18	1.25
6	H	32	THR	CA-CB	6.99	1.71	1.53
1	A	487	MET	CG-SD	6.99	1.99	1.81
1	A	551	TYR	CD1-CE1	-6.99	1.28	1.39
2	B	788	ARG	CD-NE	-6.99	1.34	1.46
4	E	201	LYS	CB-CG	6.99	1.71	1.52
1	A	999	VAL	CB-CG1	-6.99	1.38	1.52
2	B	703	ILE	C-O	6.99	1.36	1.23
1	A	1385	THR	CB-CG2	6.99	1.75	1.52
2	B	970	THR	CA-CB	-6.99	1.35	1.53
2	B	259	TYR	C-O	-6.98	1.10	1.23
2	B	692	TYR	CG-CD2	-6.98	1.30	1.39
10	L	59	ALA	N-CA	6.98	1.60	1.46
1	A	912	LEU	CA-C	-6.98	1.34	1.52
1	A	1269	GLU	CD-OE2	6.98	1.33	1.25
1	A	843	LYS	C-O	-6.98	1.10	1.23
2	B	1085	ILE	CB-CG2	-6.98	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5	GLY	CA-C	6.97	1.63	1.51
7	I	34	TYR	CE1-CZ	-6.97	1.29	1.38
2	B	865	LYS	CA-CB	6.97	1.69	1.53
2	B	982	SER	CB-OG	-6.97	1.33	1.42
1	A	1036	ARG	CZ-NH1	6.97	1.42	1.33
1	A	295	LEU	CG-CD2	6.97	1.77	1.51
1	A	826	ASP	CG-OD2	6.97	1.41	1.25
1	A	711	ARG	C-O	-6.96	1.10	1.23
2	B	299	GLU	CD-OE2	6.96	1.33	1.25
4	E	57	MET	C-O	6.96	1.36	1.23
6	H	137	GLN	CB-CG	6.96	1.71	1.52
7	I	8	ARG	CZ-NH1	6.96	1.42	1.33
1	A	430	TRP	CZ3-CH2	-6.96	1.28	1.40
2	B	348	ARG	NE-CZ	-6.96	1.24	1.33
2	B	1128	LEU	N-CA	6.96	1.60	1.46
3	C	219	PHE	CE1-CZ	-6.96	1.24	1.37
1	A	608	ILE	CB-CG2	-6.96	1.31	1.52
10	L	26	THR	CB-CG2	6.96	1.75	1.52
1	A	74	MET	CG-SD	6.96	1.99	1.81
1	A	446	ARG	NE-CZ	-6.96	1.24	1.33
3	C	209	TYR	CG-CD2	6.96	1.48	1.39
8	J	56	LEU	N-CA	-6.96	1.32	1.46
1	A	1012	ARG	CG-CD	6.95	1.69	1.51
2	B	490	SER	CB-OG	6.95	1.51	1.42
2	B	589	VAL	CB-CG1	-6.95	1.38	1.52
6	H	132	LEU	CA-CB	6.95	1.69	1.53
3	C	26	ASP	CG-OD1	6.95	1.41	1.25
10	L	61	THR	CB-CG2	6.95	1.75	1.52
1	A	722	LEU	C-O	-6.94	1.10	1.23
1	A	1135	ARG	NE-CZ	6.94	1.42	1.33
4	E	81	GLU	CD-OE1	6.94	1.33	1.25
1	A	1146	VAL	C-O	-6.93	1.10	1.23
2	B	436	VAL	CA-C	6.93	1.71	1.52
4	E	17	ARG	CZ-NH2	6.93	1.42	1.33
1	A	1078	GLN	CB-CG	6.93	1.71	1.52
2	B	1204	PHE	CD1-CE1	6.92	1.53	1.39
3	C	100	THR	C-O	6.92	1.36	1.23
4	E	185	ALA	CA-CB	-6.92	1.38	1.52
1	A	711	ARG	CB-CG	6.92	1.71	1.52
2	B	798	TYR	CE1-CZ	6.92	1.47	1.38
1	A	24	PRO	CG-CD	-6.92	1.27	1.50
5	F	103	MET	C-O	-6.91	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1032	SER	C-O	6.91	1.36	1.23
6	H	27	GLU	CA-C	6.91	1.71	1.52
4	E	210	SER	CB-OG	6.91	1.51	1.42
4	E	110	PHE	N-CA	-6.90	1.32	1.46
5	F	105	ALA	CA-CB	-6.90	1.38	1.52
4	E	200	ARG	CB-CG	-6.90	1.33	1.52
2	B	265	SER	CA-CB	6.89	1.63	1.52
1	A	264	PHE	CG-CD1	6.89	1.49	1.38
1	A	725	ALA	CA-CB	-6.89	1.38	1.52
4	E	52	ARG	CB-CG	6.89	1.71	1.52
2	B	512	ARG	CA-C	6.89	1.70	1.52
3	C	107	SER	CB-OG	-6.88	1.33	1.42
9	K	55	LYS	CD-CE	6.88	1.68	1.51
2	B	266	ALA	C-O	6.88	1.36	1.23
2	B	983	ARG	NE-CZ	-6.88	1.24	1.33
1	A	892	ALA	CA-CB	-6.87	1.38	1.52
6	H	19	ARG	CB-CG	6.87	1.71	1.52
1	A	1056	SER	CA-CB	-6.86	1.42	1.52
1	A	1005	GLU	CD-OE2	6.86	1.33	1.25
2	B	579	ARG	NE-CZ	-6.86	1.24	1.33
5	F	122	MET	SD-CE	-6.86	1.39	1.77
2	B	904	ARG	C-O	-6.86	1.10	1.23
1	A	1289	ARG	NE-CZ	-6.86	1.24	1.33
2	B	113	TYR	CD2-CE2	-6.86	1.29	1.39
2	B	567	GLU	CB-CG	6.86	1.65	1.52
7	I	15	TYR	CD2-CE2	6.86	1.49	1.39
1	A	1287	TYR	CD1-CE1	6.85	1.49	1.39
2	B	209	GLU	CD-OE1	-6.84	1.18	1.25
2	B	352	ALA	CA-CB	-6.84	1.38	1.52
6	H	127	GLY	N-CA	6.84	1.56	1.46
2	B	574	SER	CB-OG	-6.83	1.33	1.42
1	A	1302	PRO	C-O	6.83	1.36	1.23
4	E	7	ARG	CD-NE	6.83	1.58	1.46
3	C	261	ALA	C-O	-6.83	1.10	1.23
6	H	27	GLU	CG-CD	6.83	1.62	1.51
2	B	174	LEU	C-O	-6.82	1.10	1.23
1	A	954	TRP	CG-CD1	-6.82	1.27	1.36
2	B	172	ILE	CA-CB	-6.82	1.39	1.54
5	F	107	VAL	CB-CG2	-6.82	1.38	1.52
2	B	959	ASP	CA-CB	6.81	1.69	1.53
1	A	1003	LYS	CD-CE	6.81	1.68	1.51
2	B	875	GLU	CD-OE2	6.81	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	TRP	CD2-CE3	-6.81	1.30	1.40
8	J	42	LYS	C-O	6.81	1.36	1.23
2	B	995	ARG	CD-NE	-6.80	1.34	1.46
1	A	373	THR	C-O	-6.80	1.10	1.23
1	A	572	TRP	CE2-CZ2	-6.80	1.28	1.39
1	A	1050	GLU	CG-CD	6.80	1.62	1.51
2	B	25	ILE	CA-CB	6.80	1.70	1.54
1	A	792	TYR	CD1-CE1	-6.80	1.29	1.39
9	K	7	PHE	CE2-CZ	6.79	1.50	1.37
7	I	107	SER	CA-CB	-6.79	1.42	1.52
2	B	1200	ALA	C-O	-6.79	1.10	1.23
3	C	158	VAL	CA-CB	-6.79	1.40	1.54
1	A	1123	GLY	CA-C	6.78	1.62	1.51
1	A	1171	GLN	CB-CG	6.78	1.70	1.52
4	E	26	ARG	CG-CD	-6.78	1.34	1.51
1	A	1081	LEU	CG-CD2	6.78	1.76	1.51
2	B	361	LEU	C-N	-6.78	1.21	1.34
1	A	1225	PHE	C-O	-6.78	1.10	1.23
2	B	592	ASN	CB-CG	6.78	1.66	1.51
7	I	78	CYS	CB-SG	6.78	1.93	1.82
1	A	849	MET	SD-CE	-6.77	1.40	1.77
1	A	1239	ARG	CZ-NH2	-6.77	1.24	1.33
2	B	173	MET	C-O	-6.77	1.10	1.23
1	A	830	LYS	CE-NZ	6.76	1.66	1.49
2	B	114	PRO	CG-CD	-6.76	1.28	1.50
1	A	298	PHE	CG-CD2	6.76	1.48	1.38
7	I	6	PHE	C-O	-6.76	1.10	1.23
4	E	142	VAL	C-O	6.76	1.36	1.23
6	H	141	TYR	CZ-OH	-6.76	1.26	1.37
6	H	79	TRP	CB-CG	-6.75	1.38	1.50
1	A	750	GLY	C-O	-6.75	1.12	1.23
1	A	958	VAL	CA-CB	-6.75	1.40	1.54
2	B	1192	TYR	CE1-CZ	-6.75	1.29	1.38
1	A	689	LYS	CD-CE	6.75	1.68	1.51
9	K	26	LYS	CB-CG	6.75	1.70	1.52
1	A	1141	THR	C-O	6.75	1.36	1.23
8	J	13	VAL	CB-CG2	-6.75	1.38	1.52
1	A	1338	VAL	CA-CB	-6.74	1.40	1.54
4	E	67	GLU	CG-CD	6.74	1.62	1.51
2	B	587	HIS	C-O	-6.74	1.10	1.23
2	B	278	GLN	CB-CG	-6.73	1.34	1.52
1	A	828	ALA	CA-CB	-6.73	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	829	VAL	CB-CG2	6.73	1.67	1.52
2	B	617	ARG	C-O	-6.73	1.10	1.23
2	B	592	ASN	CG-ND2	6.72	1.49	1.32
2	B	875	GLU	CB-CG	6.72	1.65	1.52
1	A	604	GLY	CA-C	-6.72	1.41	1.51
1	A	1061	GLY	N-CA	-6.72	1.35	1.46
2	B	618	ASP	CG-OD1	6.72	1.40	1.25
2	B	662	MET	CG-SD	-6.72	1.63	1.81
1	A	368	LYS	CG-CD	6.72	1.75	1.52
1	A	1141	THR	CB-CG2	-6.72	1.30	1.52
1	A	1416	ALA	C-O	-6.71	1.10	1.23
7	I	48	LEU	C-O	-6.71	1.10	1.23
10	L	29	TYR	CG-CD2	-6.71	1.30	1.39
1	A	383	TYR	CE1-CZ	6.71	1.47	1.38
8	J	7	CYS	CB-SG	-6.71	1.70	1.82
6	H	139	ASN	CA-CB	6.70	1.70	1.53
1	A	1118	VAL	CB-CG2	-6.70	1.38	1.52
8	J	38	ARG	CB-CG	6.70	1.70	1.52
9	K	1	MET	N-CA	6.69	1.59	1.46
3	C	228	PHE	CG-CD2	-6.69	1.28	1.38
1	A	1191	TRP	CE2-CZ2	-6.68	1.28	1.39
2	B	267	ARG	C-O	-6.68	1.10	1.23
2	B	1004	GLU	CG-CD	6.68	1.61	1.51
1	A	661	GLY	CA-C	6.68	1.62	1.51
1	A	518	LYS	CE-NZ	-6.67	1.32	1.49
1	A	795	GLU	CD-OE1	6.67	1.32	1.25
3	C	95	CYS	CB-SG	-6.67	1.71	1.82
9	K	64	GLU	C-O	-6.67	1.10	1.23
2	B	465	ASN	CB-CG	6.66	1.66	1.51
3	C	192	TRP	CB-CG	6.66	1.62	1.50
1	A	709	THR	CB-CG2	-6.66	1.30	1.52
1	A	427	GLN	CG-CD	6.66	1.66	1.51
1	A	414	ASP	C-O	-6.66	1.10	1.23
1	A	361	LEU	C-O	-6.66	1.10	1.23
2	B	397	ASP	CG-OD1	6.66	1.40	1.25
6	H	129	TYR	CE2-CZ	6.66	1.47	1.38
1	A	599	SER	CA-CB	6.65	1.62	1.52
1	A	1146	VAL	CB-CG1	-6.65	1.38	1.52
1	A	291	GLU	C-O	-6.65	1.10	1.23
1	A	1239	ARG	CB-CG	-6.65	1.34	1.52
2	B	525	ALA	C-O	6.65	1.35	1.23
8	J	24	LEU	CA-CB	-6.65	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	711	GLU	CA-CB	-6.65	1.39	1.53
2	B	728	ARG	CZ-NH1	-6.64	1.24	1.33
1	A	1093	LYS	N-CA	6.64	1.59	1.46
2	B	90	ILE	N-CA	6.64	1.59	1.46
2	B	729	ILE	C-O	-6.64	1.10	1.23
4	E	160	GLU	CD-OE1	6.64	1.32	1.25
1	A	1045	VAL	CB-CG1	-6.64	1.39	1.52
2	B	604	ARG	N-CA	6.64	1.59	1.46
2	B	1221	SER	N-CA	6.64	1.59	1.46
1	A	53	LEU	N-CA	6.63	1.59	1.46
1	A	1228	TRP	CE2-CZ2	-6.63	1.28	1.39
2	B	105	SER	CB-OG	6.63	1.50	1.42
2	B	559	SER	CB-OG	-6.63	1.33	1.42
2	B	816	GLU	CD-OE1	6.63	1.32	1.25
4	E	79	TRP	CD2-CE3	6.63	1.50	1.40
1	A	965	GLN	CD-NE2	6.63	1.49	1.32
6	H	91	ASP	C-O	6.63	1.35	1.23
6	H	116	TYR	CE1-CZ	6.63	1.47	1.38
2	B	651	LEU	CG-CD2	-6.63	1.27	1.51
1	A	806	ARG	CZ-NH2	6.62	1.41	1.33
1	A	1262	LYS	CG-CD	6.62	1.75	1.52
4	E	205	SER	C-O	-6.62	1.10	1.23
1	A	1042	PHE	CE2-CZ	6.62	1.50	1.37
2	B	60	GLN	CB-CG	-6.62	1.34	1.52
2	B	1057	LYS	CG-CD	6.62	1.75	1.52
7	I	63	GLY	C-O	-6.62	1.13	1.23
2	B	227	LYS	CG-CD	6.61	1.75	1.52
1	A	838	GLN	CG-CD	6.61	1.66	1.51
2	B	851	PHE	CB-CG	6.61	1.62	1.51
1	A	1444	MET	SD-CE	6.61	2.14	1.77
2	B	586	TRP	CE3-CZ3	-6.61	1.27	1.38
7	I	14	LEU	C-O	-6.61	1.10	1.23
1	A	1001	ARG	NE-CZ	-6.61	1.24	1.33
1	A	1221	LYS	CB-CG	6.61	1.70	1.52
2	B	417	PHE	CE1-CZ	-6.60	1.24	1.37
2	B	249	ARG	CG-CD	6.60	1.68	1.51
2	B	1079	LYS	CE-NZ	-6.60	1.32	1.49
2	B	1096	ARG	C-O	-6.60	1.10	1.23
1	A	1418	LEU	C-O	-6.60	1.10	1.23
2	B	124	TYR	CE2-CZ	-6.60	1.29	1.38
4	E	112	TYR	CG-CD1	-6.60	1.30	1.39
3	C	215	GLU	CD-OE1	6.59	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	256	VAL	CB-CG1	-6.59	1.39	1.52
3	C	174	ALA	CA-CB	-6.59	1.38	1.52
2	B	434	ARG	NE-CZ	6.59	1.41	1.33
2	B	874	PHE	CD1-CE1	-6.59	1.26	1.39
6	H	43	ASN	CB-CG	6.59	1.66	1.51
2	B	916	THR	CB-CG2	6.59	1.74	1.52
2	B	97	VAL	CB-CG1	-6.59	1.39	1.52
1	A	591	PHE	CB-CG	6.58	1.62	1.51
1	A	919	ILE	CA-CB	6.58	1.70	1.54
3	C	216	GLY	C-O	6.58	1.34	1.23
1	A	802	ASN	CB-CG	6.58	1.66	1.51
6	H	6	PHE	CA-C	-6.58	1.35	1.52
9	K	54	ARG	CD-NE	6.58	1.57	1.46
2	B	37	PHE	CE2-CZ	-6.58	1.24	1.37
9	K	61	TYR	CD1-CE1	6.58	1.49	1.39
6	H	27	GLU	CD-OE1	6.57	1.32	1.25
1	A	624	SER	CA-CB	6.57	1.62	1.52
2	B	573	GLN	C-O	-6.57	1.10	1.23
1	A	348	SER	CA-CB	-6.57	1.43	1.52
3	C	61	GLU	N-CA	6.57	1.59	1.46
1	A	1057	VAL	CB-CG2	-6.57	1.39	1.52
2	B	238	ALA	CA-CB	6.57	1.66	1.52
6	H	131	ASN	CA-CB	6.56	1.70	1.53
2	B	608	ASP	CB-CG	6.56	1.65	1.51
5	F	127	GLU	CD-OE2	6.56	1.32	1.25
1	A	1442	ASP	CA-C	-6.56	1.35	1.52
2	B	57	TYR	CG-CD1	-6.56	1.30	1.39
2	B	710	LEU	CG-CD1	-6.56	1.27	1.51
7	I	62	ILE	C-O	-6.56	1.10	1.23
1	A	866	PHE	CB-CG	-6.55	1.40	1.51
1	A	1448	GLU	CA-C	6.55	1.70	1.52
2	B	857	ARG	NE-CZ	6.55	1.41	1.33
3	C	49	VAL	CB-CG1	6.55	1.66	1.52
3	C	39	ALA	CA-CB	-6.55	1.38	1.52
1	A	1012	ARG	NE-CZ	6.55	1.41	1.33
2	B	479	VAL	C-O	-6.55	1.10	1.23
2	B	627	PHE	CD2-CE2	-6.55	1.26	1.39
2	B	89	GLU	C-O	6.54	1.35	1.23
1	A	1428	VAL	CB-CG2	6.54	1.66	1.52
2	B	382	ILE	CG1-CD1	6.54	1.95	1.50
2	B	605	ARG	CZ-NH1	-6.54	1.24	1.33
10	L	65	VAL	CB-CG2	6.54	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	679	TYR	CE2-CZ	-6.54	1.30	1.38
7	I	54	GLU	CD-OE1	6.53	1.32	1.25
2	B	1178	ASN	CB-CG	-6.53	1.36	1.51
4	E	128	PRO	CA-C	6.53	1.66	1.52
1	A	941	LYS	CG-CD	6.53	1.74	1.52
7	I	86	PHE	CE1-CZ	6.53	1.49	1.37
4	E	185	ALA	N-CA	-6.53	1.33	1.46
1	A	871	ASP	C-O	-6.53	1.10	1.23
2	B	1224	PHE	CG-CD2	6.53	1.48	1.38
1	A	31	SER	C-O	6.53	1.35	1.23
1	A	423	ASP	CG-OD1	6.53	1.40	1.25
3	C	108	GLU	CD-OE1	6.52	1.32	1.25
7	I	118	ARG	NE-CZ	6.52	1.41	1.33
9	K	68	PHE	CG-CD1	-6.52	1.28	1.38
2	B	1224	PHE	CG-CD1	6.51	1.48	1.38
9	K	37	LYS	CA-CB	-6.51	1.39	1.53
6	H	21	ASN	C-O	-6.51	1.10	1.23
4	E	74	ASP	CB-CG	-6.51	1.38	1.51
10	L	34	CYS	CB-SG	-6.51	1.71	1.82
2	B	536	VAL	CB-CG1	-6.50	1.39	1.52
2	B	1073	TYR	CD2-CE2	-6.50	1.29	1.39
1	A	718	VAL	CA-CB	-6.49	1.41	1.54
1	A	1080	THR	CA-C	6.49	1.69	1.52
1	A	1279	ILE	N-CA	-6.49	1.33	1.46
2	B	905	VAL	CB-CG1	-6.49	1.39	1.52
1	A	298	PHE	CD2-CE2	6.49	1.52	1.39
1	A	1108	ALA	N-CA	-6.49	1.33	1.46
7	I	31	THR	N-CA	-6.49	1.33	1.46
2	B	28	GLU	CD-OE2	6.49	1.32	1.25
9	K	108	GLU	CD-OE1	6.49	1.32	1.25
1	A	854	ASN	CB-CG	6.49	1.66	1.51
1	A	1018	PHE	CE2-CZ	6.49	1.49	1.37
2	B	1063	GLY	C-O	-6.48	1.13	1.23
6	H	116	TYR	N-CA	6.48	1.59	1.46
1	A	1330	ASN	C-O	-6.48	1.11	1.23
4	E	198	ILE	CB-CG2	-6.48	1.32	1.52
3	C	119	VAL	CA-CB	6.48	1.68	1.54
1	A	1119	TYR	CD2-CE2	-6.47	1.29	1.39
3	C	57	VAL	CA-CB	-6.47	1.41	1.54
3	C	210	GLU	CD-OE1	6.47	1.32	1.25
1	A	517	ASN	CB-CG	6.47	1.66	1.51
8	J	26	GLN	CB-CG	6.47	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	695	ALA	CA-CB	-6.47	1.38	1.52
7	I	105	SER	CB-OG	6.46	1.50	1.42
2	B	643	ASP	CA-CB	6.46	1.68	1.53
6	H	115	TYR	CE1-CZ	6.46	1.47	1.38
2	B	197	PHE	CG-CD1	-6.46	1.29	1.38
2	B	1224	PHE	CD1-CE1	6.46	1.52	1.39
3	C	114	TYR	CD1-CE1	-6.46	1.29	1.39
2	B	1132	GLU	CD-OE2	6.46	1.32	1.25
3	C	181	ASP	C-O	-6.46	1.11	1.23
4	E	168	TYR	CG-CD1	-6.46	1.30	1.39
6	H	102	TYR	CD1-CE1	-6.45	1.29	1.39
2	B	851	PHE	CE1-CZ	6.45	1.49	1.37
4	E	14	ARG	CZ-NH2	-6.45	1.24	1.33
2	B	969	ARG	NE-CZ	-6.44	1.24	1.33
2	B	34	ILE	CB-CG2	-6.44	1.32	1.52
2	B	282	ILE	CA-CB	-6.44	1.40	1.54
1	A	777	PHE	CG-CD1	-6.44	1.29	1.38
2	B	1183	LYS	CA-CB	6.44	1.68	1.53
3	C	191	TYR	CE1-CZ	-6.44	1.30	1.38
6	H	104	PHE	C-O	6.44	1.35	1.23
2	B	1224	PHE	CD2-CE2	6.44	1.52	1.39
1	A	678	GLU	CD-OE1	6.43	1.32	1.25
3	C	81	GLU	C-O	6.43	1.35	1.23
2	B	366	GLN	C-O	-6.43	1.11	1.23
1	A	1003	LYS	CE-NZ	6.43	1.65	1.49
8	J	9	SER	CB-OG	6.43	1.50	1.42
1	A	264	PHE	CA-CB	6.42	1.68	1.53
1	A	895	LYS	CG-CD	6.42	1.74	1.52
1	A	1044	TRP	CE3-CZ3	6.42	1.49	1.38
2	B	732	SER	CA-CB	6.42	1.62	1.52
1	A	1093	LYS	CG-CD	6.42	1.74	1.52
2	B	1220	ARG	NE-CZ	6.42	1.41	1.33
1	A	971	PHE	CG-CD1	-6.41	1.29	1.38
3	C	254	LYS	CA-C	-6.41	1.36	1.52
9	K	81	TYR	C-O	-6.41	1.11	1.23
1	A	923	LEU	C-O	6.41	1.35	1.23
9	K	73	LEU	C-O	6.41	1.35	1.23
2	B	106	ASP	CA-C	6.40	1.69	1.52
1	A	469	ARG	NE-CZ	-6.40	1.24	1.33
2	B	1091	TYR	CD2-CE2	6.40	1.49	1.39
1	A	22	PHE	CB-CG	-6.40	1.40	1.51
5	F	148	VAL	C-O	6.40	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	44	TYR	CE1-CZ	-6.40	1.30	1.38
1	A	617	VAL	CA-CB	-6.39	1.41	1.54
2	B	1087	PHE	CD2-CE2	-6.39	1.26	1.39
2	B	369	GLY	CA-C	6.39	1.62	1.51
2	B	1134	GLU	CB-CG	6.39	1.64	1.52
1	A	1262	LYS	CB-CG	6.39	1.69	1.52
5	F	102	SER	CB-OG	-6.39	1.33	1.42
2	B	851	PHE	CD1-CE1	-6.39	1.26	1.39
7	I	45	ARG	CD-NE	6.38	1.57	1.46
1	A	288	ALA	CA-CB	6.38	1.65	1.52
3	C	208	GLU	CG-CD	6.38	1.61	1.51
4	E	40	GLU	CB-CG	6.38	1.64	1.52
1	A	975	HIS	CA-C	6.38	1.69	1.52
3	C	267	GLN	N-CA	6.38	1.59	1.46
1	A	739	ASP	CB-CG	6.37	1.65	1.51
1	A	1433	MET	SD-CE	-6.37	1.42	1.77
1	A	461	LYS	CD-CE	6.37	1.67	1.51
5	F	97	ARG	CA-CB	-6.37	1.40	1.53
1	A	1009	ASN	CG-OD1	6.37	1.38	1.24
2	B	279	ASP	CB-CG	6.37	1.65	1.51
3	C	215	GLU	CG-CD	6.37	1.61	1.51
1	A	568	PRO	CB-CG	-6.37	1.18	1.50
2	B	996	ARG	NE-CZ	-6.37	1.24	1.33
3	C	47	ASP	CG-OD2	6.37	1.40	1.25
7	I	90	GLN	C-O	-6.37	1.11	1.23
2	B	138	GLU	N-CA	6.36	1.59	1.46
1	A	934	LYS	CG-CD	6.36	1.74	1.52
1	A	1145	SER	C-O	-6.36	1.11	1.23
9	K	66	PRO	N-CD	-6.36	1.39	1.47
7	I	11	ASN	CB-CG	-6.36	1.36	1.51
10	L	66	GLN	CD-NE2	6.36	1.48	1.32
1	A	593	GLU	CD-OE1	6.36	1.32	1.25
1	A	1372	VAL	CB-CG2	-6.36	1.39	1.52
1	A	514	PRO	CA-C	-6.36	1.40	1.52
2	B	252	SER	CA-CB	6.35	1.62	1.52
4	E	99	HIS	N-CA	6.35	1.59	1.46
1	A	618	GLU	CG-CD	6.35	1.61	1.51
1	A	393	ARG	CZ-NH2	6.35	1.41	1.33
9	K	96	ASN	CB-CG	6.35	1.65	1.51
6	H	117	SER	C-O	6.34	1.35	1.23
1	A	593	GLU	CB-CG	6.34	1.64	1.52
2	B	166	PHE	CB-CG	-6.34	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1362	TYR	CD1-CE1	6.34	1.48	1.39
4	E	79	TRP	CB-CG	6.34	1.61	1.50
1	A	551	TYR	CG-CD2	-6.33	1.30	1.39
1	A	1008	GLN	CB-CG	6.33	1.69	1.52
2	B	1064	TYR	CG-CD1	-6.33	1.30	1.39
1	A	792	TYR	CA-C	-6.33	1.36	1.52
10	L	67	PHE	CG-CD2	-6.33	1.29	1.38
1	A	461	LYS	CA-CB	-6.33	1.40	1.53
2	B	312	GLU	CG-CD	6.33	1.61	1.51
10	L	65	VAL	CA-C	-6.32	1.36	1.52
2	B	908	GLU	CG-CD	6.32	1.61	1.51
2	B	1047	PHE	CD2-CE2	6.32	1.51	1.39
2	B	1106	ARG	NE-CZ	6.32	1.41	1.33
3	C	148	ARG	CZ-NH1	6.32	1.41	1.33
7	I	72	ASP	CG-OD2	6.32	1.39	1.25
2	B	962	LYS	CE-NZ	6.32	1.64	1.49
2	B	1018	PRO	CA-C	-6.32	1.40	1.52
2	B	397	ASP	CG-OD2	6.32	1.39	1.25
5	F	87	LYS	CG-CD	6.32	1.74	1.52
1	A	911	SER	C-O	6.31	1.35	1.23
2	B	526	GLU	CD-OE2	6.31	1.32	1.25
2	B	336	ARG	CZ-NH1	6.31	1.41	1.33
2	B	396	ASP	C-O	6.31	1.35	1.23
2	B	358	LYS	CB-CG	6.31	1.69	1.52
3	C	108	GLU	C-O	6.31	1.35	1.23
7	I	36	GLU	CA-CB	-6.31	1.40	1.53
1	A	274	ILE	CB-CG2	6.30	1.72	1.52
9	K	70	ARG	CZ-NH1	-6.30	1.24	1.33
2	B	343	ILE	CB-CG2	-6.30	1.33	1.52
6	H	136	LYS	CA-CB	6.30	1.67	1.53
1	A	1287	TYR	CD2-CE2	6.30	1.48	1.39
3	C	199	LYS	CG-CD	6.30	1.73	1.52
10	L	27	LEU	CA-CB	6.29	1.68	1.53
3	C	22	LEU	C-O	-6.29	1.11	1.23
1	A	292	ALA	CA-CB	6.29	1.65	1.52
9	K	16	GLU	CD-OE2	6.29	1.32	1.25
1	A	1157	ASP	C-O	6.29	1.35	1.23
9	K	38	GLU	CD-OE2	-6.29	1.18	1.25
2	B	691	GLU	CG-CD	6.28	1.61	1.51
1	A	551	TYR	CB-CG	6.28	1.61	1.51
2	B	706	GLN	CD-NE2	6.28	1.48	1.32
2	B	249	ARG	CB-CG	6.28	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	792	TYR	CE2-CZ	-6.28	1.30	1.38
5	F	87	LYS	CE-NZ	6.28	1.64	1.49
6	H	20	TYR	CD2-CE2	-6.28	1.29	1.39
6	H	115	TYR	CD1-CE1	6.28	1.48	1.39
1	A	1332	PHE	CE1-CZ	-6.27	1.25	1.37
2	B	351	TYR	C-O	6.27	1.35	1.23
1	A	1318	THR	C-O	-6.27	1.11	1.23
2	B	792	MET	C-O	-6.26	1.11	1.23
2	B	846	ILE	CA-CB	6.26	1.69	1.54
2	B	1108	ARG	N-CA	6.26	1.58	1.46
1	A	852	TYR	CZ-OH	-6.26	1.27	1.37
1	A	880	LYS	C-O	-6.26	1.11	1.23
2	B	384	ARG	CG-CD	6.26	1.67	1.51
1	A	967	ALA	CA-CB	-6.26	1.39	1.52
2	B	1087	PHE	C-O	-6.26	1.11	1.23
1	A	622	VAL	CB-CG1	-6.26	1.39	1.52
1	A	1189	SER	C-O	-6.26	1.11	1.23
2	B	579	ARG	CG-CD	6.26	1.67	1.51
4	E	35	VAL	CB-CG1	-6.25	1.39	1.52
1	A	469	ARG	CG-CD	6.25	1.67	1.51
1	A	1002	GLY	CA-C	6.25	1.61	1.51
3	C	160	LYS	CG-CD	6.25	1.73	1.52
4	E	21	GLU	CG-CD	6.24	1.61	1.51
1	A	1225	PHE	CB-CG	6.24	1.61	1.51
1	A	94	GLY	CA-C	6.24	1.61	1.51
2	B	937	ALA	CA-CB	6.24	1.65	1.52
4	E	191	LYS	C-O	-6.24	1.11	1.23
2	B	626	ILE	CA-CB	-6.24	1.40	1.54
2	B	870	ILE	C-O	6.24	1.35	1.23
1	A	885	THR	N-CA	-6.23	1.33	1.46
3	C	75	MET	CB-CG	-6.23	1.31	1.51
1	A	76	GLU	CD-OE1	6.22	1.32	1.25
9	K	88	LYS	CG-CD	6.22	1.73	1.52
1	A	95	PHE	CD1-CE1	6.22	1.51	1.39
1	A	1026	LEU	C-O	-6.22	1.11	1.23
1	A	1034	GLU	CG-CD	6.22	1.61	1.51
10	L	47	ARG	CG-CD	6.22	1.67	1.51
2	B	353	LYS	CG-CD	6.22	1.73	1.52
2	B	1108	ARG	CA-C	6.22	1.69	1.52
5	F	98	ALA	CA-CB	-6.22	1.39	1.52
1	A	640	GLN	CD-OE1	6.21	1.37	1.24
2	B	972	LYS	CA-CB	-6.21	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1001	ARG	C-O	6.21	1.35	1.23
1	A	1092	LYS	CA-C	6.21	1.69	1.52
1	A	368	LYS	CE-NZ	6.21	1.64	1.49
1	A	787	PHE	CE2-CZ	-6.21	1.25	1.37
2	B	865	LYS	CB-CG	6.21	1.69	1.52
1	A	1315	GLU	CD-OE1	6.21	1.32	1.25
2	B	186	GLU	C-O	6.21	1.35	1.23
3	C	127	ARG	N-CA	6.21	1.58	1.46
6	H	130	ARG	NE-CZ	-6.20	1.25	1.33
2	B	780	VAL	CB-CG2	-6.20	1.39	1.52
1	A	852	TYR	CE1-CZ	-6.20	1.30	1.38
4	E	23	VAL	C-O	6.20	1.35	1.23
4	E	145	THR	CA-CB	-6.20	1.37	1.53
2	B	624	LEU	CA-CB	-6.20	1.39	1.53
3	C	78	GLU	CD-OE1	6.20	1.32	1.25
1	A	347	PHE	CG-CD2	6.19	1.48	1.38
1	A	572	TRP	CZ3-CH2	-6.19	1.30	1.40
1	A	1025	ARG	CG-CD	-6.19	1.36	1.51
2	B	910	VAL	C-O	-6.19	1.11	1.23
1	A	1417	GLU	CA-CB	6.19	1.67	1.53
2	B	1087	PHE	CD1-CE1	-6.19	1.26	1.39
3	C	63	ILE	CA-CB	6.19	1.69	1.54
1	A	1349	TYR	C-O	-6.19	1.11	1.23
2	B	763	GLN	CB-CG	-6.18	1.35	1.52
2	B	803	LEU	CA-CB	-6.18	1.39	1.53
1	A	15	LYS	CB-CG	6.18	1.69	1.52
1	A	1208	THR	C-O	6.18	1.35	1.23
2	B	666	TYR	CG-CD2	6.18	1.47	1.39
2	B	263	GLY	C-O	6.18	1.33	1.23
3	C	165	LYS	CD-CE	6.18	1.66	1.51
2	B	832	GLY	CA-C	-6.18	1.42	1.51
4	E	187	TYR	CD2-CE2	6.18	1.48	1.39
6	H	118	PHE	CE2-CZ	6.18	1.49	1.37
1	A	24	PRO	CA-C	6.17	1.65	1.52
1	A	681	GLU	CB-CG	6.17	1.63	1.52
1	A	814	PHE	CE1-CZ	-6.17	1.25	1.37
5	F	144	GLU	CD-OE1	6.17	1.32	1.25
10	L	62	LYS	CE-NZ	6.17	1.64	1.49
2	B	855	PHE	CE2-CZ	-6.17	1.25	1.37
7	I	28	GLU	C-O	-6.17	1.11	1.23
1	A	491	VAL	C-O	-6.17	1.11	1.23
1	A	1417	GLU	CB-CG	6.17	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	194	GLU	C-O	-6.16	1.11	1.23
1	A	346	ASP	CA-CB	6.16	1.67	1.53
4	E	42	PHE	CD2-CE2	6.16	1.51	1.39
2	B	49	ASP	CB-CG	6.16	1.64	1.51
1	A	1151	GLU	CD-OE1	6.16	1.32	1.25
2	B	109	THR	CA-CB	6.16	1.69	1.53
10	L	67	PHE	C-O	-6.16	1.11	1.23
1	A	592	ASP	CG-OD1	6.15	1.39	1.25
1	A	22	PHE	CE1-CZ	6.15	1.49	1.37
1	A	1420	ASP	CG-OD1	6.15	1.39	1.25
7	I	120	GLN	CG-CD	6.15	1.65	1.51
6	H	105	GLU	CD-OE2	6.15	1.32	1.25
6	H	14	GLU	CD-OE2	6.15	1.32	1.25
3	C	148	ARG	CD-NE	6.15	1.56	1.46
2	B	550	ASP	C-O	6.14	1.35	1.23
3	C	241	ASP	CA-CB	6.14	1.67	1.53
1	A	808	LEU	N-CA	-6.14	1.34	1.46
2	B	224	GLN	CB-CG	6.14	1.69	1.52
2	B	602	THR	CB-CG2	-6.14	1.32	1.52
4	E	138	ALA	C-O	-6.13	1.11	1.23
1	A	1030	ARG	CZ-NH2	-6.13	1.25	1.33
2	B	793	ALA	C-O	-6.13	1.11	1.23
1	A	696	GLU	CD-OE2	-6.13	1.19	1.25
2	B	38	PHE	CD1-CE1	-6.13	1.26	1.39
2	B	137	TYR	CG-CD2	6.13	1.47	1.39
1	A	1202	MET	CG-SD	-6.13	1.65	1.81
2	B	268	THR	C-O	-6.13	1.11	1.23
2	B	368	GLU	CA-CB	6.13	1.67	1.53
2	B	1060	ARG	CB-CG	-6.12	1.36	1.52
3	C	37	MET	CA-CB	-6.12	1.40	1.53
1	A	286	HIS	CB-CG	6.12	1.61	1.50
1	A	445	ASN	C-O	6.12	1.34	1.23
1	A	1349	TYR	CE2-CZ	-6.12	1.30	1.38
1	A	1376	THR	C-O	-6.12	1.11	1.23
1	A	900	ASP	N-CA	6.12	1.58	1.46
2	B	1224	PHE	CB-CG	6.12	1.61	1.51
2	B	1168	LEU	CA-C	-6.11	1.37	1.52
2	B	256	VAL	CB-CG2	-6.11	1.40	1.52
1	A	590	ARG	CZ-NH2	-6.11	1.25	1.33
2	B	638	PHE	CD2-CE2	-6.11	1.27	1.39
3	C	205	LYS	N-CA	6.11	1.58	1.46
3	C	180	TYR	CB-CG	-6.11	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	SER	C-O	-6.11	1.11	1.23
2	B	797	TYR	CE2-CZ	-6.11	1.30	1.38
1	A	396	PRO	CA-C	-6.11	1.40	1.52
2	B	466	TRP	C-N	6.11	1.44	1.33
2	B	1181	GLU	CD-OE2	-6.11	1.19	1.25
2	B	138	GLU	CD-OE1	-6.10	1.19	1.25
2	B	1156	ASP	CA-CB	6.10	1.67	1.53
1	A	1328	TYR	C-O	-6.10	1.11	1.23
3	C	214	ASN	C-O	6.10	1.34	1.23
2	B	91	SER	C-O	6.10	1.34	1.23
2	B	974	PRO	C-O	-6.10	1.11	1.23
1	A	360	GLU	CD-OE2	6.10	1.32	1.25
8	J	1	MET	CG-SD	-6.09	1.65	1.81
1	A	238	CYS	C-O	-6.09	1.11	1.23
2	B	169	ARG	CZ-NH2	6.09	1.41	1.33
8	J	44	TYR	CG-CD2	-6.09	1.31	1.39
10	L	46	VAL	CB-CG2	6.09	1.65	1.52
4	E	37	LEU	CG-CD2	6.09	1.74	1.51
2	B	1028	GLU	CG-CD	6.08	1.61	1.51
3	C	55	THR	CB-OG1	-6.08	1.31	1.43
2	B	984	HIS	C-O	-6.08	1.11	1.23
3	C	87	PHE	CE1-CZ	6.08	1.49	1.37
4	E	77	SER	N-CA	-6.08	1.34	1.46
2	B	680	THR	CB-CG2	-6.08	1.32	1.52
2	B	646	LEU	CB-CG	6.08	1.70	1.52
7	I	118	ARG	CD-NE	6.08	1.56	1.46
1	A	630	ILE	CB-CG2	-6.07	1.34	1.52
2	B	650	GLU	CD-OE1	6.07	1.32	1.25
3	C	231	ASN	CB-CG	6.07	1.65	1.51
2	B	945	GLU	CD-OE2	6.07	1.32	1.25
2	B	1050	ILE	C-O	-6.07	1.11	1.23
1	A	768	GLN	C-O	-6.07	1.11	1.23
1	A	1018	PHE	CB-CG	-6.07	1.41	1.51
1	A	247	ARG	C-O	6.06	1.34	1.23
1	A	1222	ASN	CA-CB	6.06	1.69	1.53
1	A	387	ARG	CG-CD	6.06	1.67	1.51
1	A	880	LYS	N-CA	-6.06	1.34	1.46
2	B	24	PRO	CA-CB	-6.06	1.41	1.53
3	C	255	VAL	CA-CB	-6.06	1.42	1.54
4	E	7	ARG	CG-CD	6.06	1.67	1.51
7	I	44	TYR	CG-CD2	6.06	1.47	1.39
2	B	682	SER	CA-C	-6.06	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	65	ASP	N-CA	6.05	1.58	1.46
2	B	589	VAL	CA-CB	-6.05	1.42	1.54
3	C	157	CYS	CB-SG	-6.05	1.72	1.82
3	C	222	LYS	CG-CD	6.05	1.73	1.52
1	A	714	PHE	CE1-CZ	-6.05	1.25	1.37
8	J	45	CYS	CB-SG	6.05	1.92	1.82
1	A	53	LEU	CG-CD1	6.05	1.74	1.51
3	C	177	GLU	CD-OE1	6.05	1.32	1.25
1	A	893	PHE	CD2-CE2	6.04	1.51	1.39
7	I	101	PHE	CD2-CE2	6.04	1.51	1.39
2	B	797	TYR	CG-CD2	-6.04	1.31	1.39
1	A	668	ASP	CA-CB	-6.04	1.40	1.53
1	A	76	GLU	CD-OE2	6.04	1.32	1.25
2	B	951	GLN	N-CA	-6.04	1.34	1.46
2	B	977	GLY	C-O	-6.04	1.14	1.23
3	C	120	ILE	CA-CB	-6.04	1.41	1.54
1	A	540	PHE	C-O	-6.03	1.11	1.23
1	A	969	GLN	CD-OE1	6.03	1.37	1.24
1	A	1013	ASP	CG-OD2	6.03	1.39	1.25
9	K	66	PRO	CB-CG	-6.03	1.19	1.50
1	A	894	GLU	CD-OE2	6.03	1.32	1.25
1	A	1062	GLU	CG-CD	-6.03	1.43	1.51
1	A	1322	ILE	CB-CG2	-6.03	1.34	1.52
2	B	560	GLU	CG-CD	6.03	1.60	1.51
1	A	1281	ARG	CG-CD	6.03	1.67	1.51
2	B	983	ARG	CG-CD	6.03	1.67	1.51
4	E	176	PRO	N-CD	-6.03	1.39	1.47
1	A	1425	SER	CB-OG	6.02	1.50	1.42
6	H	115	TYR	CB-CG	-6.02	1.42	1.51
2	B	585	VAL	CB-CG2	-6.02	1.40	1.52
2	B	775	LYS	CE-NZ	6.02	1.64	1.49
3	C	211	ASP	CG-OD2	6.02	1.39	1.25
1	A	994	GLN	CA-C	-6.02	1.37	1.52
1	A	1118	VAL	N-CA	-6.02	1.34	1.46
2	B	190	TYR	CD1-CE1	6.02	1.48	1.39
1	A	1256	GLU	CA-CB	6.01	1.67	1.53
7	I	85	PHE	C-O	-6.01	1.11	1.23
3	C	49	VAL	C-O	-6.01	1.11	1.23
2	B	401	PHE	CB-CG	-6.01	1.41	1.51
1	A	702	LEU	N-CA	-6.01	1.34	1.46
1	A	866	PHE	CD2-CE2	6.01	1.51	1.39
1	A	656	TRP	CG-CD2	-6.00	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1103	GLU	CB-CG	-6.00	1.40	1.52
2	B	18	PHE	CA-CB	6.00	1.67	1.53
2	B	708	GLU	CD-OE1	6.00	1.32	1.25
5	F	92	ARG	CA-CB	-6.00	1.40	1.53
1	A	408	ASP	C-O	6.00	1.34	1.23
7	I	121	PHE	CG-CD1	-6.00	1.29	1.38
1	A	264	PHE	CE2-CZ	6.00	1.48	1.37
2	B	1132	GLU	CB-CG	6.00	1.63	1.52
1	A	1103	GLU	CG-CD	6.00	1.60	1.51
8	J	26	GLN	CG-CD	6.00	1.64	1.51
3	C	209	TYR	CG-CD1	5.99	1.47	1.39
3	C	260	LEU	CG-CD2	5.99	1.74	1.51
1	A	1071	SER	CA-CB	-5.99	1.44	1.52
5	F	149	GLU	CD-OE2	5.99	1.32	1.25
1	A	409	SER	CA-CB	5.99	1.61	1.52
1	A	954	TRP	CD2-CE2	-5.99	1.34	1.41
2	B	613	VAL	CA-CB	5.99	1.67	1.54
1	A	801	GLU	CA-CB	-5.99	1.40	1.53
7	I	67	THR	C-O	-5.99	1.11	1.23
1	A	1303	GLU	CD-OE2	5.99	1.32	1.25
2	B	691	GLU	CD-OE1	5.99	1.32	1.25
1	A	350	ARG	C-O	-5.98	1.11	1.23
2	B	203	PHE	CE2-CZ	-5.98	1.25	1.37
10	L	29	TYR	CE2-CZ	-5.98	1.30	1.38
1	A	715	GLU	CB-CG	5.98	1.63	1.52
6	H	109	LYS	CB-CG	5.98	1.68	1.52
2	B	1183	LYS	CA-C	5.98	1.68	1.52
2	B	892	LYS	CE-NZ	5.98	1.64	1.49
1	A	839	ARG	CZ-NH1	5.98	1.40	1.33
2	B	1180	PHE	CE1-CZ	5.98	1.48	1.37
1	A	1443	VAL	CB-CG1	-5.97	1.40	1.52
2	B	46	GLN	CG-CD	-5.97	1.37	1.51
7	I	72	ASP	CG-OD1	5.97	1.39	1.25
1	A	1325	THR	CB-CG2	-5.97	1.32	1.52
10	L	68	GLU	CB-CG	5.97	1.63	1.52
1	A	1159	ARG	CB-CG	5.97	1.68	1.52
1	A	1359	ASP	CG-OD1	5.97	1.39	1.25
2	B	654	ARG	CZ-NH1	-5.97	1.25	1.33
2	B	312	GLU	CD-OE2	5.96	1.32	1.25
5	F	108	PHE	N-CA	-5.96	1.34	1.46
1	A	572	TRP	CB-CG	-5.96	1.39	1.50
1	A	367	PRO	CA-C	-5.96	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	857	ARG	C-O	-5.96	1.12	1.23
3	C	205	LYS	CB-CG	5.96	1.68	1.52
1	A	1284	MET	CA-C	-5.96	1.37	1.52
2	B	835	GLN	CB-CG	5.96	1.68	1.52
1	A	299	HIS	C-O	-5.96	1.12	1.23
2	B	734	HIS	C-N	5.95	1.47	1.34
1	A	505	CYS	C-O	-5.95	1.12	1.23
1	A	1285	MET	CB-CG	5.95	1.70	1.51
2	B	96	TYR	CD1-CE1	5.95	1.48	1.39
2	B	262	GLU	CD-OE2	5.95	1.32	1.25
2	B	486	TYR	CG-CD2	5.95	1.46	1.39
3	C	169	LYS	CD-CE	5.95	1.66	1.51
1	A	655	PHE	CB-CG	-5.95	1.41	1.51
1	A	485	ASP	C-O	-5.95	1.12	1.23
1	A	1256	GLU	N-CA	5.95	1.58	1.46
2	B	582	VAL	C-O	-5.95	1.12	1.23
5	F	76	LYS	CE-NZ	5.95	1.64	1.49
2	B	702	LEU	CG-CD2	-5.94	1.29	1.51
2	B	866	TYR	CE1-CZ	5.94	1.46	1.38
3	C	158	VAL	C-O	-5.94	1.12	1.23
3	C	222	LYS	CB-CG	5.94	1.68	1.52
6	H	22	LYS	CB-CG	5.94	1.68	1.52
1	A	666	ILE	CA-CB	-5.93	1.41	1.54
2	B	866	TYR	CG-CD1	5.93	1.46	1.39
1	A	398	GLU	CD-OE1	5.93	1.32	1.25
1	A	1289	ARG	CB-CG	-5.93	1.36	1.52
1	A	672	ASP	CA-CB	5.93	1.67	1.53
1	A	1289	ARG	CZ-NH2	-5.93	1.25	1.33
2	B	1180	PHE	CD1-CE1	-5.93	1.27	1.39
6	H	90	ALA	CA-CB	-5.93	1.40	1.52
2	B	876	LYS	C-O	-5.93	1.12	1.23
1	A	858	ASN	CB-CG	-5.93	1.37	1.51
7	I	5	ARG	C-O	5.92	1.34	1.23
9	K	48	ALA	CA-CB	-5.92	1.40	1.52
4	E	44	ALA	C-O	5.92	1.34	1.23
1	A	1153	TYR	CG-CD1	-5.92	1.31	1.39
2	B	370	PHE	CG-CD1	5.92	1.47	1.38
1	A	1038	THR	CA-C	-5.91	1.37	1.52
2	B	466	TRP	C-O	5.91	1.34	1.23
2	B	125	SER	CA-CB	5.91	1.61	1.52
2	B	822	ASN	C-O	-5.91	1.12	1.23
7	I	24	ARG	CG-CD	5.91	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	82	GLU	CD-OE2	5.91	1.32	1.25
1	A	489	LEU	C-O	-5.91	1.12	1.23
10	L	40	LEU	CB-CG	5.91	1.69	1.52
1	A	867	ILE	CB-CG1	-5.90	1.37	1.54
2	B	304	ASP	N-CA	5.90	1.58	1.46
1	A	1023	ARG	CA-C	-5.90	1.37	1.52
3	C	181	ASP	CA-C	-5.90	1.37	1.52
6	H	131	ASN	N-CA	5.90	1.58	1.46
2	B	358	LYS	CE-NZ	5.90	1.63	1.49
2	B	1100	ASP	CA-CB	5.90	1.67	1.53
3	C	68	GLY	N-CA	5.90	1.54	1.46
1	A	466	SER	N-CA	5.90	1.58	1.46
4	E	113	GLN	CG-CD	5.90	1.64	1.51
7	I	59	VAL	CB-CG1	-5.90	1.40	1.52
6	H	19	ARG	N-CA	5.89	1.58	1.46
1	A	717	ASN	CG-OD1	5.89	1.36	1.24
2	B	958	GLN	N-CA	5.89	1.58	1.46
1	A	803	SER	CB-OG	5.89	1.50	1.42
1	A	897	TYR	CD1-CE1	-5.89	1.30	1.39
1	A	1077	THR	CB-CG2	5.89	1.71	1.52
3	C	15	LYS	CB-CG	5.88	1.68	1.52
3	C	79	GLN	CD-OE1	5.88	1.36	1.24
1	A	962	ARG	CG-CD	5.88	1.66	1.51
2	B	103	ASN	CA-CB	5.88	1.68	1.53
2	B	132	VAL	CB-CG1	-5.88	1.40	1.52
6	H	88	SER	N-CA	5.88	1.58	1.46
6	H	93	TYR	CE2-CZ	5.88	1.46	1.38
7	I	121	PHE	CD1-CE1	-5.88	1.27	1.39
2	B	323	VAL	C-O	-5.88	1.12	1.23
7	I	115	LYS	CD-CE	5.88	1.66	1.51
10	L	27	LEU	CG-CD1	5.87	1.73	1.51
2	B	25	ILE	C-O	-5.87	1.12	1.23
2	B	1150	ARG	CG-CD	-5.87	1.37	1.51
2	B	303	TYR	CG-CD1	5.87	1.46	1.39
1	A	1239	ARG	N-CA	-5.87	1.34	1.46
10	L	47	ARG	CB-CG	5.87	1.68	1.52
2	B	265	SER	CB-OG	5.86	1.49	1.42
2	B	737	THR	C-O	-5.86	1.12	1.23
1	A	393	ARG	NE-CZ	5.86	1.40	1.33
1	A	507	VAL	CA-CB	5.86	1.67	1.54
1	A	1311	VAL	N-CA	-5.86	1.34	1.46
5	F	121	ALA	CA-CB	-5.86	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	137	TYR	CE1-CZ	-5.86	1.30	1.38
2	B	625	LYS	CD-CE	5.86	1.65	1.51
1	A	619	LYS	CE-NZ	5.86	1.63	1.49
1	A	830	LYS	N-CA	5.85	1.58	1.46
2	B	546	SER	C-O	-5.85	1.12	1.23
3	C	56	THR	CB-CG2	-5.85	1.33	1.52
6	H	78	SER	C-O	-5.85	1.12	1.23
7	I	44	TYR	CD2-CE2	5.85	1.48	1.39
1	A	1154	TYR	CZ-OH	5.84	1.47	1.37
2	B	466	TRP	CG-CD1	5.84	1.45	1.36
2	B	1043	ASP	CG-OD2	5.84	1.38	1.25
1	A	918	GLU	CG-CD	5.84	1.60	1.51
3	C	127	ARG	CG-CD	-5.84	1.37	1.51
2	B	120	ARG	CG-CD	5.84	1.66	1.51
2	B	818	PRO	CG-CD	-5.84	1.31	1.50
3	C	102	GLN	C-O	5.84	1.34	1.23
3	C	146	LYS	CE-NZ	-5.84	1.34	1.49
6	H	78	SER	CB-OG	-5.84	1.34	1.42
8	J	6	ARG	CB-CG	5.84	1.68	1.52
2	B	165	VAL	N-CA	5.84	1.58	1.46
7	I	112	SER	CA-CB	-5.84	1.44	1.52
1	A	44	THR	N-CA	5.84	1.58	1.46
3	C	78	GLU	CG-CD	5.84	1.60	1.51
5	F	129	LYS	CD-CE	5.84	1.65	1.51
1	A	19	PHE	CG-CD1	5.83	1.47	1.38
2	B	430	ARG	NE-CZ	5.82	1.40	1.33
2	B	529	GLU	N-CA	5.82	1.57	1.46
8	J	18	TRP	CA-CB	-5.82	1.41	1.53
1	A	12	ARG	CZ-NH1	5.82	1.40	1.33
7	I	27	PHE	CG-CD2	5.82	1.47	1.38
7	I	37	GLU	CD-OE2	5.82	1.32	1.25
9	K	10	PHE	CE1-CZ	-5.82	1.26	1.37
1	A	372	LYS	CE-NZ	-5.82	1.34	1.49
2	B	327	ARG	NE-CZ	-5.82	1.25	1.33
8	J	59	LYS	C-O	5.82	1.34	1.23
2	B	535	LEU	CG-CD1	-5.81	1.30	1.51
2	B	1146	PHE	C-O	-5.81	1.12	1.23
2	B	640	VAL	CB-CG1	-5.81	1.40	1.52
2	B	1027	ILE	N-CA	-5.81	1.34	1.46
2	B	1027	ILE	CA-CB	-5.81	1.41	1.54
3	C	42	PRO	CA-CB	-5.81	1.42	1.53
1	A	1140	HIS	CB-CG	-5.81	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	155	ARG	CZ-NH1	5.81	1.40	1.33
1	A	1001	ARG	N-CA	-5.80	1.34	1.46
2	B	360	PHE	CG-CD2	-5.80	1.30	1.38
3	C	29	MET	SD-CE	5.80	2.10	1.77
4	E	195	VAL	CA-CB	-5.80	1.42	1.54
1	A	555	ASP	CA-CB	5.80	1.66	1.53
1	A	847	ASP	CG-OD2	5.80	1.38	1.25
3	C	20	PHE	CE1-CZ	5.80	1.48	1.37
4	E	154	ILE	CB-CG2	-5.80	1.34	1.52
1	A	518	LYS	CB-CG	-5.80	1.36	1.52
2	B	315	LYS	CB-CG	-5.80	1.36	1.52
2	B	1154	ALA	N-CA	5.80	1.57	1.46
1	A	439	ASN	CG-ND2	-5.79	1.18	1.32
2	B	845	SER	C-O	5.79	1.34	1.23
9	K	68	PHE	CB-CG	-5.79	1.41	1.51
1	A	1202	MET	C-O	5.79	1.34	1.23
1	A	241	VAL	CB-CG1	5.79	1.65	1.52
1	A	799	PHE	CG-CD1	5.79	1.47	1.38
6	H	117	SER	N-CA	5.79	1.57	1.46
1	A	1301	GLU	CG-CD	5.78	1.60	1.51
6	H	135	LEU	CA-CB	5.78	1.67	1.53
1	A	917	SER	CA-C	-5.78	1.38	1.52
2	B	608	ASP	CG-OD2	5.78	1.38	1.25
1	A	434	ARG	CD-NE	-5.78	1.36	1.46
4	E	136	ASN	CG-ND2	5.78	1.47	1.32
1	A	1450	LEU	N-CA	5.78	1.57	1.46
7	I	83	ASN	C-O	5.78	1.34	1.23
7	I	57	GLY	C-O	-5.78	1.14	1.23
1	A	699	ALA	C-O	-5.77	1.12	1.23
2	B	800	GLN	CG-CD	5.77	1.64	1.51
2	B	839	MET	CG-SD	5.77	1.96	1.81
6	H	77	ARG	NE-CZ	5.77	1.40	1.33
6	H	129	TYR	CG-CD1	5.77	1.46	1.39
9	K	40	HIS	CA-CB	5.77	1.66	1.53
1	A	603	ASN	N-CA	-5.77	1.34	1.46
2	B	1008	PRO	CG-CD	-5.77	1.31	1.50
2	B	1034	VAL	CB-CG1	-5.77	1.40	1.52
1	A	685	GLU	CD-OE2	5.77	1.31	1.25
1	A	894	GLU	CB-CG	5.77	1.63	1.52
2	B	353	LYS	C-O	-5.77	1.12	1.23
3	C	26	ASP	CB-CG	5.77	1.63	1.51
2	B	178	ASN	CG-OD1	5.76	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	745	PRO	CA-CB	-5.76	1.42	1.53
2	B	882	THR	CB-CG2	5.76	1.71	1.52
2	B	763	GLN	CG-CD	5.76	1.64	1.51
1	A	700	ASN	CG-ND2	-5.76	1.18	1.32
3	C	7	GLN	CD-OE1	5.76	1.36	1.24
3	C	212	PRO	C-O	-5.76	1.11	1.23
5	F	152	ILE	N-CA	-5.76	1.34	1.46
2	B	481	GLN	C-O	5.76	1.34	1.23
4	E	212	ARG	CG-CD	5.76	1.66	1.51
8	J	63	TYR	CE2-CZ	-5.76	1.31	1.38
1	A	609	ASP	CB-CG	5.76	1.63	1.51
1	A	1287	TYR	CE2-CZ	5.76	1.46	1.38
7	I	96	SER	CA-CB	-5.76	1.44	1.52
1	A	554	PRO	N-CD	-5.76	1.39	1.47
1	A	1355	VAL	CB-CG2	-5.76	1.40	1.52
1	A	1328	TYR	CD2-CE2	-5.75	1.30	1.39
2	B	644	GLU	CD-OE1	5.75	1.31	1.25
1	A	346	ASP	CG-OD1	5.75	1.38	1.25
1	A	1112	LYS	CG-CD	5.75	1.72	1.52
2	B	1181	GLU	N-CA	5.75	1.57	1.46
2	B	1224	PHE	CE1-CZ	5.75	1.48	1.37
7	I	29	CYS	C-O	5.75	1.34	1.23
1	A	293	GLU	CD-OE2	5.75	1.31	1.25
1	A	1136	SER	CB-OG	5.74	1.49	1.42
1	A	553	VAL	C-N	-5.74	1.23	1.34
1	A	874	ASP	CA-C	-5.74	1.38	1.52
2	B	488	TYR	CG-CD1	5.74	1.46	1.39
3	C	97	VAL	CB-CG2	5.74	1.65	1.52
9	K	58	PHE	CD2-CE2	-5.74	1.27	1.39
1	A	371	ALA	CA-CB	-5.74	1.40	1.52
1	A	1188	GLN	CG-CD	5.74	1.64	1.51
1	A	662	PHE	CG-CD1	-5.74	1.30	1.38
2	B	581	PHE	CE2-CZ	-5.74	1.26	1.37
4	E	155	ARG	CD-NE	5.74	1.56	1.46
6	H	98	TYR	CD1-CE1	5.74	1.48	1.39
7	I	4	PHE	CE2-CZ	5.74	1.48	1.37
1	A	774	ARG	CZ-NH1	-5.73	1.25	1.33
8	J	49	MET	SD-CE	-5.73	1.45	1.77
2	B	727	LYS	CE-NZ	-5.73	1.34	1.49
3	C	89	GLU	CG-CD	5.73	1.60	1.51
2	B	1069	PHE	CB-CG	-5.73	1.41	1.51
2	B	1137	CYS	C-O	-5.73	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	184	ASN	N-CA	5.73	1.57	1.46
1	A	240	PRO	C-O	5.72	1.34	1.23
6	H	102	TYR	CE1-CZ	-5.72	1.31	1.38
1	A	362	ASP	CB-CG	-5.72	1.39	1.51
1	A	779	PHE	CE1-CZ	-5.72	1.26	1.37
2	B	916	THR	CA-C	5.72	1.67	1.52
3	C	108	GLU	CD-OE2	5.72	1.31	1.25
4	E	6	GLU	CD-OE2	5.72	1.31	1.25
9	K	102	LYS	CD-CE	5.72	1.65	1.51
1	A	1001	ARG	CZ-NH2	5.72	1.40	1.33
1	A	1290	LYS	CB-CG	5.72	1.68	1.52
1	A	839	ARG	CZ-NH2	5.72	1.40	1.33
2	B	250	PHE	CG-CD1	5.72	1.47	1.38
2	B	425	THR	CB-CG2	5.72	1.71	1.52
1	A	74	MET	SD-CE	5.71	2.09	1.77
2	B	1033	LYS	CB-CG	-5.71	1.37	1.52
1	A	264	PHE	CD2-CE2	5.71	1.50	1.39
2	B	604	ARG	CD-NE	-5.71	1.36	1.46
4	E	57	MET	CG-SD	5.71	1.96	1.81
3	C	228	PHE	C-O	-5.71	1.12	1.23
2	B	448	ILE	CA-CB	5.70	1.68	1.54
2	B	604	ARG	C-O	-5.70	1.12	1.23
1	A	771	GLU	CG-CD	5.70	1.60	1.51
1	A	1096	SER	CB-OG	5.70	1.49	1.42
7	I	48	LEU	CG-CD2	-5.70	1.30	1.51
1	A	860	LEU	C-O	-5.70	1.12	1.23
2	B	19	GLU	CA-CB	5.70	1.66	1.53
2	B	547	VAL	N-CA	5.70	1.57	1.46
1	A	1129	GLU	CB-CG	5.70	1.62	1.52
2	B	1031	LEU	CA-CB	-5.70	1.40	1.53
7	I	111	THR	CA-CB	-5.70	1.38	1.53
4	E	150	VAL	CB-CG2	-5.69	1.40	1.52
1	A	45	GLN	CA-C	5.69	1.67	1.52
1	A	546	VAL	CA-CB	-5.69	1.42	1.54
8	J	63	TYR	CG-CD2	-5.69	1.31	1.39
2	B	883	LEU	CG-CD2	5.69	1.73	1.51
6	H	87	ARG	CG-CD	5.69	1.66	1.51
2	B	734	HIS	C-O	5.69	1.34	1.23
6	H	24	CYS	CB-SG	-5.69	1.72	1.81
1	A	63	ARG	CB-CG	5.68	1.67	1.52
1	A	274	ILE	N-CA	5.68	1.57	1.46
1	A	980	ASP	C-O	5.68	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	75	CYS	CA-C	-5.68	1.38	1.52
2	B	569	TYR	CD1-CE1	-5.68	1.30	1.39
1	A	893	PHE	CB-CG	-5.68	1.41	1.51
1	A	1342	GLU	CD-OE2	5.68	1.31	1.25
2	B	866	TYR	CG-CD2	5.68	1.46	1.39
1	A	16	GLU	N-CA	5.68	1.57	1.46
3	C	234	SER	C-O	5.68	1.34	1.23
1	A	712	GLU	C-O	-5.68	1.12	1.23
2	B	1101	ASP	CA-CB	5.68	1.66	1.53
2	B	1153	GLU	CG-CD	5.68	1.60	1.51
3	C	267	GLN	C-O	5.68	1.34	1.23
9	K	112	GLN	CB-CG	5.68	1.67	1.52
1	A	813	PHE	CD2-CE2	5.67	1.50	1.39
1	A	1366	ARG	CD-NE	-5.67	1.36	1.46
4	E	195	VAL	CB-CG2	5.67	1.64	1.52
1	A	1223	ASP	CG-OD1	5.67	1.38	1.25
2	B	70	ILE	CB-CG2	5.67	1.70	1.52
2	B	120	ARG	CZ-NH2	5.67	1.40	1.33
3	C	167	HIS	CA-C	-5.67	1.38	1.52
8	J	1	MET	CA-CB	-5.67	1.41	1.53
1	A	1131	ALA	CA-CB	-5.67	1.40	1.52
2	B	198	ASP	CB-CG	-5.67	1.39	1.51
1	A	1450	LEU	CA-CB	5.67	1.66	1.53
6	H	13	SER	CB-OG	5.67	1.49	1.42
7	I	6	PHE	CE2-CZ	5.67	1.48	1.37
7	I	98	VAL	C-O	-5.67	1.12	1.23
1	A	486	GLU	CD-OE1	-5.67	1.19	1.25
1	A	839	ARG	C-O	-5.67	1.12	1.23
1	A	358	ASN	CA-C	-5.67	1.38	1.52
1	A	625	SER	CB-OG	5.67	1.49	1.42
1	A	656	TRP	CE3-CZ3	5.67	1.48	1.38
1	A	942	PHE	C-O	-5.67	1.12	1.23
2	B	18	PHE	CG-CD1	5.67	1.47	1.38
4	E	162	ARG	CA-CB	5.66	1.66	1.53
6	H	119	GLY	C-O	5.66	1.32	1.23
2	B	883	LEU	CB-CG	5.66	1.69	1.52
6	H	146	ARG	CZ-NH2	5.66	1.40	1.33
1	A	1212	VAL	CB-CG1	-5.66	1.41	1.52
6	H	44	VAL	CB-CG1	5.65	1.64	1.52
1	A	1023	ARG	CZ-NH1	-5.65	1.25	1.33
1	A	1287	TYR	CE1-CZ	5.65	1.45	1.38
2	B	479	VAL	CA-CB	-5.65	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	16	GLU	CB-CG	5.65	1.62	1.52
1	A	913	LEU	CA-CB	5.65	1.66	1.53
2	B	286	PHE	CE2-CZ	-5.65	1.26	1.37
4	E	38	PRO	CA-C	-5.65	1.41	1.52
1	A	688	LYS	CE-NZ	5.65	1.63	1.49
1	A	1027	ALA	N-CA	-5.65	1.35	1.46
2	B	1176	ASN	CB-CG	5.65	1.64	1.51
3	C	235	VAL	CB-CG1	-5.65	1.41	1.52
2	B	190	TYR	CA-CB	-5.65	1.41	1.53
8	J	58	GLU	CB-CG	5.65	1.62	1.52
2	B	370	PHE	CE1-CZ	5.64	1.48	1.37
1	A	474	VAL	CB-CG1	-5.64	1.41	1.52
1	A	978	PRO	CB-CG	5.64	1.78	1.50
2	B	856	PHE	CD1-CE1	5.64	1.50	1.39
3	C	201	TRP	CE3-CZ3	-5.64	1.28	1.38
4	E	135	PHE	CE2-CZ	5.64	1.48	1.37
1	A	895	LYS	CE-NZ	5.63	1.63	1.49
2	B	1129	ARG	CZ-NH1	5.63	1.40	1.33
1	A	1225	PHE	CD2-CE2	5.63	1.50	1.39
2	B	287	ARG	CG-CD	5.63	1.66	1.51
9	K	8	GLU	CD-OE2	5.63	1.31	1.25
10	L	63	ARG	NE-CZ	5.63	1.40	1.33
2	B	208	SER	C-O	5.63	1.34	1.23
1	A	536	LEU	CA-C	5.63	1.67	1.52
1	A	601	LYS	C-O	-5.63	1.12	1.23
4	E	23	VAL	N-CA	-5.63	1.35	1.46
4	E	72	PHE	CD2-CE2	-5.63	1.27	1.39
1	A	711	ARG	CA-C	-5.62	1.38	1.52
2	B	617	ARG	CA-CB	-5.62	1.41	1.53
5	F	109	VAL	CB-CG1	-5.62	1.41	1.52
1	A	1441	PHE	CG-CD1	-5.62	1.30	1.38
3	C	48	SER	CB-OG	5.62	1.49	1.42
6	H	146	ARG	CZ-NH1	5.62	1.40	1.33
7	I	74	GLU	CB-CG	5.62	1.62	1.52
1	A	95	PHE	CG-CD1	5.62	1.47	1.38
1	A	248	PRO	CB-CG	5.62	1.78	1.50
1	A	37	PHE	C-O	-5.62	1.12	1.23
1	A	789	LYS	CG-CD	-5.62	1.33	1.52
7	I	25	LEU	CG-CD2	-5.62	1.31	1.51
1	A	724	GLU	CB-CG	5.61	1.62	1.52
1	A	516	SER	CB-OG	5.61	1.49	1.42
2	B	1097	HIS	CB-CG	-5.61	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	122	LYS	CA-CB	5.61	1.66	1.53
7	I	100	PHE	CD2-CE2	5.61	1.50	1.39
2	B	380	TYR	CE1-CZ	-5.61	1.31	1.38
1	A	346	ASP	C-O	-5.61	1.12	1.23
1	A	431	LYS	CD-CE	5.61	1.65	1.51
2	B	660	LYS	CG-CD	5.61	1.71	1.52
1	A	1034	GLU	CA-CB	-5.60	1.41	1.53
1	A	458	HIS	C-O	5.60	1.33	1.23
1	A	589	GLN	CA-C	-5.60	1.38	1.52
2	B	486	TYR	CD2-CE2	5.60	1.47	1.39
7	I	87	GLN	CB-CG	5.60	1.67	1.52
2	B	1102	LYS	CA-CB	5.60	1.66	1.53
4	E	207	ARG	NE-CZ	5.60	1.40	1.33
1	A	572	TRP	CG-CD1	-5.60	1.28	1.36
2	B	397	ASP	C-O	5.60	1.33	1.23
7	I	70	ARG	CZ-NH2	-5.60	1.25	1.33
1	A	926	GLN	CD-OE1	5.59	1.36	1.24
4	E	91	LYS	CB-CG	5.59	1.67	1.52
7	I	45	ARG	CA-CB	-5.59	1.41	1.53
1	A	1080	THR	N-CA	5.59	1.57	1.46
1	A	285	PRO	CB-CG	-5.59	1.22	1.50
1	A	386	ASP	CG-OD1	5.59	1.38	1.25
2	B	997	GLU	N-CA	5.59	1.57	1.46
9	K	50	LEU	CG-CD2	-5.59	1.31	1.51
2	B	100	PRO	CB-CG	-5.59	1.22	1.50
1	A	880	LYS	CB-CG	5.59	1.67	1.52
2	B	269	ILE	CA-CB	-5.59	1.42	1.54
2	B	667	GLN	CD-OE1	5.59	1.36	1.24
2	B	787	VAL	N-CA	-5.59	1.35	1.46
3	C	10	ILE	CA-CB	-5.59	1.42	1.54
7	I	27	PHE	C-O	-5.59	1.12	1.23
1	A	853	ASP	CB-CG	5.58	1.63	1.51
3	C	155	LEU	C-O	5.58	1.33	1.23
1	A	776	ALA	CA-CB	-5.58	1.40	1.52
1	A	1304	TRP	CD2-CE2	-5.58	1.34	1.41
2	B	612	GLU	C-O	-5.58	1.12	1.23
3	C	192	TRP	CE2-CZ2	-5.58	1.30	1.39
6	H	111	LEU	CA-C	5.58	1.67	1.52
2	B	971	THR	N-CA	-5.58	1.35	1.46
4	E	16	PHE	CE1-CZ	-5.58	1.26	1.37
6	H	93	TYR	CE1-CZ	5.58	1.45	1.38
2	B	855	PHE	CE1-CZ	5.58	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	32	SER	C-O	5.58	1.33	1.23
1	A	801	GLU	CG-CD	5.58	1.60	1.51
2	B	1130	PHE	N-CA	-5.58	1.35	1.46
4	E	122	LYS	CD-CE	5.58	1.65	1.51
3	C	125	MET	CG-SD	5.57	1.95	1.81
6	H	136	LYS	CA-C	5.57	1.67	1.52
8	J	53	HIS	CG-CD2	-5.57	1.26	1.35
2	B	979	LYS	CB-CG	-5.57	1.37	1.52
3	C	119	VAL	CB-CG1	-5.57	1.41	1.52
2	B	1149	GLU	CG-CD	5.57	1.60	1.51
2	B	304	ASP	CB-CG	5.56	1.63	1.51
2	B	499	ASN	C-O	-5.56	1.12	1.23
3	C	143	LEU	CA-CB	-5.56	1.41	1.53
1	A	1309	ASP	CA-C	-5.56	1.38	1.52
4	E	169	ARG	CG-CD	5.56	1.65	1.51
10	L	27	LEU	CB-CG	5.56	1.68	1.52
1	A	264	PHE	CA-C	5.56	1.67	1.52
2	B	279	ASP	CG-OD1	5.56	1.38	1.25
6	H	19	ARG	CZ-NH2	5.56	1.40	1.33
3	C	209	TYR	CD1-CE1	5.56	1.47	1.39
3	C	211	ASP	CB-CG	5.56	1.63	1.51
1	A	655	PHE	CG-CD2	-5.55	1.30	1.38
3	C	214	ASN	N-CA	5.55	1.57	1.46
1	A	358	ASN	C-O	-5.55	1.12	1.23
1	A	411	ASP	C-O	-5.55	1.12	1.23
1	A	632	VAL	CB-CG1	-5.55	1.41	1.52
1	A	882	SER	C-O	-5.55	1.12	1.23
1	A	983	ILE	C-N	-5.55	1.21	1.34
1	A	686	ALA	C-O	-5.55	1.12	1.23
1	A	1002	GLY	C-O	5.55	1.32	1.23
3	C	187	LYS	CD-CE	5.55	1.65	1.51
9	K	72	LYS	C-O	-5.55	1.12	1.23
2	B	57	TYR	CD2-CE2	5.54	1.47	1.39
5	F	79	ARG	CZ-NH2	-5.54	1.25	1.33
1	A	449	SER	CB-OG	5.54	1.49	1.42
7	I	51	ASN	CB-CG	5.54	1.63	1.51
1	A	1411	GLU	CB-CG	5.54	1.62	1.52
2	B	499	ASN	CG-ND2	5.54	1.46	1.32
2	B	1196	ILE	CA-CB	-5.54	1.42	1.54
10	L	27	LEU	CG-CD2	5.54	1.72	1.51
1	A	836	TYR	CA-C	5.53	1.67	1.52
2	B	42	GLY	C-O	5.53	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	954	VAL	CB-CG2	5.53	1.64	1.52
1	A	623	GLY	C-O	5.53	1.32	1.23
1	A	400	PRO	C-O	-5.53	1.12	1.23
1	A	576	GLN	CA-C	-5.53	1.38	1.52
2	B	259	TYR	CD2-CE2	-5.53	1.31	1.39
1	A	881	GLN	CB-CG	-5.53	1.37	1.52
1	A	1339	LEU	CA-CB	-5.53	1.41	1.53
2	B	422	LYS	CG-CD	5.52	1.71	1.52
1	A	726	ARG	CZ-NH2	5.52	1.40	1.33
1	A	1303	GLU	C-O	-5.52	1.12	1.23
4	E	93	MET	SD-CE	5.52	2.08	1.77
1	A	383	TYR	CD1-CE1	5.52	1.47	1.39
1	A	770	VAL	C-O	-5.52	1.12	1.23
3	C	165	LYS	N-CA	5.52	1.57	1.46
4	E	48	ASP	CB-CG	5.52	1.63	1.51
1	A	643	ALA	CA-CB	-5.52	1.40	1.52
2	B	1023	VAL	CB-CG2	-5.52	1.41	1.52
6	H	140	ALA	CA-CB	-5.52	1.40	1.52
2	B	371	GLU	C-O	-5.52	1.12	1.23
7	I	103	CYS	C-O	-5.52	1.12	1.23
2	B	174	LEU	CG-CD1	5.52	1.72	1.51
6	H	120	GLY	C-O	5.52	1.32	1.23
2	B	271	ALA	C-O	-5.51	1.12	1.23
2	B	635	ARG	CZ-NH2	-5.51	1.25	1.33
1	A	969	GLN	CD-NE2	5.51	1.46	1.32
1	A	420	ARG	CZ-NH2	-5.51	1.25	1.33
1	A	39	GLU	CA-C	5.51	1.67	1.52
1	A	731	ARG	CZ-NH1	5.51	1.40	1.33
3	C	188	HIS	C-O	5.51	1.33	1.23
1	A	478	TYR	CG-CD1	-5.51	1.31	1.39
1	A	811	GLN	CB-CG	-5.51	1.37	1.52
2	B	610	ASN	C-O	5.51	1.33	1.23
6	H	50	ALA	N-CA	5.51	1.57	1.46
1	A	1311	VAL	CB-CG2	-5.50	1.41	1.52
2	B	994	TYR	CE2-CZ	-5.50	1.31	1.38
3	C	239	PRO	C-N	-5.50	1.21	1.34
7	I	74	GLU	CG-CD	5.50	1.60	1.51
9	K	108	GLU	CG-CD	5.50	1.60	1.51
5	F	78	GLN	C-O	-5.50	1.12	1.23
1	A	6	TYR	CD1-CE1	5.49	1.47	1.39
2	B	1004	GLU	C-O	5.49	1.33	1.23
1	A	41	MET	CG-SD	5.49	1.95	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	788	SER	C-O	-5.49	1.12	1.23
4	E	71	LYS	CE-NZ	-5.49	1.35	1.49
5	F	147	SER	CB-OG	5.49	1.49	1.42
1	A	984	LYS	CE-NZ	5.49	1.62	1.49
6	H	85	GLY	CA-C	5.49	1.60	1.51
7	I	8	ARG	CB-CG	5.49	1.67	1.52
2	B	1096	ARG	CB-CG	-5.49	1.37	1.52
2	B	401	PHE	C-O	-5.49	1.12	1.23
2	B	458	LYS	CD-CE	5.49	1.65	1.51
3	C	228	PHE	CG-CD1	-5.48	1.30	1.38
2	B	893	LEU	CG-CD2	-5.48	1.31	1.51
7	I	7	CYS	CB-SG	-5.48	1.72	1.81
1	A	500	GLU	CB-CG	-5.48	1.41	1.52
2	B	193	LYS	CD-CE	5.48	1.65	1.51
2	B	755	ILE	C-O	5.48	1.33	1.23
2	B	1215	ARG	NE-CZ	-5.48	1.25	1.33
4	E	162	ARG	CD-NE	5.47	1.55	1.46
1	A	425	GLN	CG-CD	5.47	1.63	1.51
7	I	50	THR	CA-C	-5.47	1.38	1.52
2	B	685	LEU	CG-CD1	-5.47	1.31	1.51
1	A	956	LEU	C-N	-5.47	1.23	1.34
2	B	333	PHE	CG-CD2	-5.47	1.30	1.38
7	I	73	ARG	CA-CB	-5.47	1.42	1.53
1	A	1328	TYR	CE2-CZ	5.46	1.45	1.38
2	B	110	HIS	CA-C	5.46	1.67	1.52
2	B	629	ASP	CB-CG	5.46	1.63	1.51
4	E	44	ALA	CA-CB	5.46	1.64	1.52
1	A	368	LYS	CD-CE	5.46	1.65	1.51
1	A	486	GLU	CG-CD	5.46	1.60	1.51
1	A	1280	GLU	CB-CG	5.46	1.62	1.52
2	B	202	TYR	CG-CD1	-5.46	1.32	1.39
2	B	557	PHE	CD2-CE2	-5.46	1.28	1.39
9	K	19	LEU	CA-CB	-5.46	1.41	1.53
9	K	55	LYS	CE-NZ	5.45	1.62	1.49
2	B	250	PHE	N-CA	5.45	1.57	1.46
2	B	972	LYS	CE-NZ	5.45	1.62	1.49
1	A	563	PRO	CG-CD	5.45	1.68	1.50
3	C	9	LYS	CE-NZ	5.45	1.62	1.49
1	A	293	GLU	N-CA	5.45	1.57	1.46
1	A	565	ILE	CB-CG2	-5.45	1.35	1.52
2	B	49	ASP	C-O	-5.45	1.13	1.23
2	B	486	TYR	CB-CG	-5.45	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	9	ILE	C-O	5.45	1.33	1.23
2	B	942	ARG	CZ-NH2	5.44	1.40	1.33
9	K	35	PHE	CD1-CE1	-5.44	1.28	1.39
1	A	1373	ASP	CG-OD2	5.44	1.37	1.25
2	B	225	VAL	CB-CG2	-5.44	1.41	1.52
2	B	780	VAL	C-O	-5.44	1.13	1.23
8	J	8	PHE	CD2-CE2	5.44	1.50	1.39
2	B	348	ARG	CZ-NH1	-5.44	1.25	1.33
3	C	43	THR	C-O	5.44	1.33	1.23
6	H	127	GLY	CA-C	5.44	1.60	1.51
4	E	137	GLU	CG-CD	5.44	1.60	1.51
10	L	64	LEU	CG-CD1	5.44	1.72	1.51
10	L	44	ASP	C-O	5.44	1.33	1.23
2	B	935	ARG	NE-CZ	5.43	1.40	1.33
4	E	121	MET	SD-CE	5.43	2.08	1.77
7	I	121	PHE	CE2-CZ	-5.43	1.27	1.37
1	A	11	LEU	C-O	-5.43	1.13	1.23
1	A	393	ARG	CG-CD	5.43	1.65	1.51
2	B	173	MET	CB-CG	5.43	1.68	1.51
10	L	66	GLN	CD-OE1	5.43	1.35	1.24
1	A	799	PHE	CE2-CZ	5.43	1.47	1.37
1	A	1117	THR	CA-CB	-5.43	1.39	1.53
1	A	468	PHE	CD2-CE2	-5.43	1.28	1.39
1	A	1418	LEU	CG-CD1	5.43	1.72	1.51
2	B	223	VAL	C-O	-5.43	1.13	1.23
4	E	35	VAL	CA-CB	-5.43	1.43	1.54
1	A	992	ASP	CB-CG	5.43	1.63	1.51
2	B	732	SER	CA-C	5.42	1.67	1.52
2	B	890	TYR	CD1-CE1	5.42	1.47	1.39
6	H	141	TYR	CG-CD2	-5.42	1.32	1.39
1	A	1156	PRO	C-O	5.42	1.34	1.23
9	K	25	THR	CB-CG2	5.42	1.70	1.52
4	E	34	GLU	CG-CD	5.42	1.60	1.51
3	C	196	ASP	CG-OD1	5.42	1.37	1.25
2	B	958	GLN	CA-CB	5.42	1.65	1.53
1	A	905	ASP	CA-CB	-5.41	1.42	1.53
1	A	271	LYS	CD-CE	5.41	1.64	1.51
2	B	658	ILE	CB-CG2	-5.41	1.36	1.52
2	B	743	ILE	CB-CG2	-5.41	1.36	1.52
2	B	790	ASP	CA-C	-5.41	1.38	1.52
3	C	193	TYR	CG-CD2	5.41	1.46	1.39
9	K	54	ARG	CZ-NH1	5.41	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	863	VAL	CB-CG1	5.41	1.64	1.52
1	A	1200	ALA	C-O	5.41	1.33	1.23
1	A	417	TYR	CD2-CE2	5.41	1.47	1.39
1	A	892	ALA	C-O	-5.41	1.13	1.23
2	B	578	THR	CB-CG2	-5.41	1.34	1.52
2	B	1109	GLY	CA-C	5.41	1.60	1.51
7	I	111	THR	C-O	-5.41	1.13	1.23
9	K	63	VAL	CB-CG2	5.40	1.64	1.52
1	A	899	VAL	CB-CG1	-5.40	1.41	1.52
2	B	105	SER	CA-C	5.40	1.67	1.52
2	B	367	LEU	CA-CB	5.40	1.66	1.53
2	B	632	ARG	NE-CZ	-5.40	1.26	1.33
6	H	136	LYS	N-CA	5.40	1.57	1.46
7	I	86	PHE	CG-CD2	5.40	1.46	1.38
4	E	202	SER	CB-OG	-5.40	1.35	1.42
1	A	1356	ILE	CA-CB	-5.40	1.42	1.54
1	A	1361	SER	CB-OG	5.40	1.49	1.42
9	K	29	ASN	CG-ND2	5.40	1.46	1.32
1	A	745	GLN	CD-OE1	5.40	1.35	1.24
1	A	833	GLU	CB-CG	5.39	1.62	1.52
2	B	949	VAL	CA-CB	-5.39	1.43	1.54
7	I	97	MET	N-CA	-5.39	1.35	1.46
1	A	50	ILE	N-CA	5.39	1.57	1.46
1	A	737	LEU	CG-CD2	5.39	1.71	1.51
1	A	6	TYR	CE1-CZ	5.39	1.45	1.38
9	K	82	ASP	C-O	-5.38	1.13	1.23
1	A	1042	PHE	CG-CD1	5.38	1.46	1.38
1	A	1426	GLU	CG-CD	5.38	1.60	1.51
2	B	227	LYS	C-O	-5.38	1.13	1.23
1	A	1036	ARG	C-O	-5.38	1.13	1.23
2	B	413	LEU	C-O	-5.38	1.13	1.23
2	B	901	PRO	CG-CD	5.38	1.68	1.50
1	A	61	ILE	CB-CG2	5.38	1.69	1.52
1	A	929	LEU	N-CA	-5.38	1.35	1.46
1	A	56	PRO	C-O	5.38	1.34	1.23
3	C	9	LYS	C-O	-5.38	1.13	1.23
6	H	143	LEU	CA-C	-5.38	1.39	1.52
8	J	47	ARG	CZ-NH1	-5.38	1.26	1.33
9	K	102	LYS	CB-CG	5.38	1.67	1.52
1	A	1236	LEU	CG-CD2	5.38	1.71	1.51
4	E	31	THR	CA-CB	5.38	1.67	1.53
2	B	830	TYR	CG-CD1	-5.37	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	804	GLY	N-CA	5.37	1.54	1.46
1	A	724	GLU	N-CA	-5.37	1.35	1.46
2	B	488	TYR	C-O	5.37	1.33	1.23
1	A	815	PHE	CG-CD2	-5.37	1.30	1.38
3	C	204	SER	C-O	5.37	1.33	1.23
5	F	84	TYR	CE2-CZ	5.37	1.45	1.38
9	K	2	ASN	CA-C	5.36	1.66	1.52
7	I	24	ARG	C-O	5.36	1.33	1.23
1	A	1341	ILE	CB-CG2	-5.36	1.36	1.52
1	A	536	LEU	C-O	5.36	1.33	1.23
1	A	872	GLY	CA-C	-5.36	1.43	1.51
1	A	1079	MET	C-O	5.36	1.33	1.23
2	B	360	PHE	C-O	5.36	1.33	1.23
4	E	79	TRP	C-O	-5.36	1.13	1.23
1	A	1129	GLU	CA-CB	5.35	1.65	1.53
3	C	62	PHE	CE1-CZ	5.35	1.47	1.37
1	A	370	ILE	C-O	-5.35	1.13	1.23
1	A	813	PHE	CG-CD2	-5.35	1.30	1.38
1	A	1327	ILE	N-CA	-5.35	1.35	1.46
7	I	6	PHE	CD1-CE1	5.35	1.50	1.39
4	E	47	CYS	CA-C	5.35	1.66	1.52
2	B	1135	ARG	CD-NE	-5.35	1.37	1.46
1	A	1237	ILE	CA-CB	-5.35	1.42	1.54
6	H	79	TRP	CA-CB	-5.35	1.42	1.53
2	B	1204	PHE	CB-CG	5.34	1.60	1.51
5	F	72	LYS	CG-CD	5.34	1.70	1.52
1	A	720	ARG	CD-NE	5.34	1.55	1.46
2	B	35	SER	CA-CB	-5.34	1.45	1.52
8	J	1	MET	SD-CE	5.34	2.07	1.77
2	B	1008	PRO	CA-CB	-5.34	1.42	1.53
3	C	159	ALA	N-CA	-5.34	1.35	1.46
1	A	462	VAL	CA-CB	-5.33	1.43	1.54
4	E	203	GLU	CA-CB	-5.33	1.42	1.53
1	A	387	ARG	CD-NE	5.33	1.55	1.46
1	A	925	LEU	N-CA	-5.33	1.35	1.46
2	B	199	MET	C-O	-5.33	1.13	1.23
2	B	224	GLN	N-CA	-5.33	1.35	1.46
1	A	1426	GLU	CB-CG	5.33	1.62	1.52
7	I	18	GLU	CD-OE2	5.33	1.31	1.25
5	F	149	GLU	C-O	5.33	1.33	1.23
1	A	1447	GLU	CB-CG	5.33	1.62	1.52
1	A	409	SER	CB-OG	5.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	620	LYS	CB-CG	5.32	1.67	1.52
1	A	857	ARG	CZ-NH2	5.32	1.40	1.33
2	B	367	LEU	CG-CD2	5.32	1.71	1.51
2	B	1073	TYR	CG-CD2	-5.32	1.32	1.39
2	B	1220	ARG	CG-CD	5.32	1.65	1.51
2	B	549	THR	C-O	5.32	1.33	1.23
2	B	798	TYR	CG-CD2	5.32	1.46	1.39
1	A	500	GLU	C-O	-5.32	1.13	1.23
1	A	1450	LEU	CA-C	5.32	1.66	1.52
2	B	224	GLN	C-O	-5.32	1.13	1.23
2	B	233	PRO	CB-CG	5.32	1.76	1.50
3	C	226	ASP	C-O	-5.32	1.13	1.23
4	E	83	CYS	CB-SG	5.32	1.91	1.82
7	I	1	MET	CA-CB	5.32	1.65	1.53
1	A	1298	TYR	CG-CD2	-5.32	1.32	1.39
2	B	1060	ARG	CZ-NH2	-5.32	1.26	1.33
2	B	810	GLU	CD-OE2	5.32	1.31	1.25
3	C	244	VAL	CA-CB	-5.32	1.43	1.54
10	L	47	ARG	NE-CZ	5.32	1.40	1.33
2	B	351	TYR	CD1-CE1	5.32	1.47	1.39
2	B	1191	ILE	CA-CB	-5.32	1.42	1.54
2	B	239	GLU	C-O	5.31	1.33	1.23
2	B	993	THR	CA-C	-5.31	1.39	1.52
4	E	40	GLU	CG-CD	5.31	1.59	1.51
1	A	1194	ARG	CD-NE	-5.31	1.37	1.46
2	B	280	ILE	CB-CG2	-5.31	1.36	1.52
2	B	887	HIS	CA-CB	5.31	1.65	1.53
3	C	268	ASP	CB-CG	5.31	1.62	1.51
7	I	87	GLN	C-O	-5.31	1.13	1.23
1	A	1362	TYR	CD2-CE2	-5.31	1.31	1.39
2	B	785	TYR	CZ-OH	-5.31	1.28	1.37
1	A	826	ASP	CB-CG	5.30	1.62	1.51
2	B	337	ARG	CZ-NH2	-5.30	1.26	1.33
1	A	32	VAL	CA-C	5.30	1.66	1.52
1	A	974	ASP	N-CA	5.30	1.56	1.46
2	B	643	ASP	C-O	-5.30	1.13	1.23
2	B	1087	PHE	CE1-CZ	-5.30	1.27	1.37
3	C	214	ASN	CB-CG	5.30	1.63	1.51
7	I	60	GLN	CG-CD	5.30	1.63	1.51
7	I	93	LYS	CG-CD	5.30	1.70	1.52
9	K	26	LYS	CA-C	5.30	1.66	1.52
8	J	38	ARG	CG-CD	-5.30	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	ARG	CD-NE	5.30	1.55	1.46
2	B	37	PHE	CA-CB	-5.30	1.42	1.53
3	C	3	GLU	CG-CD	5.30	1.59	1.51
3	C	4	GLU	CD-OE1	5.30	1.31	1.25
1	A	464	PRO	C-N	-5.29	1.21	1.34
1	A	14	VAL	CB-CG1	-5.29	1.41	1.52
1	A	838	GLN	CD-OE1	5.29	1.35	1.24
1	A	1127	ASP	CG-OD2	5.29	1.37	1.25
1	A	590	ARG	CB-CG	5.29	1.66	1.52
2	B	351	TYR	CD2-CE2	5.29	1.47	1.39
6	H	2	SER	N-CA	5.29	1.56	1.46
1	A	941	LYS	CA-CB	5.29	1.65	1.53
1	A	1225	PHE	CG-CD2	5.29	1.46	1.38
2	B	20	ASP	CB-CG	5.29	1.62	1.51
1	A	529	CYS	C-O	-5.29	1.13	1.23
1	A	1326	ARG	CZ-NH1	-5.29	1.26	1.33
5	F	135	ARG	CG-CD	5.29	1.65	1.51
6	H	22	LYS	C-O	5.29	1.33	1.23
6	H	104	PHE	CG-CD2	5.29	1.46	1.38
2	B	781	PHE	CE2-CZ	5.29	1.47	1.37
2	B	815	ARG	CD-NE	-5.29	1.37	1.46
2	B	371	GLU	CA-C	-5.29	1.39	1.52
2	B	904	ARG	CG-CD	-5.29	1.38	1.51
2	B	1021	MET	CG-SD	-5.28	1.67	1.81
1	A	1256	GLU	CB-CG	5.28	1.62	1.52
1	A	1308	THR	N-CA	-5.28	1.35	1.46
1	A	515	GLN	CG-CD	5.28	1.63	1.51
3	C	123	ASN	CB-CG	5.28	1.63	1.51
2	B	945	GLU	CG-CD	5.28	1.59	1.51
4	E	23	VAL	CB-CG1	5.28	1.64	1.52
7	I	1	MET	SD-CE	5.28	2.07	1.77
1	A	1224	LEU	C-O	-5.28	1.13	1.23
2	B	235	SER	N-CA	-5.28	1.35	1.46
2	B	328	GLU	CB-CG	5.28	1.62	1.52
2	B	606	LYS	CB-CG	-5.27	1.38	1.52
2	B	275	TYR	CD1-CE1	-5.27	1.31	1.39
2	B	561	TRP	CE3-CZ3	5.27	1.47	1.38
2	B	1211	ASN	CB-CG	-5.27	1.39	1.51
3	C	13	ALA	C-O	-5.27	1.13	1.23
2	B	165	VAL	CA-CB	5.27	1.65	1.54
2	B	1135	ARG	CG-CD	-5.27	1.38	1.51
1	A	821	ARG	NE-CZ	-5.26	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	35	PHE	CG-CD1	-5.26	1.30	1.38
1	A	469	ARG	CB-CG	5.26	1.66	1.52
1	A	598	LEU	CG-CD1	5.26	1.71	1.51
2	B	350	GLN	CA-CB	-5.26	1.42	1.53
3	C	240	VAL	CA-C	-5.26	1.39	1.52
1	A	303	TYR	CG-CD2	-5.26	1.32	1.39
2	B	776	GLN	CG-CD	5.26	1.63	1.51
3	C	154	LYS	CE-NZ	5.26	1.62	1.49
4	E	21	GLU	CD-OE2	5.26	1.31	1.25
4	E	30	ILE	CA-CB	5.26	1.67	1.54
1	A	556	TRP	CB-CG	-5.25	1.40	1.50
1	A	1040	GLN	CD-OE1	5.25	1.35	1.24
1	A	1353	TYR	CD1-CE1	5.25	1.47	1.39
2	B	199	MET	CG-SD	5.25	1.94	1.81
1	A	98	LYS	CB-CG	-5.25	1.38	1.52
5	F	108	PHE	CE2-CZ	5.25	1.47	1.37
2	B	315	LYS	CA-CB	-5.25	1.42	1.53
2	B	567	GLU	CG-CD	5.25	1.59	1.51
2	B	1021	MET	CB-CG	5.25	1.68	1.51
2	B	1174	LYS	CB-CG	5.25	1.66	1.52
1	A	889	SER	C-O	-5.24	1.13	1.23
1	A	927	VAL	CB-CG1	-5.24	1.41	1.52
2	B	483	LEU	C-O	-5.24	1.13	1.23
2	B	1155	SER	C-O	5.24	1.33	1.23
9	K	69	ALA	N-CA	5.24	1.56	1.46
3	C	104	PHE	CB-CG	-5.24	1.42	1.51
2	B	973	ILE	N-CA	-5.24	1.35	1.46
1	A	8	SER	CA-CB	5.24	1.60	1.52
4	E	169	ARG	C-O	5.24	1.33	1.23
1	A	1346	ALA	CA-CB	-5.24	1.41	1.52
2	B	404	LYS	N-CA	-5.24	1.35	1.46
3	C	90	ASP	N-CA	5.24	1.56	1.46
5	F	88	TYR	CG-CD1	-5.24	1.32	1.39
2	B	60	GLN	C-O	-5.23	1.13	1.23
2	B	333	PHE	CE1-CZ	-5.23	1.27	1.37
5	F	79	ARG	CD-NE	-5.23	1.37	1.46
5	F	95	GLY	C-O	-5.23	1.15	1.23
5	F	110	ASP	CG-OD1	5.23	1.37	1.25
3	C	60	ASP	CA-C	-5.23	1.39	1.52
1	A	944	ARG	CZ-NH2	-5.23	1.26	1.33
2	B	816	GLU	CG-CD	5.23	1.59	1.51
2	B	862	GLN	CD-OE1	5.23	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	113	THR	CB-CG2	5.23	1.69	1.52
1	A	646	PHE	CG-CD1	-5.23	1.30	1.38
7	I	87	GLN	CA-C	-5.23	1.39	1.52
1	A	961	ARG	CG-CD	5.22	1.65	1.51
2	B	455	SER	CB-OG	5.22	1.49	1.42
2	B	1005	GLY	C-O	5.22	1.32	1.23
5	F	106	PRO	CG-CD	-5.22	1.33	1.50
7	I	30	ARG	CA-CB	-5.22	1.42	1.53
1	A	1274	ARG	CZ-NH2	5.22	1.39	1.33
2	B	610	ASN	CG-ND2	-5.22	1.19	1.32
3	C	193	TYR	CD2-CE2	5.22	1.47	1.39
7	I	18	GLU	CG-CD	-5.22	1.44	1.51
1	A	411	ASP	CG-OD1	5.22	1.37	1.25
1	A	1127	ASP	CB-CG	5.22	1.62	1.51
4	E	29	PHE	CD2-CE2	-5.22	1.28	1.39
1	A	1235	LYS	CB-CG	5.21	1.66	1.52
9	K	38	GLU	CG-CD	5.21	1.59	1.51
4	E	6	GLU	CG-CD	5.21	1.59	1.51
1	A	653	VAL	C-O	-5.21	1.13	1.23
1	A	1308	THR	CB-CG2	-5.21	1.35	1.52
2	B	230	ALA	N-CA	5.21	1.56	1.46
9	K	99	GLY	C-O	5.21	1.31	1.23
1	A	652	VAL	CB-CG1	-5.21	1.42	1.52
1	A	973	ILE	C-O	5.21	1.33	1.23
2	B	1094	ARG	NE-CZ	-5.21	1.26	1.33
1	A	351	THR	CB-CG2	-5.21	1.35	1.52
1	A	567	LYS	CB-CG	-5.21	1.38	1.52
2	B	556	THR	C-O	5.21	1.33	1.23
1	A	905	ASP	CG-OD2	5.20	1.37	1.25
2	B	89	GLU	CG-CD	5.20	1.59	1.51
2	B	650	GLU	CG-CD	5.20	1.59	1.51
2	B	728	ARG	CG-CD	5.20	1.65	1.51
1	A	493	GLN	CB-CG	-5.20	1.38	1.52
2	B	627	PHE	CE1-CZ	5.20	1.47	1.37
2	B	892	LYS	C-O	-5.20	1.13	1.23
6	H	103	LYS	CA-C	-5.20	1.39	1.52
1	A	1142	THR	C-O	5.20	1.33	1.23
4	E	90	VAL	CA-CB	5.20	1.65	1.54
4	E	70	SER	CB-OG	-5.19	1.35	1.42
4	E	78	LEU	C-O	5.19	1.33	1.23
6	H	112	ILE	CB-CG2	-5.19	1.36	1.52
2	B	678	GLU	CG-CD	5.19	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	3	VAL	CB-CG1	-5.19	1.42	1.52
1	A	987	VAL	CB-CG2	-5.19	1.42	1.52
2	B	995	ARG	NE-CZ	-5.19	1.26	1.33
1	A	857	ARG	C-O	5.19	1.33	1.23
1	A	1303	GLU	N-CA	-5.19	1.35	1.46
2	B	730	ARG	CZ-NH1	-5.19	1.26	1.33
1	A	532	ARG	CB-CG	-5.18	1.38	1.52
1	A	1304	TRP	CG-CD1	-5.18	1.29	1.36
2	B	534	GLY	C-O	5.18	1.31	1.23
3	C	10	ILE	C-O	-5.18	1.13	1.23
1	A	1228	TRP	CZ3-CH2	-5.18	1.31	1.40
6	H	111	LEU	N-CA	5.18	1.56	1.46
1	A	380	VAL	C-O	5.18	1.33	1.23
1	A	463	ILE	CB-CG2	-5.18	1.36	1.52
2	B	820	GLY	N-CA	-5.17	1.38	1.46
2	B	1183	LYS	CB-CG	5.17	1.66	1.52
1	A	1048	ASN	N-CA	-5.17	1.36	1.46
2	B	899	ILE	CA-CB	-5.17	1.43	1.54
2	B	958	GLN	CD-NE2	5.17	1.45	1.32
9	K	89	ASN	CB-CG	5.17	1.62	1.51
9	K	107	THR	C-O	5.17	1.33	1.23
1	A	1255	GLU	CG-CD	5.17	1.59	1.51
2	B	1077	THR	C-O	-5.17	1.13	1.23
3	C	20	PHE	C-O	-5.17	1.13	1.23
9	K	16	GLU	C-O	-5.17	1.13	1.23
1	A	23	SER	C-O	5.17	1.33	1.23
1	A	248	PRO	N-CD	5.17	1.55	1.47
1	A	992	ASP	C-O	-5.17	1.13	1.23
2	B	654	ARG	CA-CB	-5.17	1.42	1.53
1	A	387	ARG	NE-CZ	5.17	1.39	1.33
1	A	965	GLN	CD-OE1	5.17	1.35	1.24
2	B	136	THR	C-O	5.17	1.33	1.23
1	A	513	SER	CB-OG	-5.16	1.35	1.42
2	B	265	SER	CA-C	5.16	1.66	1.52
1	A	431	LYS	CE-NZ	5.16	1.61	1.49
9	K	50	LEU	C-O	-5.16	1.13	1.23
1	A	25	GLU	CB-CG	5.16	1.61	1.52
1	A	994	GLN	CG-CD	-5.16	1.39	1.51
1	A	1209	MET	N-CA	-5.16	1.36	1.46
4	E	212	ARG	CD-NE	-5.16	1.37	1.46
1	A	894	GLU	CD-OE1	5.16	1.31	1.25
2	B	678	GLU	CD-OE1	5.16	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	855	PHE	CG-CD1	-5.16	1.31	1.38
2	B	395	GLN	CB-CG	-5.16	1.38	1.52
2	B	1139	ILE	C-O	-5.16	1.13	1.23
1	A	15	LYS	CD-CE	5.15	1.64	1.51
1	A	821	ARG	CG-CD	5.15	1.64	1.51
2	B	49	ASP	CG-OD2	5.15	1.37	1.25
2	B	394	ASP	CG-OD2	5.15	1.37	1.25
1	A	779	PHE	CG-CD2	-5.15	1.31	1.38
3	C	109	SER	CA-CB	5.15	1.60	1.52
2	B	23	ALA	CA-CB	-5.15	1.41	1.52
3	C	199	LYS	CA-C	-5.15	1.39	1.52
1	A	1446	ASP	N-CA	5.15	1.56	1.46
2	B	807	ARG	NE-CZ	-5.15	1.26	1.33
1	A	933	TYR	CG-CD2	-5.14	1.32	1.39
2	B	1157	ALA	CA-CB	5.14	1.63	1.52
9	K	2	ASN	CB-CG	5.14	1.62	1.51
2	B	306	ASN	CB-CG	5.14	1.62	1.51
1	A	404	TYR	CZ-OH	-5.14	1.29	1.37
8	J	18	TRP	CE3-CZ3	-5.14	1.29	1.38
2	B	452	THR	CA-CB	5.14	1.66	1.53
1	A	350	ARG	CG-CD	-5.14	1.39	1.51
1	A	711	ARG	N-CA	-5.14	1.36	1.46
1	A	911	SER	CA-CB	5.14	1.60	1.52
1	A	1137	ALA	C-O	5.14	1.33	1.23
8	J	31	ASP	CG-OD1	5.14	1.37	1.25
1	A	786	HIS	CA-CB	-5.13	1.42	1.53
1	A	1030	ARG	CB-CG	-5.13	1.38	1.52
2	B	722	ASP	CB-CG	5.13	1.62	1.51
1	A	1170	ILE	CA-CB	5.13	1.66	1.54
1	A	976	THR	CA-CB	5.13	1.66	1.53
1	A	303	TYR	CG-CD1	-5.13	1.32	1.39
1	A	977	LYS	CG-CD	5.13	1.69	1.52
1	A	1304	TRP	CE2-CZ2	-5.13	1.31	1.39
6	H	141	TYR	CE2-CZ	-5.13	1.31	1.38
1	A	607	ILE	CB-CG1	-5.13	1.39	1.54
1	A	1191	TRP	C-O	5.13	1.33	1.23
2	B	106	ASP	CA-CB	5.13	1.65	1.53
8	J	42	LYS	CG-CD	5.13	1.69	1.52
2	B	37	PHE	CD1-CE1	-5.12	1.29	1.39
1	A	1220	PHE	CD2-CE2	5.12	1.49	1.39
6	H	10	PHE	CD2-CE2	5.12	1.49	1.39
2	B	605	ARG	NE-CZ	-5.12	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1243	VAL	CA-CB	5.12	1.65	1.54
3	C	158	VAL	CB-CG1	-5.12	1.42	1.52
6	H	115	TYR	CD2-CE2	5.12	1.47	1.39
1	A	942	PHE	CB-CG	-5.12	1.42	1.51
2	B	1079	LYS	CA-C	-5.12	1.39	1.52
2	B	137	TYR	CD1-CE1	5.11	1.47	1.39
1	A	549	MET	C-O	-5.11	1.13	1.23
1	A	664	THR	CB-CG2	-5.11	1.35	1.52
2	B	758	PHE	CD2-CE2	5.11	1.49	1.39
1	A	971	PHE	CB-CG	-5.11	1.42	1.51
1	A	1003	LYS	C-O	5.11	1.33	1.23
7	I	41	PRO	CA-CB	-5.11	1.43	1.53
8	J	24	LEU	CG-CD2	-5.11	1.32	1.51
1	A	833	GLU	C-O	5.11	1.33	1.23
5	F	77	ASP	CG-OD1	5.11	1.37	1.25
1	A	940	ARG	CZ-NH1	-5.10	1.26	1.33
1	A	1029	ARG	CA-CB	-5.10	1.42	1.53
2	B	294	ASP	CB-CG	5.10	1.62	1.51
2	B	627	PHE	CE2-CZ	-5.10	1.27	1.37
2	B	889	THR	N-CA	5.10	1.56	1.46
4	E	42	PHE	CE1-CZ	-5.10	1.27	1.37
1	A	776	ALA	C-O	-5.10	1.13	1.23
1	A	1195	LEU	N-CA	5.10	1.56	1.46
2	B	869	SER	CA-C	5.10	1.66	1.52
1	A	1151	GLU	CB-CG	-5.10	1.42	1.52
1	A	1344	GLY	C-O	-5.09	1.15	1.23
2	B	565	PRO	CG-CD	-5.09	1.33	1.50
10	L	63	ARG	CD-NE	5.09	1.55	1.46
1	A	1077	THR	C-O	-5.09	1.13	1.23
3	C	223	ALA	CA-CB	-5.09	1.41	1.52
3	C	247	GLY	N-CA	-5.09	1.38	1.46
1	A	1052	GLN	N-CA	-5.09	1.36	1.46
2	B	57	TYR	CA-CB	5.09	1.65	1.53
2	B	68	THR	CA-CB	5.09	1.66	1.53
7	I	114	GLN	C-O	-5.09	1.13	1.23
1	A	1195	LEU	C-N	-5.09	1.22	1.34
3	C	218	PRO	CG-CD	5.09	1.67	1.50
1	A	244	PRO	C-O	5.08	1.33	1.23
1	A	459	ARG	CD-NE	-5.08	1.37	1.46
3	C	82	TYR	CD1-CE1	-5.08	1.31	1.39
1	A	635	ARG	C-O	-5.08	1.13	1.23
2	B	344	LYS	CG-CD	5.08	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	561	TRP	CZ3-CH2	5.08	1.48	1.40
1	A	446	ARG	CZ-NH2	5.08	1.39	1.33
4	E	67	GLU	CB-CG	5.08	1.61	1.52
4	E	124	VAL	CB-CG2	-5.08	1.42	1.52
1	A	677	ARG	CD-NE	5.08	1.55	1.46
1	A	74	MET	CA-CB	5.08	1.65	1.53
2	B	694	ASP	CG-OD2	5.08	1.37	1.25
4	E	211	TYR	C-O	5.08	1.32	1.23
2	B	275	TYR	CZ-OH	-5.08	1.29	1.37
2	B	852	ARG	CZ-NH2	-5.08	1.26	1.33
2	B	1128	LEU	CA-C	5.08	1.66	1.52
1	A	593	GLU	C-N	5.08	1.42	1.33
2	B	308	TRP	CA-C	-5.08	1.39	1.52
4	E	126	SER	CA-CB	5.08	1.60	1.52
7	I	15	TYR	C-O	-5.08	1.13	1.23
1	A	89	PRO	CA-C	-5.07	1.42	1.52
1	A	556	TRP	CD2-CE3	-5.07	1.32	1.40
1	A	1049	ILE	CA-CB	-5.07	1.43	1.54
1	A	1286	LYS	C-O	-5.07	1.13	1.23
2	B	217	ARG	CD-NE	-5.07	1.37	1.46
2	B	643	ASP	CA-C	-5.07	1.39	1.52
2	B	827	ILE	CB-CG2	-5.07	1.37	1.52
2	B	1091	TYR	CB-CG	-5.07	1.44	1.51
2	B	310	MET	C-O	5.07	1.32	1.23
1	A	285	PRO	C-O	-5.07	1.13	1.23
3	C	211	ASP	CG-OD1	5.07	1.37	1.25
1	A	805	LEU	CG-CD1	-5.07	1.33	1.51
2	B	451	LYS	CG-CD	5.07	1.69	1.52
1	A	920	LEU	CA-CB	-5.07	1.42	1.53
1	A	1274	ARG	CB-CG	-5.07	1.38	1.52
1	A	1298	TYR	CE1-CZ	-5.07	1.31	1.38
10	L	42	ARG	CD-NE	5.07	1.55	1.46
1	A	1446	ASP	CA-CB	5.07	1.65	1.53
2	B	106	ASP	CG-OD2	5.07	1.37	1.25
3	C	117	ASP	CG-OD1	5.07	1.37	1.25
10	L	63	ARG	CG-CD	5.07	1.64	1.51
1	A	404	TYR	CE1-CZ	-5.06	1.31	1.38
3	C	79	GLN	CG-CD	5.06	1.62	1.51
9	K	78	THR	CA-CB	-5.06	1.40	1.53
1	A	621	THR	CB-CG2	-5.06	1.35	1.52
1	A	803	SER	CA-CB	5.06	1.60	1.52
1	A	360	GLU	CD-OE1	5.06	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	378	GLU	CG-CD	-5.06	1.44	1.51
2	B	745	PRO	N-CD	-5.06	1.40	1.47
1	A	367	PRO	N-CD	-5.06	1.40	1.47
3	C	191	TYR	CD1-CE1	5.06	1.47	1.39
6	H	56	THR	CA-CB	5.06	1.66	1.53
2	B	226	PHE	CE1-CZ	5.05	1.47	1.37
2	B	552	MET	CA-CB	-5.05	1.42	1.53
2	B	1223	ASP	CA-C	5.05	1.66	1.52
1	A	982	THR	CB-OG1	-5.05	1.33	1.43
3	C	191	TYR	N-CA	-5.05	1.36	1.46
7	I	117	LYS	CE-NZ	5.05	1.61	1.49
1	A	781	ASP	C-O	5.05	1.32	1.23
2	B	1082	MET	CA-C	-5.05	1.39	1.52
4	E	110	PHE	CG-CD2	-5.05	1.31	1.38
5	F	84	TYR	CZ-OH	5.05	1.46	1.37
1	A	1228	TRP	CA-C	-5.05	1.39	1.52
2	B	388	CYS	CB-SG	-5.05	1.73	1.81
2	B	735	ALA	CA-CB	-5.05	1.41	1.52
6	H	37	LYS	CA-C	5.05	1.66	1.52
2	B	660	LYS	CB-CG	5.05	1.66	1.52
2	B	30	SER	C-O	-5.05	1.13	1.23
7	I	20	LYS	CG-CD	5.05	1.69	1.52
1	A	297	GLN	C-O	-5.04	1.13	1.23
1	A	359	LEU	CG-CD2	-5.04	1.33	1.51
2	B	257	LYS	C-O	-5.04	1.13	1.23
2	B	1188	LYS	CG-CD	5.04	1.69	1.52
1	A	1116	LEU	CA-CB	-5.04	1.42	1.53
6	H	130	ARG	CA-C	5.04	1.66	1.52
1	A	626	ASN	CG-OD1	5.04	1.35	1.24
2	B	96	TYR	CD2-CE2	5.04	1.47	1.39
1	A	568	PRO	N-CD	-5.04	1.40	1.47
1	A	656	TRP	CD2-CE3	-5.04	1.32	1.40
3	C	167	HIS	CA-CB	-5.04	1.42	1.53
5	F	148	VAL	CA-CB	-5.04	1.44	1.54
8	J	1	MET	CB-CG	-5.04	1.35	1.51
1	A	883	LEU	C-O	5.04	1.32	1.23
1	A	1282	VAL	CA-CB	-5.04	1.44	1.54
1	A	712	GLU	CB-CG	5.04	1.61	1.52
1	A	897	TYR	N-CA	5.04	1.56	1.46
2	B	513	GLN	CD-NE2	5.03	1.45	1.32
2	B	854	LEU	CA-C	-5.03	1.39	1.52
2	B	964	VAL	CA-CB	-5.03	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	39	ALA	C-O	5.03	1.32	1.23
7	I	27	PHE	CE1-CZ	-5.03	1.27	1.37
3	C	158	VAL	N-CA	-5.03	1.36	1.46
3	C	244	VAL	CB-CG1	-5.03	1.42	1.52
1	A	93	VAL	CB-CG1	5.03	1.63	1.52
1	A	586	ILE	CB-CG2	-5.03	1.37	1.52
2	B	398	ARG	CZ-NH1	5.03	1.39	1.33
1	A	537	ARG	CZ-NH1	5.03	1.39	1.33
2	B	1140	ALA	C-O	5.03	1.32	1.23
1	A	953	ASN	CG-OD1	5.02	1.35	1.24
5	F	153	VAL	CA-C	-5.02	1.39	1.52
1	A	477	PRO	CG-CD	5.02	1.67	1.50
1	A	578	LEU	N-CA	5.02	1.56	1.46
9	K	61	TYR	CZ-OH	-5.02	1.29	1.37
2	B	291	ILE	CB-CG2	-5.02	1.37	1.52
2	B	829	CYS	CB-SG	5.02	1.90	1.82
1	A	1050	GLU	CD-OE1	5.02	1.31	1.25
8	J	38	ARG	N-CA	-5.02	1.36	1.46
1	A	661	GLY	C-O	5.02	1.31	1.23
9	K	66	PRO	C-O	-5.01	1.13	1.23
1	A	471	ASN	CA-C	-5.01	1.40	1.52
1	A	944	ARG	CZ-NH1	-5.01	1.26	1.33
1	A	601	LYS	CE-NZ	5.01	1.61	1.49
1	A	940	ARG	CZ-NH2	-5.01	1.26	1.33
1	A	994	GLN	CD-OE1	-5.01	1.12	1.24
2	B	231	PRO	N-CA	5.01	1.55	1.47
2	B	1154	ALA	C-N	5.01	1.45	1.34
6	H	14	GLU	CD-OE1	5.01	1.31	1.25
2	B	1130	PHE	C-O	-5.01	1.13	1.23
2	B	130	VAL	CA-C	5.00	1.66	1.52
1	A	611	GLN	CD-NE2	5.00	1.45	1.32
2	B	660	LYS	N-CA	-5.00	1.36	1.46
1	A	1168	GLU	CB-CG	5.00	1.61	1.52
3	C	58	LEU	CG-CD2	-5.00	1.33	1.51

All (1625) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1366	ARG	NE-CZ-NH2	-34.23	103.18	120.30
1	A	774	ARG	NE-CZ-NH1	32.19	136.39	120.30
3	C	34	ARG	NE-CZ-NH2	-31.55	104.53	120.30
2	B	995	ARG	NE-CZ-NH2	-30.46	105.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1366	ARG	NE-CZ-NH1	28.94	134.77	120.30
9	K	47	ARG	NE-CZ-NH2	-27.69	106.45	120.30
1	A	469	ARG	NE-CZ-NH2	-26.96	106.82	120.30
3	C	35	ARG	NE-CZ-NH2	-24.26	108.17	120.30
2	B	496	ARG	NE-CZ-NH1	24.02	132.31	120.30
1	A	940	ARG	NE-CZ-NH1	23.85	132.22	120.30
1	A	469	ARG	NE-CZ-NH1	23.64	132.12	120.30
2	B	995	ARG	NE-CZ-NH1	23.07	131.83	120.30
2	B	1135	ARG	NE-CZ-NH2	-22.80	108.90	120.30
1	A	446	ARG	NE-CZ-NH2	-22.60	109.00	120.30
2	B	604	ARG	NE-CZ-NH1	21.98	131.29	120.30
1	A	459	ARG	NE-CZ-NH2	-21.91	109.35	120.30
3	C	35	ARG	NE-CZ-NH1	20.90	130.75	120.30
3	C	34	ARG	NE-CZ-NH1	20.81	130.70	120.30
2	B	620	ARG	NE-CZ-NH1	-20.38	110.11	120.30
2	B	496	ARG	NE-CZ-NH2	-19.91	110.35	120.30
3	C	66	ARG	NE-CZ-NH1	-19.84	110.38	120.30
1	A	1336	MET	CG-SD-CE	19.29	131.07	100.20
2	B	807	ARG	NE-CZ-NH2	-19.12	110.74	120.30
2	B	106	ASP	CB-CG-OD2	19.06	135.46	118.30
3	C	66	ARG	NE-CZ-NH2	18.64	129.62	120.30
1	A	434	ARG	NE-CZ-NH2	-18.48	111.06	120.30
1	A	896	ARG	NE-CZ-NH2	-18.46	111.07	120.30
1	A	590	ARG	NE-CZ-NH2	-18.33	111.13	120.30
3	C	16	ASP	CB-CG-OD2	18.08	134.57	118.30
1	A	821	ARG	NE-CZ-NH2	-17.81	111.39	120.30
2	B	996	ARG	NE-CZ-NH1	-17.48	111.56	120.30
2	B	983	ARG	NE-CZ-NH2	-17.00	111.80	120.30
1	A	1135	ARG	NE-CZ-NH1	-17.00	111.80	120.30
2	B	287	ARG	NE-CZ-NH2	-16.82	111.89	120.30
2	B	909	ASP	CB-CG-OD2	16.77	133.39	118.30
1	A	434	ARG	NE-CZ-NH1	16.72	128.66	120.30
1	A	1100	ARG	NE-CZ-NH2	-16.55	112.02	120.30
2	B	839	MET	CG-SD-CE	-16.26	74.18	100.20
2	B	1150	ARG	NE-CZ-NH1	-16.25	112.17	120.30
1	A	1241	ARG	NE-CZ-NH2	-16.21	112.19	120.30
2	B	405	ARG	NE-CZ-NH1	16.13	128.37	120.30
1	A	962	ARG	NE-CZ-NH2	-15.84	112.38	120.30
2	B	394	ASP	CB-CG-OD2	15.79	132.51	118.30
2	B	604	ARG	NE-CZ-NH2	-15.76	112.42	120.30
1	A	949	ASP	CB-CG-OD2	15.73	132.46	118.30
1	A	985	ASP	CB-CG-OD1	-15.64	104.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	249	ARG	NE-CZ-NH1	15.62	128.11	120.30
9	K	22	ASP	CB-CG-OD1	15.50	132.25	118.30
1	A	1100	ARG	NE-CZ-NH1	15.46	128.03	120.30
1	A	940	ARG	NE-CZ-NH2	-15.45	112.57	120.30
1	A	481	ASP	CB-CG-OD1	15.40	132.16	118.30
8	J	43	ARG	NE-CZ-NH1	-15.31	112.64	120.30
1	A	1422	ARG	NE-CZ-NH1	15.27	127.93	120.30
1	A	774	ARG	NE-CZ-NH2	-15.26	112.67	120.30
10	L	70	ARG	NE-CZ-NH1	15.21	127.90	120.30
2	B	497	ARG	NE-CZ-NH2	-15.14	112.73	120.30
10	L	68	GLU	OE1-CD-OE2	-15.11	105.17	123.30
3	C	220	ASP	CB-CG-OD1	15.00	131.80	118.30
1	A	1036	ARG	NE-CZ-NH2	-14.99	112.81	120.30
8	J	6	ARG	NE-CZ-NH2	14.95	127.77	120.30
7	I	61	ASP	CB-CG-OD2	14.93	131.74	118.30
1	A	1241	ARG	NE-CZ-NH1	14.90	127.75	120.30
2	B	1043	ASP	CB-CG-OD2	14.90	131.71	118.30
2	B	983	ARG	NE-CZ-NH1	14.89	127.75	120.30
9	K	47	ARG	NE-CZ-NH1	14.85	127.72	120.30
2	B	39	ARG	NE-CZ-NH1	14.83	127.71	120.30
2	B	287	ARG	NE-CZ-NH1	14.78	127.69	120.30
9	K	5	ASP	CB-CG-OD1	-14.74	105.04	118.30
1	A	420	ARG	NE-CZ-NH1	14.59	127.59	120.30
1	A	1442	ASP	CB-CG-OD2	14.53	131.38	118.30
1	A	961	ARG	NE-CZ-NH1	-14.45	113.07	120.30
1	A	172	PRO	CA-N-CD	-14.41	91.33	111.50
3	C	84	ARG	NE-CZ-NH2	14.39	127.50	120.30
2	B	998	ASP	CB-CG-OD2	14.39	131.25	118.30
2	B	326	ASP	CB-CG-OD2	14.34	131.20	118.30
2	B	620	ARG	NH1-CZ-NH2	14.20	135.02	119.40
8	J	48	ARG	NE-CZ-NH1	14.20	127.40	120.30
9	K	114	LEU	CB-CG-CD2	14.19	135.12	111.00
8	J	38	ARG	NE-CZ-NH1	14.17	127.39	120.30
2	B	373	ARG	NE-CZ-NH2	-14.04	113.28	120.30
8	J	43	ARG	NE-CZ-NH2	14.03	127.31	120.30
4	E	14	ARG	NE-CZ-NH1	13.95	127.27	120.30
3	C	93	ASP	CB-CG-OD2	13.81	130.73	118.30
1	A	483	ASP	CB-CG-OD2	13.69	130.62	118.30
1	A	483	ASP	CB-CG-OD1	-13.65	106.01	118.30
1	A	407	ARG	NE-CZ-NH2	-13.55	113.52	120.30
8	J	49	MET	CG-SD-CE	-13.51	78.58	100.20
5	F	92	ARG	NE-CZ-NH1	13.48	127.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	591	ARG	NE-CZ-NH1	13.48	127.04	120.30
1	A	1006	ILE	CG1-CB-CG2	-13.45	81.80	111.40
6	H	77	ARG	NE-CZ-NH1	13.29	126.94	120.30
2	B	1019	SER	CB-CA-C	-13.21	84.99	110.10
4	E	11	ARG	NE-CZ-NH1	-13.18	113.71	120.30
3	C	268	ASP	CB-CG-OD2	13.11	130.09	118.30
1	A	153	PRO	CA-N-CD	-13.06	93.21	111.50
2	B	790	ASP	CB-CG-OD2	-13.06	106.55	118.30
1	A	884	ASP	CB-CG-OD1	-13.01	106.59	118.30
2	B	642	ASP	CB-CG-OD1	12.94	129.95	118.30
1	A	806	ARG	NE-CZ-NH1	-12.84	113.88	120.30
2	B	790	ASP	CB-CG-OD1	12.79	129.81	118.30
1	A	538	ASP	CB-CA-C	-12.79	84.83	110.40
2	B	241	ARG	NE-CZ-NH1	12.74	126.67	120.30
4	E	212	ARG	NE-CZ-NH2	-12.66	113.97	120.30
9	K	5	ASP	CB-CG-OD2	12.65	129.69	118.30
5	F	81	THR	N-CA-CB	-12.61	86.34	110.30
4	E	207	ARG	NE-CZ-NH1	12.59	126.60	120.30
1	A	826	ASP	CB-CG-OD2	12.54	129.59	118.30
2	B	348	ARG	NE-CZ-NH2	-12.52	114.04	120.30
4	E	212	ARG	CD-NE-CZ	12.49	141.09	123.60
2	B	106	ASP	CB-CG-OD1	-12.36	107.17	118.30
9	K	114	LEU	CA-CB-CG	12.33	143.65	115.30
2	B	807	ARG	NE-CZ-NH1	12.32	126.46	120.30
10	L	68	GLU	CG-CD-OE1	12.31	142.93	118.30
2	B	49	ASP	CB-CG-OD2	12.13	129.22	118.30
2	B	391	ASP	CB-CG-OD2	12.13	129.22	118.30
2	B	883	LEU	CA-CB-CG	12.13	143.20	115.30
1	A	446	ARG	NH1-CZ-NH2	12.12	132.74	119.40
2	B	294	ASP	CB-CG-OD2	12.12	129.21	118.30
4	E	200	ARG	NE-CZ-NH1	-12.12	114.24	120.30
2	B	188	ASP	CB-CG-OD2	12.07	129.17	118.30
2	B	1150	ARG	NH1-CZ-NH2	12.01	132.61	119.40
2	B	120	ARG	NE-CZ-NH1	-11.95	114.33	120.30
4	E	204	THR	CA-CB-CG2	11.94	129.12	112.40
7	I	70	ARG	NE-CZ-NH2	-11.93	114.33	120.30
1	A	557	ASP	CB-CG-OD2	11.81	128.93	118.30
2	B	635	ARG	NE-CZ-NH1	11.80	126.20	120.30
10	L	34	CYS	CA-CB-SG	-11.78	92.79	114.00
1	A	1269	GLU	OE1-CD-OE2	11.74	137.38	123.30
1	A	423	ASP	CB-CG-OD1	11.70	128.83	118.30
2	B	1043	ASP	CB-CG-OD1	-11.70	107.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1062	GLU	CB-CA-C	-11.67	87.05	110.40
1	A	518	LYS	CD-CE-NZ	-11.63	84.96	111.70
1	A	1196	GLU	OE1-CD-OE2	11.62	137.24	123.30
2	B	1220	ARG	NE-CZ-NH2	11.62	126.11	120.30
1	A	944	ARG	NE-CZ-NH2	11.62	126.11	120.30
1	A	459	ARG	NE-CZ-NH1	11.59	126.09	120.30
6	H	130	ARG	NE-CZ-NH1	-11.52	114.54	120.30
3	C	86	CYS	CA-CB-SG	11.45	134.61	114.00
1	A	884	ASP	CB-CG-OD2	11.41	128.57	118.30
4	E	24	LYS	CD-CE-NZ	-11.39	85.49	111.70
1	A	42	ASP	CB-CG-OD2	11.37	128.53	118.30
9	K	42	LEU	CB-CG-CD1	-11.36	91.68	111.00
1	A	857	ARG	NE-CZ-NH1	-11.34	114.63	120.30
1	A	728	LYS	CD-CE-NZ	11.30	137.69	111.70
2	B	747	MET	CG-SD-CE	-11.30	82.12	100.20
1	A	801	GLU	OE1-CD-OE2	11.29	136.84	123.30
2	B	1219	ASP	CB-CG-OD2	11.23	128.41	118.30
6	H	135	LEU	CA-CB-CG	11.14	140.92	115.30
2	B	485	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	A	740	LEU	CB-CG-CD1	11.12	129.90	111.00
7	I	45	ARG	NE-CZ-NH1	-11.11	114.74	120.30
1	A	609	ASP	CB-CG-OD2	11.04	128.24	118.30
1	A	416	ARG	NE-CZ-NH2	-11.03	114.78	120.30
2	B	568	ASP	CB-CG-OD2	11.02	128.22	118.30
1	A	372	LYS	CD-CE-NZ	-11.00	86.40	111.70
1	A	544	ASP	CB-CG-OD1	10.99	128.19	118.30
2	B	1135	ARG	NH1-CZ-NH2	10.97	131.47	119.40
1	A	197	PRO	CA-N-CD	-10.94	96.18	111.50
1	A	748	MET	CG-SD-CE	10.91	117.66	100.20
2	B	579	ARG	NE-CZ-NH1	-10.88	114.86	120.30
1	A	1043	ASP	CB-CG-OD2	10.87	128.08	118.30
2	B	620	ARG	NE-CZ-NH2	-10.87	114.87	120.30
1	A	36	ARG	NE-CZ-NH1	10.84	125.72	120.30
3	C	246	ARG	NE-CZ-NH1	10.83	125.71	120.30
1	A	949	ASP	N-CA-CB	-10.80	91.16	110.60
7	I	81	ARG	NE-CZ-NH1	10.77	125.68	120.30
2	B	552	MET	CG-SD-CE	10.76	117.41	100.20
1	A	93	VAL	CB-CA-C	-10.75	90.97	111.40
1	A	537	ARG	NE-CZ-NH1	10.73	125.67	120.30
6	H	110	ASP	CB-CG-OD2	10.70	127.93	118.30
9	K	6	ARG	NE-CZ-NH2	-10.66	114.97	120.30
2	B	326	ASP	CB-CG-OD1	-10.66	108.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	941	LYS	CD-CE-NZ	-10.59	87.34	111.70
1	A	1055	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	857	ARG	NE-CZ-NH2	10.56	125.58	120.30
1	A	352	VAL	CG1-CB-CG2	-10.55	94.02	110.90
1	A	592	ASP	CB-CG-OD2	-10.54	108.81	118.30
1	A	537	ARG	NE-CZ-NH2	-10.46	115.07	120.30
2	B	1097	HIS	CB-CA-C	10.40	131.21	110.40
2	B	56	ASP	CB-CG-OD2	10.40	127.66	118.30
1	A	771	GLU	OE1-CD-OE2	10.38	135.75	123.30
1	A	1284	MET	CA-CB-CG	-10.36	95.69	113.30
1	A	771	GLU	CG-CD-OE1	-10.36	97.58	118.30
2	B	1006	ILE	CG1-CB-CG2	-10.34	88.65	111.40
4	E	25	ASP	CB-CG-OD2	10.32	127.59	118.30
1	A	605	MET	CG-SD-CE	-10.31	83.70	100.20
1	A	961	ARG	NE-CZ-NH2	10.27	125.44	120.30
1	A	1207	LEU	CB-CG-CD1	-10.26	93.57	111.00
1	A	1422	ARG	NE-CZ-NH2	-10.23	115.19	120.30
4	E	50	MET	CG-SD-CE	10.20	116.52	100.20
1	A	53	LEU	CA-CB-CG	10.18	138.72	115.30
8	J	1	MET	CG-SD-CE	-10.18	83.91	100.20
2	B	1150	ARG	NE-CZ-NH2	-10.17	115.22	120.30
2	B	652	LYS	CD-CE-NZ	10.14	135.03	111.70
1	A	853	ASP	CB-CG-OD2	10.11	127.40	118.30
2	B	337	ARG	CG-CD-NE	-10.04	90.72	111.80
1	A	455	MET	CG-SD-CE	-10.01	84.18	100.20
1	A	28	ARG	NE-CZ-NH1	10.01	125.30	120.30
3	C	172	PRO	N-CD-CG	9.98	118.17	103.20
1	A	1366	ARG	CD-NE-CZ	9.97	137.55	123.60
3	C	160	LYS	CD-CE-NZ	9.96	134.61	111.70
2	B	1160	VAL	CB-CA-C	-9.93	92.53	111.40
7	I	81	ARG	NE-CZ-NH2	-9.92	115.34	120.30
2	B	605	ARG	NE-CZ-NH1	-9.91	115.34	120.30
1	A	620	LYS	CD-CE-NZ	9.90	134.47	111.70
2	B	547	VAL	CG1-CB-CG2	9.86	126.67	110.90
1	A	466	SER	CB-CA-C	-9.86	91.38	110.10
2	B	408	LEU	CB-CG-CD2	-9.84	94.27	111.00
4	E	14	ARG	NE-CZ-NH2	-9.83	115.39	120.30
3	C	163	ILE	CA-CB-CG2	9.82	130.54	110.90
4	E	162	ARG	NE-CZ-NH1	9.80	125.20	120.30
2	B	598	GLU	OE1-CD-OE2	-9.78	111.56	123.30
1	A	974	ASP	N-CA-CB	9.77	128.19	110.60
1	A	1228	TRP	CB-CA-C	-9.77	90.86	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	51	LEU	CB-CG-CD1	9.75	127.58	111.00
1	A	1376	THR	N-CA-CB	-9.74	91.78	110.30
2	B	24	PRO	N-CD-CG	-9.74	88.59	103.20
1	A	1157	ASP	CB-CG-OD2	9.74	127.06	118.30
7	I	113	ASP	CB-CG-OD2	9.74	127.06	118.30
2	B	996	ARG	NH1-CZ-NH2	9.73	130.11	119.40
2	B	188	ASP	CB-CG-OD1	-9.73	109.55	118.30
1	A	438	ASP	CB-CG-OD2	9.72	127.05	118.30
3	C	18	VAL	CB-CA-C	-9.71	92.94	111.40
1	A	16	GLU	OE1-CD-OE2	9.69	134.92	123.30
4	E	182	ASP	CB-CG-OD1	9.67	127.00	118.30
1	A	1062	GLU	OE1-CD-OE2	9.66	134.89	123.30
2	B	1097	HIS	CB-CG-ND1	-9.65	99.07	123.20
1	A	305	ASP	CB-CG-OD2	9.64	126.98	118.30
5	F	119	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	1204	ASP	CB-CG-OD2	9.63	126.97	118.30
2	B	337	ARG	NE-CZ-NH2	-9.62	115.49	120.30
2	B	118	ARG	NE-CZ-NH1	9.61	125.11	120.30
2	B	563	MET	CG-SD-CE	9.61	115.57	100.20
3	C	93	ASP	CB-CG-OD1	-9.58	109.67	118.30
1	A	1420	ASP	CB-CG-OD1	-9.55	109.71	118.30
2	B	348	ARG	NE-CZ-NH1	9.53	125.06	120.30
8	J	6	ARG	NE-CZ-NH1	-9.51	115.54	120.30
7	I	109	ILE	CG1-CB-CG2	-9.50	90.49	111.40
1	A	982	THR	CA-CB-CG2	9.48	125.68	112.40
3	C	136	ASP	CB-CG-OD2	9.48	126.83	118.30
1	A	291	GLU	OE1-CD-OE2	-9.46	111.94	123.30
8	J	3	VAL	CB-CA-C	-9.46	93.43	111.40
2	B	760	ASP	CB-CG-OD2	9.44	126.80	118.30
1	A	1081	LEU	CB-CG-CD2	9.44	127.05	111.00
3	C	85	ASP	CB-CG-OD2	9.40	126.76	118.30
1	A	549	MET	CG-SD-CE	9.38	115.22	100.20
1	A	1055	ARG	CG-CD-NE	-9.38	92.09	111.80
1	A	962	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	28	ARG	NE-CZ-NH2	-9.38	115.61	120.30
7	I	43	VAL	N-CA-CB	-9.36	90.90	111.50
7	I	54	GLU	OE1-CD-OE2	9.35	134.52	123.30
1	A	1285	MET	CG-SD-CE	9.35	115.15	100.20
2	B	564	GLU	OE1-CD-OE2	9.34	134.50	123.30
1	A	486	GLU	OE1-CD-OE2	-9.33	112.10	123.30
2	B	137	TYR	CA-CB-CG	9.32	131.12	113.40
2	B	384	ARG	NE-CZ-NH1	9.32	124.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	113	ASP	CB-CG-OD1	9.32	126.69	118.30
9	K	82	ASP	CB-CG-OD2	9.30	126.67	118.30
1	A	472	LEU	CA-CB-CG	-9.27	93.98	115.30
1	A	389	THR	OG1-CB-CG2	-9.24	88.76	110.00
2	B	791	THR	OG1-CB-CG2	-9.23	88.76	110.00
2	B	837	ASP	CB-CG-OD1	9.23	126.61	118.30
2	B	1159	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	A	346	ASP	CB-CG-OD1	9.23	126.61	118.30
1	A	982	THR	N-CA-CB	-9.22	92.78	110.30
1	A	726	ARG	NE-CZ-NH1	-9.21	115.69	120.30
2	B	629	ASP	CB-CG-OD2	9.20	126.58	118.30
1	A	909	ASP	CB-CG-OD1	9.18	126.56	118.30
4	E	201	LYS	CD-CE-NZ	-9.18	90.59	111.70
2	B	391	ASP	OD1-CG-OD2	-9.14	105.94	123.30
2	B	788	ARG	NE-CZ-NH1	9.13	124.86	120.30
2	B	1050	ILE	CG1-CB-CG2	-9.10	91.38	111.40
2	B	367	LEU	CB-CG-CD2	9.10	126.47	111.00
1	A	944	ARG	NH1-CZ-NH2	-9.10	109.40	119.40
1	A	85	ASP	CB-CG-OD1	-9.09	110.12	118.30
1	A	1326	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	A	596	THR	CA-CB-CG2	-9.04	99.74	112.40
1	A	1198	ASP	CB-CG-OD1	9.04	126.44	118.30
6	H	132	LEU	CA-CB-CG	9.03	136.06	115.30
3	C	125	MET	CG-SD-CE	8.98	114.58	100.20
7	I	113	ASP	OD1-CG-OD2	-8.98	106.23	123.30
10	L	48	CYS	N-CA-CB	-8.98	94.44	110.60
3	C	155	LEU	CB-CA-C	-8.98	93.15	110.20
10	L	27	LEU	CA-CB-CG	8.97	135.94	115.30
9	K	73	LEU	CB-CG-CD1	-8.97	95.75	111.00
2	B	567	GLU	O-C-N	-8.96	108.37	122.70
3	C	165	LYS	CD-CE-NZ	8.94	132.26	111.70
8	J	61	LEU	CB-CG-CD2	8.93	126.18	111.00
2	B	1041	GLU	OE1-CD-OE2	8.92	134.01	123.30
2	B	857	ARG	NE-CZ-NH1	8.91	124.76	120.30
2	B	484	ASN	CB-CA-C	-8.91	92.58	110.40
1	A	821	ARG	CG-CD-NE	-8.90	93.11	111.80
2	B	316	PRO	N-CD-CG	-8.90	89.85	103.20
2	B	680	THR	N-CA-CB	-8.90	93.39	110.30
1	A	1373	ASP	CB-CG-OD2	8.89	126.30	118.30
9	K	24	ASP	CB-CG-OD2	8.89	126.30	118.30
1	A	53	LEU	CB-CG-CD1	8.89	126.11	111.00
1	A	557	ASP	OD1-CG-OD2	-8.89	106.41	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1176	LEU	N-CA-C	-8.89	87.00	111.00
9	K	78	THR	CA-CB-CG2	-8.86	99.99	112.40
8	J	48	ARG	NE-CZ-NH2	-8.85	115.87	120.30
1	A	360	GLU	OE1-CD-OE2	-8.84	112.69	123.30
3	C	76	ASP	CB-CG-OD1	8.84	126.26	118.30
2	B	405	ARG	NE-CZ-NH2	-8.83	115.89	120.30
2	B	552	MET	CA-CB-CG	8.81	128.28	113.30
1	A	231	PRO	CA-N-CD	-8.81	99.17	111.50
2	B	963	PHE	CB-CA-C	-8.78	92.84	110.40
1	A	787	PHE	CB-CG-CD2	8.77	126.94	120.80
2	B	95	ILE	CG1-CB-CG2	-8.77	92.11	111.40
2	B	601	ARG	NE-CZ-NH2	-8.75	115.92	120.30
2	B	964	VAL	CA-CB-CG2	-8.74	97.79	110.90
9	K	36	GLU	OE1-CD-OE2	8.74	133.78	123.30
1	A	590	ARG	NE-CZ-NH1	8.72	124.66	120.30
2	B	642	ASP	N-CA-C	-8.72	87.45	111.00
2	B	1067	ARG	NE-CZ-NH1	8.72	124.66	120.30
2	B	1010	LEU	CB-CG-CD1	-8.71	96.19	111.00
1	A	1064	VAL	N-CA-CB	-8.71	92.34	111.50
4	E	25	ASP	OD1-CG-OD2	-8.71	106.75	123.30
1	A	1271	ILE	CG1-CB-CG2	-8.71	92.25	111.40
2	B	416	LEU	CB-CA-C	-8.70	93.67	110.20
2	B	710	LEU	CB-CG-CD2	8.68	125.76	111.00
2	B	336	ARG	CB-CA-C	-8.68	93.05	110.40
5	F	135	ARG	NE-CZ-NH1	-8.68	115.96	120.30
1	A	261	ASP	CB-CG-OD2	8.66	126.09	118.30
1	A	821	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	A	1195	LEU	CB-CG-CD1	-8.66	96.28	111.00
1	A	672	ASP	CB-CG-OD1	8.65	126.09	118.30
2	B	101	MET	CG-SD-CE	8.65	114.05	100.20
2	B	582	VAL	CG1-CB-CG2	-8.65	97.05	110.90
4	E	1	MET	CG-SD-CE	8.65	114.05	100.20
1	A	1289	ARG	NE-CZ-NH1	-8.65	115.97	120.30
1	A	1442	ASP	CB-CG-OD1	-8.65	110.52	118.30
2	B	1098	MET	CG-SD-CE	8.65	114.04	100.20
1	A	913	LEU	CB-CG-CD1	-8.64	96.32	111.00
8	J	62	ARG	NE-CZ-NH1	8.63	124.61	120.30
3	C	9	LYS	CD-CE-NZ	8.63	131.54	111.70
1	A	992	ASP	CB-CG-OD2	8.63	126.06	118.30
5	F	150	GLU	N-CA-CB	-8.62	95.08	110.60
1	A	414	ASP	CB-CG-OD2	8.60	126.04	118.30
2	B	118	ARG	CD-NE-CZ	8.59	135.63	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	245	GLU	OE1-CD-OE2	-8.59	113.00	123.30
2	B	513	GLN	CA-CB-CG	8.59	132.29	113.40
1	A	720	ARG	NE-CZ-NH2	8.57	124.59	120.30
9	K	1	MET	CG-SD-CE	8.54	113.86	100.20
2	B	1020	ARG	NE-CZ-NH2	8.53	124.56	120.30
4	E	20	LYS	CA-CB-CG	8.53	132.16	113.40
7	I	61	ASP	CB-CG-OD1	-8.53	110.63	118.30
1	A	495	GLU	N-CA-CB	-8.52	95.26	110.60
2	B	730	ARG	NE-CZ-NH2	8.51	124.55	120.30
7	I	5	ARG	NE-CZ-NH2	8.50	124.55	120.30
1	A	481	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	A	555	ASP	CB-CG-OD1	8.49	125.94	118.30
1	A	1257	ASP	CB-CG-OD2	8.49	125.94	118.30
2	B	559	SER	CA-CB-OG	-8.46	88.35	111.20
6	H	89	LEU	CA-CB-CG	8.43	134.69	115.30
2	B	368	GLU	C-N-CA	-8.43	104.60	122.30
2	B	668	ASP	CB-CG-OD1	8.41	125.87	118.30
1	A	740	LEU	CB-CG-CD2	-8.40	96.72	111.00
2	B	120	ARG	NE-CZ-NH2	8.39	124.50	120.30
1	A	652	VAL	CG1-CB-CG2	-8.39	97.48	110.90
3	C	235	VAL	CG1-CB-CG2	-8.39	97.48	110.90
1	A	268	ASP	CB-CG-OD2	8.38	125.84	118.30
1	A	618	GLU	OE1-CD-OE2	8.38	133.36	123.30
10	L	60	ARG	NE-CZ-NH1	-8.37	116.11	120.30
1	A	909	ASP	CB-CG-OD2	-8.37	110.77	118.30
3	C	11	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	726	ARG	NE-CZ-NH2	8.36	124.48	120.30
7	I	13	MET	CG-SD-CE	-8.35	86.83	100.20
1	A	1226	VAL	CB-CA-C	-8.34	95.55	111.40
3	C	149	LYS	CD-CE-NZ	-8.34	92.52	111.70
5	F	119	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	856	THR	OG1-CB-CG2	-8.31	90.89	110.00
1	A	96	ILE	CG1-CB-CG2	-8.31	93.12	111.40
1	A	283	GLY	N-CA-C	-8.30	92.34	113.10
1	A	419	LYS	CD-CE-NZ	-8.29	92.62	111.70
2	B	56	ASP	CB-CG-OD1	-8.29	110.83	118.30
1	A	12	ARG	NE-CZ-NH2	-8.29	116.16	120.30
2	B	1077	THR	N-CA-CB	-8.28	94.57	110.30
8	J	38	ARG	NE-CZ-NH2	-8.28	116.16	120.30
2	B	605	ARG	NE-CZ-NH2	8.27	124.43	120.30
2	B	542	MET	CG-SD-CE	-8.23	87.04	100.20
7	I	32	CYS	CB-CA-C	-8.23	93.94	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	HIS	C-N-CD	-8.22	102.51	120.60
2	B	398	ARG	CB-CA-C	-8.22	93.96	110.40
2	B	722	ASP	CB-CG-OD1	8.22	125.70	118.30
1	A	50	ILE	CB-CA-C	-8.20	95.21	111.60
2	B	169	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	1281	ARG	NE-CZ-NH1	8.19	124.39	120.30
2	B	304	ASP	CB-CG-OD1	8.18	125.66	118.30
3	C	183	TRP	C-N-CA	-8.17	101.28	121.70
10	L	50	ASP	CB-CG-OD1	8.17	125.65	118.30
4	E	41	ASP	CB-CG-OD1	8.16	125.65	118.30
2	B	633	VAL	CG1-CB-CG2	-8.16	97.85	110.90
2	B	641	GLU	OE1-CD-OE2	-8.14	113.53	123.30
9	K	53	ASP	CB-CG-OD2	8.14	125.63	118.30
1	A	1135	ARG	NE-CZ-NH2	8.12	124.36	120.30
2	B	297	ILE	CA-CB-CG1	8.12	126.42	111.00
1	A	1161	THR	OG1-CB-CG2	-8.12	91.33	110.00
1	A	266	LEU	CA-CB-CG	8.10	133.93	115.30
2	B	654	ARG	NE-CZ-NH1	-8.10	116.25	120.30
1	A	32	VAL	CG1-CB-CG2	-8.08	97.97	110.90
2	B	89	GLU	N-CA-C	8.07	132.80	111.00
10	L	47	ARG	NE-CZ-NH2	8.07	124.34	120.30
3	C	143	LEU	CB-CG-CD2	-8.05	97.31	111.00
1	A	475	THR	CA-CB-CG2	8.05	123.67	112.40
2	B	942	ARG	NE-CZ-NH1	-8.05	116.28	120.30
3	C	226	ASP	CB-CG-OD2	8.03	125.52	118.30
2	B	622	LYS	CA-CB-CG	8.02	131.04	113.40
1	A	1438	THR	N-CA-CB	-8.02	95.07	110.30
1	A	645	LEU	CB-CG-CD1	-8.00	97.40	111.00
7	I	31	THR	N-CA-CB	-8.00	95.10	110.30
2	B	137	TYR	CB-CG-CD1	7.99	125.79	121.00
1	A	914	GLU	CG-CD-OE2	-7.98	102.34	118.30
4	E	167	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	A	731	ARG	NE-CZ-NH1	-7.97	116.32	120.30
2	B	711	GLU	OE1-CD-OE2	-7.95	113.76	123.30
1	A	1151	GLU	OE1-CD-OE2	-7.92	113.80	123.30
1	A	1005	GLU	CG-CD-OE1	7.92	134.13	118.30
2	B	1167	GLY	N-CA-C	7.91	132.88	113.10
2	B	477	ALA	N-CA-CB	7.91	121.18	110.10
4	E	81	GLU	OE1-CD-OE2	7.91	132.79	123.30
1	A	905	ASP	CB-CG-OD1	-7.90	111.19	118.30
1	A	898	ARG	NE-CZ-NH1	7.90	124.25	120.30
2	B	46	GLN	CA-CB-CG	-7.88	96.06	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1034	GLU	OE1-CD-OE2	-7.88	113.84	123.30
6	H	91	ASP	CB-CG-OD2	7.87	125.38	118.30
1	A	74	MET	CG-SD-CE	7.86	112.77	100.20
1	A	1136	SER	CB-CA-C	7.86	125.03	110.10
2	B	259	TYR	CB-CG-CD2	7.86	125.72	121.00
1	A	498	ARG	NE-CZ-NH1	-7.85	116.38	120.30
4	E	163	GLU	OE1-CD-OE2	-7.83	113.91	123.30
2	B	394	ASP	CB-CG-OD1	-7.82	111.26	118.30
3	C	26	ASP	CB-CG-OD1	7.82	125.33	118.30
8	J	17	LYS	CD-CE-NZ	-7.82	93.72	111.70
9	K	61	TYR	CB-CG-CD1	7.81	125.69	121.00
1	A	928	LEU	CB-CG-CD1	-7.80	97.74	111.00
1	A	1239	ARG	CB-CA-C	7.80	126.00	110.40
4	E	25	ASP	CB-CG-OD1	7.80	125.32	118.30
1	A	1012	ARG	CG-CD-NE	-7.79	95.44	111.80
1	A	942	PHE	CB-CG-CD2	-7.79	115.35	120.80
2	B	303	TYR	CB-CG-CD1	7.79	125.67	121.00
2	B	390	LEU	CB-CG-CD1	-7.78	97.77	111.00
2	B	620	ARG	CG-CD-NE	-7.78	95.45	111.80
1	A	547	LEU	CB-CG-CD2	-7.78	97.78	111.00
1	A	774	ARG	NH1-CZ-NH2	-7.76	110.86	119.40
2	B	320	ASP	CB-CG-OD1	7.76	125.28	118.30
7	I	35	VAL	CA-CB-CG2	-7.76	99.26	110.90
1	A	708	MET	N-CA-CB	-7.76	96.64	110.60
1	A	1005	GLU	CG-CD-OE2	-7.75	102.79	118.30
2	B	387	LEU	CB-CG-CD1	-7.75	97.82	111.00
2	B	1101	ASP	CB-CG-OD2	7.75	125.27	118.30
1	A	1196	GLU	CG-CD-OE2	-7.74	102.81	118.30
2	B	764	SER	N-CA-CB	-7.74	98.88	110.50
4	E	198	ILE	CG1-CB-CG2	-7.74	94.37	111.40
1	A	22	PHE	CB-CG-CD1	-7.74	115.38	120.80
1	A	949	ASP	CB-CG-OD1	-7.73	111.34	118.30
1	A	361	LEU	CB-CG-CD2	-7.72	97.87	111.00
3	C	11	ARG	NE-CZ-NH2	-7.71	116.45	120.30
3	C	90	ASP	CB-CG-OD2	-7.71	111.37	118.30
1	A	571	LEU	CB-CG-CD1	-7.70	97.91	111.00
9	K	22	ASP	OD1-CG-OD2	-7.70	108.67	123.30
2	B	598	GLU	N-CA-CB	7.70	124.46	110.60
2	B	498	THR	N-CA-CB	-7.69	95.68	110.30
3	C	124	LEU	CB-CG-CD1	-7.69	97.92	111.00
2	B	959	ASP	CB-CG-OD2	7.67	125.20	118.30
6	H	87	ARG	NE-CZ-NH2	-7.67	116.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	944	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	567	LYS	CD-CE-NZ	7.66	129.31	111.70
1	A	709	THR	N-CA-CB	-7.66	95.75	110.30
2	B	653	VAL	CB-CA-C	-7.66	96.86	111.40
2	B	1129	ARG	NE-CZ-NH1	7.65	124.13	120.30
3	C	254	LYS	CD-CE-NZ	-7.65	94.11	111.70
1	A	1415	SER	CB-CA-C	-7.62	95.61	110.10
1	A	1280	GLU	CG-CD-OE2	7.61	133.52	118.30
2	B	654	ARG	NE-CZ-NH2	7.61	124.10	120.30
1	A	1036	ARG	NH1-CZ-NH2	7.61	127.77	119.40
2	B	329	THR	OG1-CB-CG2	-7.59	92.53	110.00
2	B	404	LYS	CD-CE-NZ	-7.59	94.24	111.70
2	B	967	ARG	NE-CZ-NH1	-7.59	116.50	120.30
2	B	766	ARG	NE-CZ-NH2	7.58	124.09	120.30
2	B	303	TYR	CD1-CE1-CZ	-7.56	112.99	119.80
2	B	90	ILE	CB-CA-C	-7.56	96.48	111.60
4	E	17	ARG	NE-CZ-NH2	7.56	124.08	120.30
6	H	19	ARG	CD-NE-CZ	7.54	134.16	123.60
1	A	830	LYS	CB-CA-C	-7.54	95.32	110.40
4	E	142	VAL	CG1-CB-CG2	-7.54	98.84	110.90
3	C	11	ARG	CB-CA-C	-7.54	95.33	110.40
1	A	1259	MET	CG-SD-CE	7.53	112.25	100.20
1	A	1318	THR	CA-CB-CG2	7.53	122.94	112.40
2	B	305	VAL	CG1-CB-CG2	7.52	122.93	110.90
2	B	618	ASP	CB-CG-OD2	-7.51	111.54	118.30
2	B	662	MET	CA-CB-CG	-7.51	100.53	113.30
4	E	58	MET	CG-SD-CE	-7.50	88.20	100.20
3	C	118	LEU	CB-CG-CD2	7.50	123.75	111.00
1	A	469	ARG	CG-CD-NE	-7.49	96.06	111.80
2	B	1129	ARG	NE-CZ-NH2	-7.48	116.56	120.30
2	B	346	GLU	OE1-CD-OE2	-7.48	114.33	123.30
1	A	600	PRO	N-CD-CG	-7.47	91.99	103.20
1	A	537	ARG	CB-CG-CD	7.47	131.02	111.60
6	H	135	LEU	CB-CG-CD2	7.47	123.70	111.00
8	J	62	ARG	CG-CD-NE	-7.46	96.12	111.80
2	B	595	ARG	NE-CZ-NH2	7.46	124.03	120.30
2	B	1096	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	1274	ARG	NE-CZ-NH1	-7.46	116.57	120.30
2	B	539	LEU	CB-CG-CD2	7.45	123.67	111.00
2	B	910	VAL	CG1-CB-CG2	-7.45	98.97	110.90
7	I	30	ARG	NE-CZ-NH1	-7.45	116.57	120.30
1	A	158	PRO	CA-N-CD	-7.45	101.07	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	116	ASP	CB-CG-OD2	7.44	125.00	118.30
8	J	44	TYR	CB-CG-CD1	7.44	125.47	121.00
2	B	550	ASP	CB-CG-OD1	7.43	124.99	118.30
1	A	706	HIS	N-CA-CB	7.43	123.97	110.60
1	A	636	GLU	OE1-CD-OE2	-7.42	114.40	123.30
2	B	1129	ARG	CG-CD-NE	-7.42	96.23	111.80
1	A	12	ARG	CG-CD-NE	-7.41	96.23	111.80
1	A	1385	THR	N-CA-CB	-7.41	96.22	110.30
1	A	1349	TYR	CZ-CE2-CD2	7.41	126.47	119.80
6	H	111	LEU	CA-CB-CG	7.40	132.31	115.30
1	A	895	LYS	N-CA-CB	7.39	123.91	110.60
1	A	1385	THR	N-CA-C	7.39	130.96	111.00
3	C	230	MET	CG-SD-CE	7.39	112.03	100.20
1	A	1418	LEU	CB-CG-CD1	7.39	123.56	111.00
1	A	1055	ARG	NE-CZ-NH2	-7.38	116.61	120.30
9	K	24	ASP	CB-CG-OD1	-7.38	111.65	118.30
1	A	918	GLU	OE1-CD-OE2	-7.38	114.44	123.30
2	B	241	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	440	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	65	LEU	CA-CB-CG	7.37	132.24	115.30
1	A	655	PHE	CB-CG-CD2	-7.36	115.65	120.80
1	A	1012	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	629	LEU	CB-CG-CD2	-7.36	98.49	111.00
3	C	217	ASP	CB-CG-OD2	7.36	124.92	118.30
2	B	397	ASP	CB-CG-OD1	-7.34	111.69	118.30
1	A	557	ASP	C-N-CA	-7.33	106.91	122.30
1	A	61	ILE	N-CA-C	-7.31	91.26	111.00
2	B	57	TYR	CB-CG-CD2	7.31	125.39	121.00
1	A	424	ILE	CG1-CB-CG2	-7.31	95.32	111.40
2	B	1223	ASP	CB-CG-OD2	7.31	124.88	118.30
4	E	148	GLU	CG-CD-OE2	7.30	132.90	118.30
8	J	43	ARG	CG-CD-NE	-7.30	96.47	111.80
3	C	252	GLN	CA-CB-CG	7.29	129.44	113.40
6	H	102	TYR	CG-CD1-CE1	7.29	127.13	121.30
1	A	1057	VAL	CA-CB-CG2	-7.29	99.97	110.90
1	A	592	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	1286	LYS	CD-CE-NZ	-7.26	94.99	111.70
2	B	997	GLU	CA-CB-CG	-7.26	97.42	113.40
2	B	825	VAL	CG1-CB-CG2	-7.26	99.29	110.90
2	B	39	ARG	NH1-CZ-NH2	-7.25	111.42	119.40
1	A	1298	TYR	CG-CD2-CE2	7.25	127.10	121.30
4	E	98	ILE	CG1-CB-CG2	-7.25	95.45	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	29	MET	CG-SD-CE	7.24	111.79	100.20
1	A	737	LEU	CB-CG-CD1	-7.23	98.70	111.00
2	B	694	ASP	CB-CG-OD2	7.23	124.81	118.30
8	J	48	ARG	CA-CB-CG	7.22	129.29	113.40
2	B	601	ARG	NH1-CZ-NH2	7.21	127.34	119.40
1	A	464	PRO	O-C-N	-7.21	111.16	122.70
2	B	252	SER	N-CA-CB	7.21	121.32	110.50
6	H	41	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	59	GLY	N-CA-C	7.21	131.12	113.10
1	A	1223	ASP	CB-CG-OD1	7.21	124.79	118.30
7	I	73	ARG	NE-CZ-NH2	-7.20	116.70	120.30
7	I	19	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	414	ASP	OD1-CG-OD2	-7.20	109.62	123.30
3	C	57	VAL	CG1-CB-CG2	7.20	122.42	110.90
1	A	850	VAL	CG1-CB-CG2	-7.19	99.40	110.90
3	C	84	ARG	NH1-CZ-NH2	-7.19	111.50	119.40
1	A	1301	GLU	OE1-CD-OE2	7.18	131.91	123.30
8	J	1	MET	CA-CB-CG	7.18	125.50	113.30
2	B	796	LEU	CA-CB-CG	7.17	131.80	115.30
2	B	601	ARG	NE-CZ-NH1	-7.17	116.71	120.30
5	F	82	THR	CB-CA-C	-7.17	92.24	111.60
7	I	75	CYS	CB-CA-C	-7.17	96.06	110.40
10	L	70	ARG	NH1-CZ-NH2	-7.17	111.52	119.40
1	A	1119	TYR	CG-CD2-CE2	7.16	127.03	121.30
2	B	942	ARG	CB-CA-C	-7.16	96.08	110.40
1	A	1334	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	1305	VAL	CG1-CB-CG2	-7.14	99.47	110.90
1	A	1042	PHE	CB-CG-CD2	-7.14	115.80	120.80
2	B	983	ARG	CA-CB-CG	7.13	129.09	113.40
1	A	487	MET	CG-SD-CE	-7.12	88.80	100.20
8	J	22	LEU	CA-CB-CG	7.12	131.69	115.30
9	K	39	ASP	CB-CG-OD1	7.12	124.71	118.30
2	B	1166	CYS	O-C-N	-7.11	111.12	123.20
4	E	128	PRO	N-CD-CG	7.11	113.86	103.20
1	A	408	ASP	CB-CG-OD2	7.11	124.69	118.30
6	H	143	LEU	CB-CG-CD1	7.10	123.08	111.00
2	B	1026	LEU	CB-CG-CD1	-7.09	98.94	111.00
6	H	86	ASP	CB-CA-C	7.09	124.58	110.40
7	I	45	ARG	CD-NE-CZ	-7.08	113.68	123.60
3	C	210	GLU	CG-CD-OE2	-7.06	104.17	118.30
2	B	999	MET	CG-SD-CE	-7.05	88.92	100.20
1	A	557	ASP	O-C-N	-7.05	111.22	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	249	ARG	CD-NE-CZ	7.05	133.47	123.60
3	C	117	ASP	CB-CG-OD1	7.05	124.64	118.30
2	B	1004	GLU	OE1-CD-OE2	-7.05	114.84	123.30
1	A	630	ILE	CG1-CB-CG2	-7.04	95.91	111.40
3	C	121	VAL	CA-CB-CG1	7.03	121.45	110.90
1	A	460	VAL	CG1-CB-CG2	-7.03	99.65	110.90
1	A	907	THR	CB-CA-C	-7.03	92.62	111.60
2	B	165	VAL	CB-CA-C	-7.03	98.05	111.40
2	B	558	LEU	CB-CG-CD1	-7.03	99.05	111.00
2	B	122	LEU	CB-CG-CD1	-7.02	99.06	111.00
1	A	983	ILE	CG1-CB-CG2	-7.02	95.96	111.40
2	B	40	GLU	OE1-CD-OE2	7.02	131.72	123.30
8	J	22	LEU	N-CA-CB	-7.01	96.38	110.40
1	A	929	LEU	CB-CG-CD2	-6.99	99.12	111.00
5	F	72	LYS	C-N-CA	6.98	139.15	121.70
9	K	64	GLU	OE1-CD-OE2	-6.97	114.94	123.30
1	A	1198	ASP	OD1-CG-OD2	-6.96	110.07	123.30
5	F	72	LYS	N-CA-C	6.96	129.80	111.00
1	A	833	GLU	CG-CD-OE1	6.96	132.22	118.30
7	I	111	THR	CB-CA-C	-6.96	92.82	111.60
1	A	1280	GLU	CA-C-N	6.95	132.48	117.20
5	F	77	ASP	C-N-CA	-6.95	104.34	121.70
5	F	79	ARG	CB-CG-CD	-6.95	93.54	111.60
2	B	1185	CYS	CA-CB-SG	6.94	126.50	114.00
3	C	100	THR	OG1-CB-CG2	-6.94	94.03	110.00
10	L	27	LEU	CB-CG-CD2	6.93	122.78	111.00
1	A	940	ARG	CG-CD-NE	-6.93	97.25	111.80
1	A	603	ASN	N-CA-CB	-6.93	98.13	110.60
3	C	53	THR	OG1-CB-CG2	-6.92	94.08	110.00
8	J	1	MET	N-CA-CB	-6.92	98.14	110.60
1	A	555	ASP	OD1-CG-OD2	-6.92	110.15	123.30
2	B	691	GLU	CA-CB-CG	6.91	128.61	113.40
1	A	557	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	649	ILE	CA-CB-CG1	6.90	124.11	111.00
2	B	587	HIS	CA-C-N	6.89	129.98	116.20
9	K	6	ARG	CG-CD-NE	-6.89	97.34	111.80
1	A	291	GLU	CA-CB-CG	6.88	128.55	113.40
2	B	435	THR	OG1-CB-CG2	-6.88	94.17	110.00
1	A	1411	GLU	OE1-CD-OE2	-6.88	115.04	123.30
7	I	5	ARG	NH1-CZ-NH2	-6.88	111.83	119.40
1	A	1111	MET	CG-SD-CE	-6.88	89.19	100.20
4	E	2	ASP	CB-CG-OD2	6.88	124.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	676	MET	CG-SD-CE	6.87	111.19	100.20
1	A	727	ASP	CB-CG-OD1	6.87	124.48	118.30
8	J	3	VAL	CG1-CB-CG2	6.87	121.89	110.90
2	B	227	LYS	CD-CE-NZ	6.86	127.49	111.70
2	B	175	ARG	NE-CZ-NH2	6.85	123.73	120.30
2	B	137	TYR	CB-CG-CD2	-6.85	116.89	121.00
2	B	393	LYS	N-CA-CB	6.85	122.92	110.60
2	B	960	GLY	N-CA-C	6.85	130.21	113.10
2	B	591	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	B	712	PRO	N-CD-CG	-6.83	92.95	103.20
2	B	1019	SER	N-CA-CB	6.83	120.74	110.50
2	B	125	SER	CB-CA-C	6.83	123.07	110.10
4	E	162	ARG	CB-CG-CD	6.83	129.35	111.60
2	B	327	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	374	LEU	CB-CG-CD1	6.81	122.58	111.00
5	F	123	LYS	CD-CE-NZ	-6.81	96.03	111.70
1	A	1409	LEU	CB-CG-CD2	-6.81	99.42	111.00
2	B	391	ASP	CB-CG-OD1	6.81	124.43	118.30
2	B	722	ASP	OD1-CG-OD2	-6.81	110.37	123.30
1	A	86	LEU	CB-CG-CD1	-6.79	99.45	111.00
1	A	1176	LEU	CA-CB-CG	6.79	130.92	115.30
2	B	399	ASP	N-CA-CB	-6.79	98.37	110.60
2	B	170	LEU	CB-CG-CD1	-6.79	99.47	111.00
7	I	91	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	504	LEU	CA-CB-CG	6.78	130.90	115.30
1	A	960	ILE	CG1-CB-CG2	-6.77	96.51	111.40
1	A	565	ILE	CG1-CB-CG2	-6.76	96.52	111.40
2	B	303	TYR	CZ-CE2-CD2	6.76	125.89	119.80
8	J	16	ASP	CB-CG-OD2	6.76	124.39	118.30
8	J	59	LYS	CD-CE-NZ	-6.76	96.15	111.70
1	A	1280	GLU	O-C-N	-6.76	111.89	122.70
4	E	148	GLU	OE1-CD-OE2	-6.75	115.20	123.30
2	B	972	LYS	CD-CE-NZ	-6.75	96.19	111.70
1	A	464	PRO	CA-C-N	6.74	132.04	117.20
9	K	12	LEU	CA-CB-CG	-6.74	99.79	115.30
1	A	470	LEU	CB-CA-C	-6.74	97.39	110.20
1	A	705	LYS	N-CA-CB	6.74	122.73	110.60
10	L	55	ILE	CB-CA-C	-6.74	98.12	111.60
9	K	105	PHE	CZ-CE2-CD2	-6.74	112.01	120.10
6	H	80	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	A	386	ASP	CB-CG-OD2	-6.74	112.24	118.30
5	F	92	ARG	NE-CZ-NH2	-6.74	116.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	683	ILE	CG1-CB-CG2	-6.73	96.60	111.40
1	A	532	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	1318	THR	N-CA-CB	-6.72	97.53	110.30
7	I	111	THR	OG1-CB-CG2	-6.71	94.56	110.00
1	A	1433	MET	CG-SD-CE	6.71	110.94	100.20
2	B	894	ASP	CB-CG-OD1	6.71	124.34	118.30
2	B	1223	ASP	CB-CG-OD1	-6.71	112.26	118.30
4	E	11	ARG	NH1-CZ-NH2	6.71	126.78	119.40
1	A	239	LEU	CA-CB-CG	6.71	130.72	115.30
7	I	98	VAL	CA-CB-CG2	-6.71	100.84	110.90
1	A	351	THR	CB-CA-C	-6.70	93.50	111.60
5	F	94	LEU	C-N-CA	-6.70	108.22	122.30
1	A	1004	ASN	N-CA-C	6.68	129.05	111.00
2	B	501	PRO	O-C-N	6.68	133.40	122.70
2	B	813	LYS	CD-CE-NZ	-6.68	96.33	111.70
10	L	58	LYS	CA-C-N	6.68	131.90	117.20
10	L	25	ALA	C-N-CA	6.68	138.40	121.70
6	H	63	LEU	CA-CB-CG	6.67	130.64	115.30
2	B	543	SER	CB-CA-C	-6.67	97.44	110.10
4	E	121	MET	CB-CG-SD	6.67	132.40	112.40
2	B	1099	VAL	CG1-CB-CG2	6.66	121.56	110.90
3	C	38	ILE	CG1-CB-CG2	-6.66	96.75	111.40
2	B	655	LYS	CD-CE-NZ	6.65	127.00	111.70
2	B	131	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	1284	MET	CG-SD-CE	-6.65	89.57	100.20
2	B	1201	LYS	CD-CE-NZ	-6.65	96.42	111.70
2	B	1135	ARG	CG-CD-NE	-6.64	97.85	111.80
4	E	161	LYS	CA-CB-CG	6.64	128.01	113.40
6	H	94	ASP	CB-CG-OD2	6.64	124.28	118.30
7	I	5	ARG	NE-CZ-NH1	6.63	123.62	120.30
2	B	993	THR	OG1-CB-CG2	-6.63	94.75	110.00
3	C	204	SER	N-CA-CB	-6.62	100.57	110.50
1	A	755	PHE	CB-CG-CD2	6.61	125.43	120.80
5	F	115	THR	OG1-CB-CG2	-6.61	94.79	110.00
2	B	1017	ILE	CA-CB-CG1	-6.61	98.44	111.00
2	B	699	GLU	CB-CA-C	-6.61	97.18	110.40
7	I	55	THR	CA-CB-CG2	6.61	121.65	112.40
1	A	655	PHE	CB-CG-CD1	6.60	125.42	120.80
2	B	642	ASP	N-CA-CB	6.59	122.47	110.60
2	B	1083	ALA	N-CA-CB	-6.59	100.87	110.10
1	A	726	ARG	CG-CD-NE	-6.59	97.97	111.80
3	C	263	THR	CA-CB-CG2	6.59	121.62	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1085	ILE	CG1-CB-CG2	-6.58	96.91	111.40
1	A	414	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	1025	ARG	NE-CZ-NH2	6.58	123.59	120.30
7	I	17	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	781	ASP	CB-CG-OD1	6.57	124.22	118.30
1	A	1375	MET	CG-SD-CE	6.57	110.72	100.20
1	A	279	LEU	CB-CG-CD1	6.57	122.17	111.00
8	J	47	ARG	NE-CZ-NH2	-6.57	117.02	120.30
4	E	78	LEU	CB-CG-CD2	6.56	122.16	111.00
1	A	597	LEU	CB-CG-CD2	-6.56	99.84	111.00
3	C	34	ARG	CD-NE-CZ	6.56	132.79	123.60
1	A	1349	TYR	CG-CD1-CE1	6.56	126.55	121.30
2	B	884	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	1203	ASN	CB-CA-C	6.56	123.52	110.40
2	B	576	ASP	CB-CG-OD2	6.55	124.20	118.30
3	C	253	LYS	CD-CE-NZ	-6.55	96.63	111.70
4	E	4	GLU	OE1-CD-OE2	-6.55	115.44	123.30
5	F	135	ARG	NE-CZ-NH2	6.54	123.57	120.30
2	B	1183	LYS	CA-CB-CG	6.54	127.78	113.40
2	B	959	ASP	OD1-CG-OD2	-6.53	110.89	123.30
2	B	452	THR	OG1-CB-CG2	-6.53	94.98	110.00
2	B	1156	ASP	CB-CG-OD1	6.53	124.18	118.30
2	B	650	GLU	CG-CD-OE1	-6.53	105.25	118.30
1	A	1172	LEU	CB-CA-C	-6.52	97.81	110.20
10	L	58	LYS	N-CA-C	6.52	128.61	111.00
1	A	519	PRO	N-CD-CG	6.52	112.98	103.20
4	E	17	ARG	CG-CD-NE	-6.51	98.13	111.80
3	C	23	SER	N-CA-C	-6.50	93.46	111.00
1	A	1170	ILE	CG1-CB-CG2	-6.49	97.12	111.40
1	A	62	ASP	CB-CG-OD2	6.49	124.14	118.30
2	B	895	ASP	CB-CG-OD2	6.49	124.14	118.30
2	B	1219	ASP	OD1-CG-OD2	-6.49	110.97	123.30
1	A	1357	ALA	CB-CA-C	-6.49	100.37	110.10
7	I	84	VAL	N-CA-CB	-6.49	97.23	111.50
9	K	73	LEU	CA-CB-CG	6.48	130.21	115.30
1	A	1006	ILE	CA-CB-CG1	6.48	123.31	111.00
3	C	193	TYR	CD1-CE1-CZ	6.48	125.63	119.80
10	L	40	LEU	CB-CA-C	6.48	122.51	110.20
1	A	1326	ARG	NH1-CZ-NH2	-6.48	112.27	119.40
1	A	79	GLY	N-CA-C	-6.47	96.91	113.10
2	B	273	LEU	CB-CG-CD1	6.47	122.00	111.00
6	H	142	LEU	CB-CG-CD1	-6.47	100.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1001	ARG	CG-CD-NE	-6.45	98.25	111.80
2	B	217	ARG	CG-CD-NE	-6.45	98.26	111.80
1	A	634	THR	CA-CB-CG2	-6.45	103.38	112.40
9	K	19	LEU	CB-CG-CD1	-6.44	100.05	111.00
1	A	830	LYS	N-CA-CB	6.43	122.18	110.60
2	B	38	PHE	CB-CG-CD1	-6.43	116.30	120.80
1	A	923	LEU	CB-CG-CD1	-6.43	100.07	111.00
2	B	272	THR	OG1-CB-CG2	-6.43	95.22	110.00
2	B	401	PHE	CB-CG-CD2	-6.42	116.30	120.80
3	C	35	ARG	CG-CD-NE	-6.42	98.31	111.80
2	B	854	LEU	CB-CG-CD2	-6.42	100.08	111.00
1	A	1405	THR	OG1-CB-CG2	-6.41	95.26	110.00
3	C	124	LEU	N-CA-C	6.41	128.31	111.00
6	H	102	TYR	CD1-CE1-CZ	-6.41	114.03	119.80
6	H	103	LYS	CB-CG-CD	6.41	128.26	111.60
9	K	114	LEU	CB-CG-CD1	-6.41	100.11	111.00
1	A	1281	ARG	CB-CA-C	-6.40	97.60	110.40
1	A	1241	ARG	CD-NE-CZ	6.39	132.55	123.60
1	A	1299	VAL	CB-CA-C	6.39	123.55	111.40
1	A	938	LYS	CB-CA-C	-6.39	97.62	110.40
1	A	1154	TYR	N-CA-C	-6.39	93.75	111.00
2	B	646	LEU	CB-CG-CD1	6.39	121.86	111.00
1	A	407	ARG	NH1-CZ-NH2	6.38	126.42	119.40
7	I	83	ASN	CB-CA-C	-6.38	97.64	110.40
1	A	985	ASP	OD1-CG-OD2	6.38	135.41	123.30
2	B	759	PRO	N-CD-CG	-6.37	93.64	103.20
1	A	720	ARG	CG-CD-NE	6.37	125.17	111.80
1	A	934	LYS	CD-CE-NZ	-6.37	97.06	111.70
3	C	239	PRO	CA-C-O	6.36	135.47	120.20
4	E	77	SER	N-CA-C	-6.36	93.82	111.00
1	A	446	ARG	CG-CD-NE	6.36	125.16	111.80
2	B	336	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	475	THR	N-CA-CB	-6.36	98.22	110.30
1	A	44	THR	N-CA-CB	6.36	122.37	110.30
1	A	857	ARG	CB-CA-C	-6.36	97.69	110.40
10	L	68	GLU	CB-CG-CD	6.35	131.34	114.20
1	A	416	ARG	NE-CZ-NH1	6.34	123.47	120.30
3	C	183	TRP	CA-C-N	6.34	131.16	117.20
1	A	672	ASP	OD1-CG-OD2	-6.34	111.25	123.30
2	B	709	ASP	CB-CG-OD2	6.34	124.00	118.30
1	A	1171	GLN	N-CA-CB	6.33	122.00	110.60
2	B	914	LYS	CD-CE-NZ	-6.33	97.14	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1155	ASP	CB-CG-OD1	6.32	123.99	118.30
2	B	399	ASP	CB-CG-OD2	6.32	123.99	118.30
2	B	1108	ARG	N-CA-C	6.32	128.07	111.00
2	B	270	LYS	CD-CE-NZ	-6.32	97.16	111.70
1	A	939	ASP	CB-CG-OD2	6.32	123.99	118.30
2	B	608	ASP	CB-CG-OD2	6.32	123.99	118.30
2	B	1103	ILE	CB-CA-C	-6.32	98.97	111.60
3	C	16	ASP	OD1-CG-OD2	-6.32	111.30	123.30
7	I	92	ARG	NE-CZ-NH1	-6.32	117.14	120.30
2	B	446	LEU	CB-CA-C	6.31	122.19	110.20
2	B	634	TYR	CB-CG-CD1	-6.30	117.22	121.00
5	F	97	ARG	CG-CD-NE	-6.30	98.57	111.80
2	B	56	ASP	O-C-N	-6.30	112.62	122.70
1	A	462	VAL	CG1-CB-CG2	-6.30	100.82	110.90
2	B	434	ARG	CG-CD-NE	6.29	125.01	111.80
1	A	761	MET	CG-SD-CE	6.29	110.26	100.20
2	B	312	GLU	N-CA-CB	-6.29	99.28	110.60
2	B	324	ILE	CG1-CB-CG2	-6.29	97.57	111.40
2	B	1073	TYR	CZ-CE2-CD2	6.28	125.45	119.80
9	K	79	GLU	OE1-CD-OE2	-6.28	115.76	123.30
3	C	193	TYR	CZ-CE2-CD2	-6.28	114.15	119.80
1	A	1062	GLU	CA-CB-CG	6.28	127.21	113.40
2	B	1060	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	659	HIS	CB-CG-ND1	-6.27	107.52	123.20
9	K	26	LYS	CG-CD-CE	6.27	130.71	111.90
2	B	961	LEU	CB-CG-CD1	6.27	121.66	111.00
7	I	35	VAL	CB-CA-C	-6.27	99.49	111.40
2	B	735	ALA	O-C-N	6.27	132.73	122.70
2	B	629	ASP	CB-CG-OD1	-6.26	112.66	118.30
1	A	843	LYS	CB-CA-C	6.25	122.91	110.40
1	A	544	ASP	OD1-CG-OD2	-6.25	111.42	123.30
1	A	1325	THR	N-CA-CB	-6.25	98.42	110.30
1	A	731	ARG	NH1-CZ-NH2	6.24	126.27	119.40
2	B	124	TYR	CB-CG-CD2	6.24	124.74	121.00
1	A	375	THR	CA-CB-CG2	-6.24	103.67	112.40
1	A	804	TYR	CB-CG-CD1	6.24	124.74	121.00
2	B	1127	GLY	N-CA-C	6.24	128.69	113.10
2	B	722	ASP	CB-CG-OD2	6.23	123.91	118.30
9	K	75	ILE	CA-CB-CG1	6.23	122.84	111.00
1	A	555	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	1103	GLU	CB-CA-C	6.23	122.85	110.40
2	B	167	ILE	CB-CA-C	-6.23	99.15	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	ILE	CB-CA-C	-6.23	99.15	111.60
7	I	82	GLU	OE1-CD-OE2	-6.22	115.83	123.30
1	A	739	ASP	CB-CG-OD2	6.22	123.90	118.30
2	B	653	VAL	CA-CB-CG1	6.22	120.23	110.90
2	B	759	PRO	CA-CB-CG	-6.22	92.18	104.00
5	F	154	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	541	ILE	CG1-CB-CG2	-6.21	97.73	111.40
7	I	24	ARG	CB-CA-C	-6.21	97.97	110.40
7	I	78	CYS	CA-CB-SG	6.21	125.18	114.00
1	A	461	LYS	CB-CA-C	-6.21	97.98	110.40
6	H	142	LEU	CA-CB-CG	-6.20	101.03	115.30
10	L	70	ARG	N-CA-C	6.20	127.75	111.00
7	I	24	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	B	68	THR	OG1-CB-CG2	-6.20	95.74	110.00
2	B	365	THR	OG1-CB-CG2	-6.20	95.75	110.00
2	B	419	THR	OG1-CB-CG2	-6.20	95.74	110.00
1	A	1373	ASP	OD1-CG-OD2	-6.20	111.53	123.30
1	A	1235	LYS	CD-CE-NZ	6.19	125.95	111.70
3	C	127	ARG	NE-CZ-NH1	6.19	123.40	120.30
2	B	43	LEU	CB-CG-CD2	-6.19	100.47	111.00
1	A	728	LYS	CB-CG-CD	6.19	127.70	111.60
7	I	4	PHE	CB-CG-CD1	-6.19	116.47	120.80
1	A	376	TYR	CZ-CE2-CD2	-6.19	114.23	119.80
4	E	103	LYS	N-CA-CB	6.18	121.73	110.60
1	A	1192	LEU	CB-CG-CD1	-6.17	100.50	111.00
2	B	942	ARG	CA-CB-CG	6.17	126.98	113.40
2	B	477	ALA	CB-CA-C	6.17	119.36	110.10
1	A	486	GLU	CG-CD-OE1	6.17	130.63	118.30
2	B	1216	LEU	CB-CG-CD2	-6.16	100.52	111.00
1	A	879	GLU	OE1-CD-OE2	6.16	130.69	123.30
1	A	1155	ASP	OD1-CG-OD2	-6.16	111.59	123.30
1	A	1342	GLU	OE1-CD-OE2	6.16	130.69	123.30
9	K	68	PHE	CB-CG-CD1	-6.16	116.49	120.80
1	A	325	ILE	CG1-CB-CG2	-6.16	97.86	111.40
1	A	1155	ASP	CB-CG-OD2	6.15	123.84	118.30
3	C	252	GLN	CB-CA-C	6.15	122.71	110.40
10	L	57	LEU	N-CA-C	6.15	127.61	111.00
1	A	493	GLN	CB-CG-CD	6.15	127.59	111.60
4	E	87	SER	CB-CA-C	6.15	121.78	110.10
1	A	1348	LEU	CB-CG-CD1	-6.15	100.55	111.00
1	A	1445	ILE	O-C-N	6.15	132.54	122.70
2	B	909	ASP	OD1-CG-OD2	-6.14	111.64	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	THR	CB-CA-C	-6.13	95.04	111.60
2	B	297	ILE	CA-CB-CG2	-6.13	98.63	110.90
4	E	180	ARG	CD-NE-CZ	6.13	132.19	123.60
1	A	416	ARG	CG-CD-NE	-6.13	98.93	111.80
9	K	74	ARG	CG-CD-NE	-6.13	98.93	111.80
2	B	138	GLU	OE1-CD-OE2	-6.13	115.95	123.30
1	A	923	LEU	CB-CA-C	-6.12	98.57	110.20
1	A	1066	VAL	CG1-CB-CG2	-6.12	101.11	110.90
1	A	922	ASP	CB-CG-OD1	6.12	123.80	118.30
1	A	885	THR	OG1-CB-CG2	-6.11	95.94	110.00
2	B	979	LYS	CD-CE-NZ	-6.11	97.64	111.70
1	A	466	SER	N-CA-C	6.11	127.49	111.00
4	E	41	ASP	OD1-CG-OD2	-6.11	111.70	123.30
1	A	1377	THR	CA-CB-CG2	6.10	120.94	112.40
2	B	212	LEU	CB-CG-CD2	6.10	121.37	111.00
2	B	959	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	1111	MET	N-CA-CB	-6.10	99.63	110.60
2	B	304	ASP	N-CA-CB	6.10	121.57	110.60
2	B	690	VAL	CG1-CB-CG2	-6.10	101.14	110.90
3	C	249	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	A	839	ARG	NE-CZ-NH1	6.09	123.35	120.30
2	B	89	GLU	OE1-CD-OE2	-6.09	115.99	123.30
2	B	990	ILE	CA-CB-CG1	6.09	122.57	111.00
3	C	210	GLU	CG-CD-OE1	6.09	130.48	118.30
4	E	204	THR	N-CA-CB	-6.09	98.73	110.30
3	C	183	TRP	O-C-N	-6.09	112.96	122.70
4	E	16	PHE	CB-CG-CD1	6.09	125.06	120.80
1	A	1013	ASP	CB-CG-OD1	6.08	123.78	118.30
1	A	1234	GLU	CA-CB-CG	6.08	126.79	113.40
4	E	62	ALA	N-CA-CB	-6.08	101.58	110.10
4	E	195	VAL	CA-CB-CG2	-6.08	101.78	110.90
7	I	30	ARG	CG-CD-NE	-6.08	99.03	111.80
1	A	898	ARG	CB-CA-C	-6.08	98.25	110.40
1	A	608	ILE	CA-CB-CG1	6.08	122.54	111.00
1	A	664	THR	CB-CA-C	-6.08	95.20	111.60
6	H	82	PRO	N-CA-C	-6.08	96.30	112.10
3	C	85	ASP	CB-CG-OD1	-6.07	112.83	118.30
2	B	596	LEU	CB-CG-CD1	-6.07	100.68	111.00
1	A	512	VAL	CA-CB-CG1	6.07	120.00	110.90
3	C	55	THR	OG1-CB-CG2	-6.06	96.06	110.00
2	B	97	VAL	CG1-CB-CG2	-6.06	101.20	110.90
1	A	386	ASP	CB-CG-OD1	6.06	123.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	116	TYR	N-CA-C	6.06	127.35	111.00
8	J	64	ASN	CB-CA-C	6.06	122.51	110.40
1	A	895	LYS	CD-CE-NZ	-6.05	97.78	111.70
1	A	1371	LEU	CB-CG-CD1	-6.05	100.71	111.00
7	I	118	ARG	CA-CB-CG	6.05	126.71	113.40
1	A	305	ASP	OD1-CG-OD2	-6.05	111.81	123.30
4	E	26	ARG	NE-CZ-NH2	6.05	123.33	120.30
2	B	537	LYS	CD-CE-NZ	-6.04	97.80	111.70
1	A	918	GLU	CA-CB-CG	6.04	126.69	113.40
4	E	55	ARG	NE-CZ-NH2	6.04	123.32	120.30
2	B	212	LEU	CB-CG-CD1	-6.04	100.73	111.00
2	B	711	GLU	CB-CA-C	-6.04	98.33	110.40
6	H	11	GLN	CB-CA-C	-6.03	98.33	110.40
7	I	1	MET	CB-CG-SD	6.03	130.49	112.40
7	I	112	SER	N-CA-CB	-6.03	101.46	110.50
8	J	48	ARG	CD-NE-CZ	6.03	132.04	123.60
2	B	1220	ARG	NH1-CZ-NH2	-6.03	112.77	119.40
2	B	884	ARG	CG-CD-NE	-6.03	99.15	111.80
2	B	904	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	A	578	LEU	CB-CG-CD1	-6.02	100.76	111.00
1	A	96	ILE	CA-CB-CG1	6.02	122.44	111.00
3	C	206	ASN	O-C-N	-6.02	113.07	122.70
2	B	19	GLU	OE1-CD-OE2	-6.02	116.08	123.30
2	B	135	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	B	354	ASP	CB-CG-OD2	-6.01	112.89	118.30
4	E	17	ARG	NE-CZ-NH1	-6.01	117.29	120.30
9	K	41	THR	CA-CB-CG2	-6.01	103.98	112.40
2	B	807	ARG	CG-CD-NE	-6.01	99.18	111.80
7	I	92	ARG	CA-C-N	-6.00	103.99	117.20
3	C	63	ILE	CG1-CB-CG2	-6.00	98.19	111.40
1	A	1227	ILE	CG1-CB-CG2	-6.00	98.20	111.40
1	A	677	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	B	1033	LYS	CD-CE-NZ	-5.99	97.92	111.70
5	F	116	ASP	OD1-CG-OD2	-5.99	111.92	123.30
1	A	56	PRO	O-C-N	5.98	132.27	122.70
6	H	7	ASP	CB-CG-OD2	5.98	123.68	118.30
10	L	42	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	A	680	THR	OG1-CB-CG2	-5.97	96.27	110.00
1	A	720	ARG	NE-CZ-NH1	-5.97	117.31	120.30
2	B	579	ARG	NH1-CZ-NH2	5.97	125.97	119.40
2	B	1181	GLU	CA-CB-CG	5.97	126.54	113.40
7	I	55	THR	N-CA-CB	-5.97	98.96	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1359	ASP	CB-CG-OD1	5.97	123.67	118.30
2	B	942	ARG	CG-CD-NE	-5.97	99.27	111.80
2	B	598	GLU	CG-CD-OE2	5.97	130.23	118.30
2	B	381	MET	CG-SD-CE	-5.96	90.66	100.20
2	B	836	GLU	O-C-N	5.96	132.24	122.70
1	A	1225	PHE	CB-CG-CD2	5.96	124.97	120.80
7	I	5	ARG	CB-CG-CD	5.96	127.10	111.60
1	A	295	LEU	CA-CB-CG	5.96	129.00	115.30
1	A	666	ILE	CG1-CB-CG2	5.96	124.51	111.40
2	B	249	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	724	GLU	N-CA-C	-5.96	94.92	111.00
2	B	889	THR	CB-CA-C	-5.96	95.52	111.60
1	A	327	ALA	CA-C-N	-5.95	104.11	117.20
2	B	276	ILE	CG1-CB-CG2	-5.95	98.31	111.40
2	B	852	ARG	N-CA-CB	-5.95	99.89	110.60
6	H	107	VAL	N-CA-C	-5.95	94.94	111.00
1	A	885	THR	CA-CB-CG2	5.95	120.73	112.40
1	A	896	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	B	621	GLU	CG-CD-OE2	5.94	130.18	118.30
1	A	790	ASP	CB-CG-OD1	5.94	123.64	118.30
2	B	895	ASP	CB-CG-OD1	5.93	123.64	118.30
6	H	87	ARG	CA-CB-CG	5.93	126.46	113.40
2	B	397	ASP	CB-CG-OD2	5.93	123.64	118.30
5	F	149	GLU	N-CA-CB	5.93	121.28	110.60
2	B	883	LEU	CB-CG-CD2	5.93	121.08	111.00
2	B	1154	ALA	CB-CA-C	5.93	118.99	110.10
3	C	183	TRP	N-CA-C	-5.93	94.99	111.00
7	I	88	SER	CB-CA-C	-5.92	98.84	110.10
1	A	589	GLN	CB-CA-C	-5.92	98.56	110.40
1	A	708	MET	CG-SD-CE	5.92	109.67	100.20
4	E	39	LEU	CB-CG-CD1	5.92	121.06	111.00
10	L	63	ARG	N-CA-CB	5.90	121.23	110.60
1	A	858	ASN	CB-CG-OD1	-5.90	109.80	121.60
1	A	1377	THR	N-CA-CB	5.90	121.51	110.30
8	J	7	CYS	CB-CA-C	-5.90	98.60	110.40
1	A	438	ASP	OD1-CG-OD2	-5.90	112.09	123.30
3	C	40	GLU	N-CA-C	5.90	126.93	111.00
2	B	511	PRO	N-CD-CG	-5.90	94.35	103.20
2	B	954	VAL	CB-CA-C	-5.90	100.19	111.40
2	B	1153	GLU	CG-CD-OE1	-5.90	106.50	118.30
7	I	24	ARG	CG-CD-NE	-5.89	99.42	111.80
2	B	589	VAL	CB-CA-C	5.89	122.59	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1019	SER	C-N-CA	-5.89	106.98	121.70
3	C	76	ASP	CB-CG-OD2	-5.89	113.00	118.30
3	C	191	TYR	CZ-CE2-CD2	5.89	125.10	119.80
1	A	728	LYS	N-CA-CB	5.89	121.19	110.60
1	A	1243	VAL	CA-CB-CG2	5.89	119.73	110.90
1	A	897	TYR	CB-CG-CD1	5.88	124.53	121.00
9	K	74	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	1204	ASP	OD1-CG-OD2	-5.88	112.14	123.30
2	B	378	LEU	CB-CG-CD1	-5.88	101.01	111.00
6	H	63	LEU	CB-CA-C	5.87	121.36	110.20
10	L	48	CYS	N-CA-C	5.87	126.85	111.00
1	A	16	GLU	CG-CD-OE2	-5.87	106.57	118.30
1	A	658	LEU	CB-CG-CD2	-5.86	101.03	111.00
4	E	200	ARG	N-CA-CB	5.86	121.15	110.60
7	I	8	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	1193	LEU	CB-CG-CD2	-5.86	101.04	111.00
10	L	40	LEU	CB-CG-CD2	5.86	120.96	111.00
3	C	238	ILE	CA-CB-CG2	5.85	122.60	110.90
1	A	516	SER	N-CA-CB	-5.85	101.72	110.50
3	C	165	LYS	N-CA-CB	5.85	121.13	110.60
6	H	128	ASN	N-CA-C	5.85	126.78	111.00
2	B	65	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	A	1370	LEU	CD1-CG-CD2	-5.84	92.98	110.50
1	A	1371	LEU	CB-CG-CD2	5.84	120.93	111.00
3	C	18	VAL	N-CA-C	-5.84	95.23	111.00
1	A	41	MET	CG-SD-CE	5.84	109.54	100.20
2	B	1101	ASP	OD1-CG-OD2	-5.84	112.20	123.30
1	A	1035	TYR	CD1-CE1-CZ	5.84	125.05	119.80
4	E	162	ARG	CB-CA-C	5.84	122.07	110.40
6	H	127	GLY	N-CA-C	5.84	127.69	113.10
2	B	895	ASP	OD1-CG-OD2	-5.83	112.21	123.30
2	B	853	SER	CB-CA-C	-5.83	99.02	110.10
5	F	150	GLU	CG-CD-OE1	-5.83	106.64	118.30
8	J	64	ASN	N-CA-CB	-5.83	100.11	110.60
1	A	613	ILE	CG1-CB-CG2	-5.82	98.59	111.40
3	C	127	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	A	914	GLU	CG-CD-OE1	5.82	129.94	118.30
2	B	260	GLY	N-CA-C	-5.82	98.55	113.10
2	B	436	VAL	CB-CA-C	5.82	122.46	111.40
9	K	93	SER	N-CA-CB	5.82	119.22	110.50
1	A	416	ARG	CA-CB-CG	5.81	126.19	113.40
3	C	90	ASP	N-CA-C	5.81	126.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	110	ASP	OD1-CG-OD2	-5.81	112.27	123.30
1	A	436	ILE	CG1-CB-CG2	-5.80	98.63	111.40
3	C	89	GLU	N-CA-C	-5.80	95.33	111.00
2	B	20	ASP	CB-CG-OD1	5.80	123.52	118.30
2	B	644	GLU	N-CA-CB	-5.80	100.16	110.60
2	B	788	ARG	NE-CZ-NH2	-5.79	117.40	120.30
2	B	957	ASN	N-CA-CB	-5.79	100.17	110.60
4	E	149	LEU	CB-CG-CD1	5.79	120.85	111.00
1	A	86	LEU	CB-CG-CD2	5.79	120.85	111.00
1	A	1176	LEU	CB-CG-CD2	5.79	120.84	111.00
1	A	1241	ARG	CG-CD-NE	-5.79	99.65	111.80
2	B	795	ILE	CB-CA-C	-5.79	100.03	111.60
9	K	47	ARG	NH1-CZ-NH2	5.79	125.76	119.40
9	K	39	ASP	OD1-CG-OD2	-5.78	112.31	123.30
6	H	117	SER	CB-CA-C	-5.78	99.12	110.10
1	A	1134	ILE	CG1-CB-CG2	-5.78	98.69	111.40
3	C	116	LYS	CD-CE-NZ	-5.78	98.42	111.70
7	I	45	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	A	238	CYS	CA-CB-SG	-5.77	103.61	114.00
2	B	381	MET	CB-CA-C	-5.77	98.86	110.40
2	B	336	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	A	731	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	1409	LEU	CB-CG-CD1	5.75	120.78	111.00
1	A	1014	ALA	CA-C-O	5.75	132.17	120.10
1	A	1237	ILE	CG1-CB-CG2	-5.75	98.75	111.40
2	B	589	VAL	O-C-N	-5.75	113.50	122.70
1	A	1120	LEU	CB-CG-CD1	5.74	120.77	111.00
1	A	1129	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	A	1135	ARG	CD-NE-CZ	5.74	131.64	123.60
1	A	1198	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	980	ASP	CB-CA-C	-5.74	98.92	110.40
2	B	1212	ILE	CA-CB-CG1	-5.74	100.09	111.00
4	E	53	PRO	N-CD-CG	-5.74	94.59	103.20
4	E	112	TYR	OH-CZ-CE2	5.74	135.60	120.10
7	I	17	ARG	N-CA-CB	5.74	120.93	110.60
1	A	836	TYR	CB-CG-CD1	-5.74	117.56	121.00
2	B	319	GLU	OE1-CD-OE2	-5.74	116.42	123.30
4	E	154	ILE	CG1-CB-CG2	-5.74	98.78	111.40
3	C	94	LYS	CA-CB-CG	5.73	126.02	113.40
3	C	34	ARG	CG-CD-NE	-5.73	99.76	111.80
1	A	434	ARG	CD-NE-CZ	5.73	131.62	123.60
2	B	245	GLU	CG-CD-OE2	5.73	129.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	684	LEU	CB-CG-CD1	-5.73	101.26	111.00
6	H	116	TYR	CB-CA-C	-5.73	98.95	110.40
4	E	30	ILE	CG1-CB-CG2	-5.73	98.80	111.40
7	I	18	GLU	N-CA-C	-5.73	95.54	111.00
9	K	32	VAL	CG1-CB-CG2	-5.73	101.74	110.90
1	A	1208	THR	CB-CA-C	-5.72	96.14	111.60
1	A	1425	SER	CA-CB-OG	-5.72	95.75	111.20
2	B	289	LEU	O-C-N	-5.72	113.47	123.20
1	A	945	GLU	OE1-CD-OE2	5.72	130.17	123.30
2	B	589	VAL	N-CA-CB	-5.72	98.91	111.50
3	C	47	ASP	CB-CG-OD1	-5.72	113.16	118.30
1	A	739	ASP	CB-CG-OD1	5.71	123.44	118.30
6	H	52	GLN	CA-C-N	5.71	129.77	117.20
1	A	1280	GLU	CG-CD-OE1	-5.71	106.88	118.30
1	A	243	PRO	N-CD-CG	-5.71	94.64	103.20
3	C	263	THR	N-CA-CB	-5.71	99.45	110.30
1	A	235	ILE	CB-CG1-CD1	5.71	129.88	113.90
4	E	194	GLU	OE1-CD-OE2	-5.71	116.45	123.30
8	J	31	ASP	CB-CG-OD1	5.71	123.44	118.30
9	K	47	ARG	CG-CD-NE	5.71	123.79	111.80
2	B	773	MET	CA-CB-CG	-5.70	103.61	113.30
1	A	1212	VAL	CG1-CB-CG2	-5.70	101.78	110.90
2	B	239	GLU	CB-CA-C	5.70	121.80	110.40
8	J	58	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	A	968	GLN	CA-CB-CG	-5.70	100.87	113.40
2	B	268	THR	N-CA-CB	-5.70	99.47	110.30
8	J	28	ASP	N-CA-CB	5.70	120.85	110.60
2	B	911	ILE	CG1-CB-CG2	-5.69	98.87	111.40
8	J	51	LEU	CB-CG-CD2	-5.69	101.32	111.00
3	C	35	ARG	CD-NE-CZ	5.69	131.57	123.60
9	K	6	ARG	N-CA-CB	-5.69	100.36	110.60
1	A	1287	TYR	CD1-CE1-CZ	-5.69	114.68	119.80
2	B	1018	PRO	CA-C-O	-5.69	106.55	120.20
4	E	57	MET	CG-SD-CE	5.69	109.30	100.20
6	H	16	ASP	CB-CA-C	-5.69	99.03	110.40
9	K	93	SER	CB-CA-C	-5.68	99.30	110.10
1	A	896	ARG	NH1-CZ-NH2	5.68	125.65	119.40
1	A	1080	THR	CA-CB-CG2	5.68	120.35	112.40
2	B	479	VAL	CG1-CB-CG2	-5.68	101.81	110.90
2	B	1026	LEU	CB-CG-CD2	5.68	120.65	111.00
2	B	341	LEU	CB-CG-CD1	5.67	120.65	111.00
2	B	131	ASP	N-CA-C	-5.67	95.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	331	LEU	CB-CG-CD1	5.67	120.64	111.00
1	A	701	LEU	CB-CG-CD2	-5.67	101.36	111.00
1	A	1025	ARG	NE-CZ-NH1	-5.67	117.47	120.30
2	B	289	LEU	C-N-CA	-5.67	110.40	122.30
1	A	1135	ARG	CA-CB-CG	5.67	125.87	113.40
9	K	17	SER	CB-CA-C	-5.67	99.33	110.10
4	E	72	PHE	CG-CD2-CE2	-5.67	114.57	120.80
1	A	266	LEU	CB-CA-C	-5.66	99.44	110.20
8	J	24	LEU	CB-CA-C	-5.66	99.44	110.20
3	C	58	LEU	CB-CG-CD1	-5.66	101.38	111.00
1	A	720	ARG	CB-CG-CD	5.66	126.31	111.60
4	E	169	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	1116	LEU	CA-CB-CG	5.66	128.31	115.30
9	K	111	LEU	CD1-CG-CD2	5.66	127.47	110.50
5	F	133	VAL	CA-CB-CG2	-5.65	102.42	110.90
6	H	112	ILE	CG1-CB-CG2	-5.65	98.96	111.40
2	B	239	GLU	N-CA-CB	-5.65	100.43	110.60
2	B	797	TYR	CB-CG-CD2	5.65	124.39	121.00
3	C	254	LYS	N-CA-CB	5.65	120.77	110.60
10	L	26	THR	CA-CB-CG2	5.65	120.31	112.40
7	I	54	GLU	CG-CD-OE2	-5.65	107.01	118.30
1	A	871	ASP	CB-CG-OD2	5.64	123.38	118.30
2	B	857	ARG	NE-CZ-NH2	-5.64	117.48	120.30
4	E	80	VAL	CB-CA-C	-5.64	100.67	111.40
1	A	764	CYS	N-CA-CB	-5.64	100.44	110.60
1	A	1192	LEU	CB-CG-CD2	5.64	120.59	111.00
2	B	595	ARG	N-CA-CB	5.64	120.75	110.60
2	B	642	ASP	C-N-CA	-5.64	107.60	121.70
2	B	1064	TYR	C-N-CA	-5.64	107.60	121.70
5	F	97	ARG	CB-CG-CD	5.64	126.26	111.60
1	A	962	ARG	CG-CD-NE	-5.64	99.96	111.80
2	B	643	ASP	CB-CG-OD1	5.64	123.37	118.30
7	I	10	CYS	N-CA-C	5.63	126.21	111.00
1	A	290	GLU	OE1-CD-OE2	5.63	130.06	123.30
1	A	635	ARG	CG-CD-NE	-5.63	99.97	111.80
6	H	52	GLN	O-C-N	-5.63	113.69	122.70
2	B	315	LYS	CB-CA-C	-5.63	99.14	110.40
1	A	886	ILE	CG1-CB-CG2	-5.63	99.02	111.40
1	A	1231	ASP	CB-CG-OD2	5.63	123.36	118.30
2	B	1183	LYS	CB-CA-C	5.62	121.65	110.40
7	I	9	ASP	CB-CG-OD1	-5.62	113.24	118.30
2	B	646	LEU	N-CA-C	5.62	126.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	136	LYS	CD-CE-NZ	5.62	124.63	111.70
1	A	571	LEU	CB-CG-CD2	5.62	120.55	111.00
2	B	1089	PRO	N-CD-CG	5.62	111.63	103.20
7	I	4	PHE	N-CA-C	5.62	126.17	111.00
1	A	1418	LEU	CB-CG-CD2	-5.62	101.45	111.00
1	A	1012	ARG	CD-NE-CZ	5.62	131.46	123.60
1	A	1440	ALA	N-CA-CB	-5.62	102.24	110.10
1	A	913	LEU	CB-CG-CD2	5.61	120.54	111.00
3	C	215	GLU	OE1-CD-OE2	-5.61	116.57	123.30
7	I	31	THR	C-N-CA	5.61	135.72	121.70
2	B	245	GLU	CA-CB-CG	5.61	125.73	113.40
1	A	1116	LEU	N-CA-C	-5.60	95.87	111.00
1	A	74	MET	CB-CG-SD	5.60	129.21	112.40
1	A	739	ASP	OD1-CG-OD2	-5.60	112.66	123.30
3	C	152	GLU	OE1-CD-OE2	5.60	130.02	123.30
3	C	191	TYR	CB-CG-CD1	5.60	124.36	121.00
1	A	1284	MET	O-C-N	5.60	131.66	122.70
6	H	56	THR	N-CA-C	-5.60	95.88	111.00
8	J	34	THR	OG1-CB-CG2	-5.60	97.12	110.00
1	A	1003	LYS	CA-CB-CG	-5.60	101.08	113.40
3	C	260	LEU	CB-CG-CD2	5.60	120.51	111.00
4	E	81	GLU	N-CA-CB	-5.60	100.53	110.60
1	A	586	ILE	CG1-CB-CG2	-5.59	99.09	111.40
4	E	63	ASN	N-CA-C	5.59	126.10	111.00
7	I	24	ARG	N-CA-CB	5.59	120.67	110.60
1	A	1263	ILE	CG1-CB-CG2	-5.59	99.09	111.40
2	B	452	THR	C-N-CA	5.59	135.68	121.70
2	B	370	PHE	CB-CA-C	5.59	121.58	110.40
2	B	234	ILE	CG1-CB-CG2	5.59	123.69	111.40
2	B	346	GLU	CG-CD-OE1	5.59	129.48	118.30
1	A	244	PRO	CA-C-O	-5.59	106.79	120.20
2	B	522	VAL	N-CA-CB	-5.59	99.21	111.50
3	C	127	ARG	NH1-CZ-NH2	-5.59	113.25	119.40
1	A	466	SER	N-CA-CB	5.58	118.88	110.50
4	E	52	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	1450	LEU	CA-CB-CG	5.58	128.14	115.30
2	B	57	TYR	CD1-CE1-CZ	5.58	124.83	119.80
2	B	483	LEU	CB-CG-CD2	5.58	120.49	111.00
3	C	163	ILE	CB-CA-C	5.58	122.77	111.60
2	B	1019	SER	CA-CB-OG	-5.58	96.13	111.20
9	K	14	GLU	CB-CA-C	5.58	121.56	110.40
7	I	1	MET	CG-SD-CE	5.58	109.12	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	LYS	CB-CG-CD	-5.58	97.10	111.60
1	A	465	TYR	O-C-N	-5.58	113.78	122.70
2	B	459	TYR	CB-CG-CD1	-5.58	117.66	121.00
2	B	705	MET	CB-CG-SD	-5.57	95.69	112.40
9	K	4	PRO	N-CA-C	-5.57	97.62	112.10
2	B	903	VAL	CG1-CB-CG2	-5.57	101.99	110.90
2	B	1106	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	1307	GLU	OE1-CD-OE2	-5.57	116.62	123.30
2	B	353	LYS	CD-CE-NZ	5.57	124.51	111.70
2	B	133	LYS	CD-CE-NZ	-5.56	98.90	111.70
1	A	173	THR	N-CA-C	-5.56	95.98	111.00
1	A	495	GLU	OE1-CD-OE2	-5.56	116.63	123.30
1	A	1442	ASP	O-C-N	5.56	131.59	122.70
2	B	940	PRO	N-CD-CG	-5.56	94.86	103.20
1	A	58	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	908	LEU	CB-CG-CD2	-5.55	101.56	111.00
2	B	273	LEU	CB-CA-C	-5.55	99.65	110.20
1	A	441	PRO	N-CD-CG	-5.55	94.87	103.20
2	B	852	ARG	NE-CZ-NH2	5.55	123.07	120.30
2	B	56	ASP	N-CA-C	5.54	125.97	111.00
2	B	817	LEU	CB-CG-CD2	-5.54	101.57	111.00
8	J	14	VAL	O-C-N	-5.54	113.77	123.20
1	A	1231	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	1192	LEU	CB-CA-C	-5.54	99.67	110.20
4	E	38	PRO	O-C-N	5.54	131.56	122.70
5	F	81	THR	CA-CB-CG2	5.54	120.16	112.40
2	B	1010	LEU	CB-CA-C	-5.54	99.68	110.20
4	E	166	LYS	CD-CE-NZ	5.54	124.43	111.70
1	A	992	ASP	N-CA-CB	-5.53	100.64	110.60
1	A	1017	LEU	CB-CG-CD2	-5.53	101.59	111.00
2	B	1099	VAL	CB-CA-C	-5.53	100.89	111.40
7	I	9	ASP	CB-CG-OD2	5.53	123.28	118.30
9	K	111	LEU	CB-CG-CD1	-5.53	101.60	111.00
1	A	933	TYR	CB-CG-CD2	5.53	124.32	121.00
2	B	134	LYS	CD-CE-NZ	5.53	124.41	111.70
1	A	1257	ASP	CB-CG-OD1	-5.53	113.33	118.30
5	F	144	GLU	OE1-CD-OE2	5.52	129.93	123.30
6	H	117	SER	O-C-N	5.52	131.54	122.70
1	A	1146	VAL	N-CA-CB	-5.52	99.36	111.50
2	B	665	GLU	CA-CB-CG	5.52	125.54	113.40
1	A	433	GLU	OE1-CD-OE2	5.51	129.92	123.30
2	B	336	ARG	NH1-CZ-NH2	5.51	125.47	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	119	VAL	CA-CB-CG1	-5.51	102.63	110.90
9	K	61	TYR	CZ-CE2-CD2	5.51	124.76	119.80
1	A	434	ARG	CG-CD-NE	-5.51	100.24	111.80
1	A	52	GLY	CA-C-O	-5.50	110.69	120.60
2	B	841	MET	CG-SD-CE	5.50	109.00	100.20
1	A	1113	THR	OG1-CB-CG2	-5.50	97.35	110.00
1	A	934	LYS	N-CA-CB	5.50	120.50	110.60
1	A	1109	LYS	CB-CA-C	5.50	121.40	110.40
2	B	737	THR	CA-CB-CG2	-5.49	104.71	112.40
9	K	54	ARG	CD-NE-CZ	5.49	131.29	123.60
7	I	16	PRO	N-CD-CG	-5.49	94.97	103.20
7	I	92	ARG	O-C-N	5.49	131.48	122.70
7	I	93	LYS	CA-CB-CG	5.49	125.48	113.40
3	C	180	TYR	CD1-CE1-CZ	5.49	124.74	119.80
8	J	18	TRP	CD1-NE1-CE2	-5.48	104.06	109.00
10	L	58	LYS	O-C-N	-5.48	113.94	122.70
2	B	166	PHE	N-CA-CB	-5.48	100.74	110.60
1	A	672	ASP	CB-CA-C	-5.47	99.45	110.40
2	B	302	CYS	CA-CB-SG	-5.47	104.15	114.00
2	B	387	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	948	VAL	N-CA-CB	-5.47	99.46	111.50
2	B	108	VAL	CB-CA-C	5.47	121.80	111.40
3	C	14	SER	N-CA-C	-5.47	96.23	111.00
9	K	1	MET	CB-CG-SD	-5.47	96.00	112.40
1	A	66	LYS	CA-CB-CG	5.46	125.42	113.40
6	H	87	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	1274	ARG	CB-CA-C	-5.46	99.49	110.40
2	B	973	ILE	CG1-CB-CG2	-5.46	99.40	111.40
1	A	836	TYR	CB-CG-CD2	5.45	124.27	121.00
1	A	1290	LYS	CD-CE-NZ	5.45	124.24	111.70
2	B	710	LEU	CB-CG-CD1	-5.45	101.73	111.00
1	A	85	ASP	N-CA-CB	5.45	120.41	110.60
1	A	1228	TRP	CA-CB-CG	5.45	124.05	113.70
1	A	437	MET	CB-CA-C	-5.45	99.51	110.40
2	B	277	LYS	N-CA-CB	-5.45	100.80	110.60
2	B	1166	CYS	N-CA-CB	-5.44	100.80	110.60
4	E	182	ASP	OD1-CG-OD2	-5.44	112.97	123.30
1	A	567	LYS	CA-C-O	-5.44	108.69	120.10
6	H	9	ILE	N-CA-CB	5.44	123.30	110.80
1	A	607	ILE	N-CA-C	-5.43	96.34	111.00
2	B	106	ASP	N-CA-CB	-5.43	100.83	110.60
2	B	497	ARG	NH1-CZ-NH2	5.43	125.37	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	118	PHE	CG-CD2-CE2	-5.43	114.83	120.80
2	B	198	ASP	CB-CG-OD1	5.42	123.18	118.30
2	B	638	PHE	CD1-CE1-CZ	-5.42	113.59	120.10
1	A	743	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	A	1233	ASP	N-CA-CB	5.42	120.36	110.60
4	E	192	ARG	CD-NE-CZ	5.42	131.19	123.60
1	A	1259	MET	N-CA-C	-5.41	96.38	111.00
2	B	961	LEU	CA-CB-CG	5.41	127.75	115.30
2	B	903	VAL	CB-CA-C	-5.41	101.12	111.40
2	B	164	LYS	CA-C-N	5.41	129.10	117.20
9	K	70	ARG	CB-CA-C	5.41	121.22	110.40
3	C	180	TYR	CG-CD2-CE2	5.41	125.63	121.30
1	A	764	CYS	CA-CB-SG	5.41	123.73	114.00
1	A	938	LYS	CG-CD-CE	-5.40	95.69	111.90
2	B	501	PRO	CA-C-O	-5.40	107.24	120.20
2	B	773	MET	CG-SD-CE	5.40	108.84	100.20
2	B	1028	GLU	OE1-CD-OE2	-5.40	116.82	123.30
1	A	352	VAL	CA-CB-CG1	5.40	119.00	110.90
10	L	57	LEU	CB-CA-C	-5.40	99.95	110.20
2	B	990	ILE	CB-CA-C	-5.40	100.81	111.60
2	B	1073	TYR	CB-CG-CD2	5.40	124.24	121.00
1	A	1081	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	A	739	ASP	N-CA-C	5.39	125.56	111.00
2	B	303	TYR	CB-CG-CD2	-5.39	117.77	121.00
5	F	109	VAL	CG1-CB-CG2	-5.39	102.28	110.90
2	B	224	GLN	CA-CB-CG	-5.38	101.55	113.40
6	H	60	ALA	C-N-CA	-5.38	108.24	121.70
2	B	743	ILE	CG1-CB-CG2	-5.38	99.56	111.40
2	B	217	ARG	CB-CG-CD	5.38	125.59	111.60
9	K	73	LEU	CB-CG-CD2	5.38	120.15	111.00
1	A	894	GLU	CA-C-O	-5.38	108.80	120.10
2	B	633	VAL	CB-CA-C	-5.38	101.18	111.40
2	B	731	VAL	N-CA-C	-5.38	96.48	111.00
4	E	118	PRO	N-CD-CG	5.38	111.27	103.20
2	B	775	LYS	CB-CG-CD	-5.38	97.62	111.60
3	C	240	VAL	N-CA-C	5.38	125.51	111.00
1	A	469	ARG	CA-CB-CG	5.37	125.21	113.40
1	A	1289	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	A	443	LEU	CB-CG-CD1	-5.37	101.88	111.00
2	B	1020	ARG	CA-CB-CG	5.36	125.20	113.40
1	A	1239	ARG	CG-CD-NE	-5.36	100.54	111.80
2	B	635	ARG	NH1-CZ-NH2	-5.36	113.50	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	607	GLY	O-C-N	-5.36	114.12	122.70
1	A	1311	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	A	840	ARG	CD-NE-CZ	5.36	131.10	123.60
1	A	72	GLU	N-CA-C	5.35	125.46	111.00
1	A	913	LEU	N-CA-CB	-5.35	99.69	110.40
7	I	23	ASN	CB-CA-C	5.35	121.11	110.40
2	B	463	THR	N-CA-C	5.35	125.45	111.00
2	B	604	ARG	CD-NE-CZ	5.35	131.09	123.60
6	H	8	ASP	CB-CG-OD2	5.35	123.11	118.30
7	I	17	ARG	CB-CG-CD	5.35	125.50	111.60
1	A	1264	GLU	OE1-CD-OE2	-5.35	116.89	123.30
2	B	396	ASP	O-C-N	5.34	131.25	122.70
2	B	434	ARG	CA-CB-CG	5.34	125.16	113.40
1	A	678	GLU	OE1-CD-OE2	-5.34	116.89	123.30
2	B	707	PRO	N-CD-CG	-5.34	95.19	103.20
2	B	889	THR	N-CA-CB	5.34	120.44	110.30
2	B	95	ILE	CB-CA-C	-5.34	100.93	111.60
2	B	406	LEU	CB-CG-CD2	-5.34	101.93	111.00
8	J	21	TYR	CG-CD1-CE1	5.34	125.57	121.30
9	K	110	ASN	CB-CA-C	5.34	121.07	110.40
1	A	576	GLN	CB-CA-C	-5.33	99.73	110.40
1	A	883	LEU	N-CA-C	-5.33	96.59	111.00
4	E	18	THR	OG1-CB-CG2	-5.33	97.73	110.00
1	A	385	ILE	CG1-CB-CG2	5.33	123.12	111.40
1	A	917	SER	CB-CA-C	-5.33	99.98	110.10
3	C	109	SER	CB-CA-C	5.33	120.22	110.10
2	B	995	ARG	CD-NE-CZ	5.32	131.05	123.60
1	A	995	GLU	CG-CD-OE1	-5.32	107.66	118.30
2	B	781	PHE	CB-CG-CD1	-5.32	117.08	120.80
2	B	35	SER	CB-CA-C	-5.32	99.99	110.10
2	B	950	ASP	N-CA-CB	-5.32	101.03	110.60
1	A	602	ASP	C-N-CA	5.31	134.98	121.70
2	B	1030	LEU	CB-CG-CD2	-5.31	101.97	111.00
4	E	74	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	1039	LYS	CD-CE-NZ	-5.31	99.50	111.70
2	B	895	ASP	N-CA-CB	5.31	120.16	110.60
7	I	118	ARG	N-CA-C	5.31	125.33	111.00
4	E	31	THR	CA-CB-CG2	5.31	119.83	112.40
2	B	568	ASP	OD1-CG-OD2	-5.30	113.22	123.30
5	F	103	MET	CG-SD-CE	5.30	108.69	100.20
1	A	366	VAL	N-CA-C	-5.30	96.69	111.00
1	A	739	ASP	N-CA-CB	-5.30	101.06	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	359	GLU	CB-CA-C	-5.30	99.80	110.40
4	E	181	ALA	N-CA-CB	-5.30	102.68	110.10
1	A	577	ILE	CG1-CB-CG2	-5.30	99.74	111.40
9	K	11	LEU	CB-CA-C	-5.30	100.14	110.20
2	B	122	LEU	CA-CB-CG	-5.29	103.13	115.30
2	B	1110	PRO	CA-C-O	5.29	132.90	120.20
10	L	41	SER	N-CA-C	5.29	125.29	111.00
2	B	96	TYR	CB-CG-CD2	-5.29	117.83	121.00
4	E	66	GLU	N-CA-CB	5.29	120.12	110.60
1	A	1377	THR	CB-CA-C	-5.29	97.32	111.60
3	C	207	CYS	CB-CA-C	-5.29	99.82	110.40
2	B	639	ILE	CA-CB-CG1	5.29	121.04	111.00
4	E	204	THR	CA-CB-OG1	5.28	120.09	109.00
1	A	710	LEU	CB-CG-CD2	5.28	119.98	111.00
1	A	596	THR	CA-C-O	-5.28	109.02	120.10
1	A	481	ASP	N-CA-CB	-5.28	101.10	110.60
9	K	78	THR	N-CA-CB	5.28	120.33	110.30
1	A	1154	TYR	OH-CZ-CE2	5.27	134.34	120.10
1	A	1003	LYS	CB-CG-CD	5.27	125.30	111.60
3	C	202	PRO	N-CD-CG	-5.27	95.30	103.20
1	A	54	ASN	CA-C-N	5.27	128.79	117.20
1	A	1301	GLU	CG-CD-OE2	-5.27	107.76	118.30
1	A	426	LEU	CB-CG-CD1	5.26	119.95	111.00
2	B	331	LEU	CB-CG-CD2	-5.26	102.05	111.00
9	K	101	LEU	CA-CB-CG	5.26	127.40	115.30
2	B	310	MET	CG-SD-CE	5.26	108.61	100.20
2	B	299	GLU	CA-CB-CG	5.26	124.96	113.40
5	F	93	ILE	CG1-CB-CG2	-5.25	99.85	111.40
2	B	254	LEU	N-CA-C	-5.25	96.83	111.00
2	B	957	ASN	N-CA-C	5.25	125.17	111.00
4	E	28	TYR	CD1-CE1-CZ	5.25	124.53	119.80
8	J	42	LYS	CD-CE-NZ	5.25	123.78	111.70
7	I	91	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	1012	ARG	CA-CB-CG	5.24	124.93	113.40
2	B	567	GLU	CA-CB-CG	5.24	124.94	113.40
3	C	119	VAL	CA-CB-CG2	5.24	118.77	110.90
2	B	114	PRO	N-CD-CG	5.24	111.06	103.20
1	A	399	HIS	C-N-CA	5.24	144.01	122.00
1	A	834	THR	CA-CB-CG2	-5.24	105.07	112.40
1	A	1102	LYS	N-CA-CB	-5.24	101.17	110.60
1	A	1147	THR	OG1-CB-CG2	-5.24	97.95	110.00
1	A	686	ALA	N-CA-CB	5.24	117.43	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	848	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	795	GLU	CA-CB-CG	-5.23	101.89	113.40
3	C	232	VAL	CG1-CB-CG2	5.23	119.27	110.90
6	H	6	PHE	N-CA-C	-5.23	96.88	111.00
4	E	76	GLY	N-CA-C	-5.23	100.03	113.10
1	A	15	LYS	CA-CB-CG	5.23	124.90	113.40
1	A	1022	LEU	CB-CG-CD1	-5.23	102.11	111.00
2	B	705	MET	CG-SD-CE	-5.23	91.84	100.20
1	A	812	GLU	OE1-CD-OE2	-5.23	117.03	123.30
1	A	912	LEU	CA-CB-CG	-5.22	103.29	115.30
2	B	539	LEU	CB-CG-CD1	-5.22	102.12	111.00
5	F	116	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	1307	GLU	CG-CD-OE1	5.22	128.75	118.30
4	E	108	GLY	CA-C-O	5.22	130.00	120.60
2	B	1082	MET	CB-CG-SD	5.22	128.06	112.40
1	A	918	GLU	CG-CD-OE2	5.22	128.74	118.30
1	A	941	LYS	N-CA-CB	5.22	120.00	110.60
1	A	1027	ALA	N-CA-CB	-5.21	102.80	110.10
3	C	57	VAL	N-CA-CB	-5.21	100.03	111.50
1	A	63	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	B	648	HIS	N-CA-C	5.21	125.07	111.00
7	I	70	ARG	NH1-CZ-NH2	5.21	125.13	119.40
2	B	20	ASP	N-CA-CB	5.21	119.98	110.60
1	A	901	LEU	CB-CA-C	-5.21	100.30	110.20
2	B	969	ARG	CD-NE-CZ	-5.21	116.31	123.60
3	C	220	ASP	OD1-CG-OD2	-5.21	113.41	123.30
3	C	37	MET	CG-SD-CE	5.21	108.53	100.20
10	L	70	ARG	N-CA-CB	-5.21	101.23	110.60
6	H	32	THR	N-CA-CB	5.20	120.19	110.30
2	B	916	THR	N-CA-C	5.20	125.04	111.00
3	C	195	GLN	N-CA-CB	5.20	119.96	110.60
3	C	262	LEU	CB-CG-CD1	5.20	119.84	111.00
1	A	369	SER	CB-CA-C	-5.20	100.22	110.10
1	A	896	ARG	CD-NE-CZ	-5.20	116.32	123.60
4	E	46	TYR	CD1-CE1-CZ	5.20	124.48	119.80
2	B	702	LEU	CB-CG-CD2	5.20	119.83	111.00
1	A	26	GLU	OE1-CD-OE2	-5.19	117.07	123.30
2	B	890	TYR	CB-CG-CD1	5.19	124.11	121.00
1	A	446	ARG	NE-CZ-NH1	-5.19	117.71	120.30
2	B	310	MET	CA-CB-CG	-5.19	104.48	113.30
1	A	11	LEU	CB-CG-CD2	5.18	119.81	111.00
1	A	476	SER	CA-CB-OG	-5.18	97.20	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	857	ARG	CG-CD-NE	-5.18	100.91	111.80
10	L	57	LEU	CB-CG-CD2	-5.18	102.19	111.00
2	B	898	LEU	CB-CG-CD2	5.18	119.81	111.00
6	H	39	THR	CA-CB-CG2	-5.18	105.15	112.40
2	B	392	ARG	NE-CZ-NH2	-5.18	117.71	120.30
2	B	514	LEU	CB-CG-CD2	-5.18	102.20	111.00
2	B	1007	VAL	N-CA-CB	-5.18	100.11	111.50
1	A	984	LYS	CA-CB-CG	5.17	124.78	113.40
1	A	651	LYS	CB-CA-C	5.17	120.75	110.40
7	I	1	MET	CA-CB-CG	5.17	122.09	113.30
1	A	900	ASP	CB-CG-OD2	-5.17	113.64	118.30
4	E	144	ILE	CG1-CB-CG2	5.17	122.78	111.40
2	B	646	LEU	CB-CG-CD2	5.17	119.79	111.00
2	B	165	VAL	N-CA-CB	5.17	122.87	111.50
8	J	63	TYR	CB-CG-CD1	5.17	124.10	121.00
1	A	497	THR	N-CA-CB	-5.17	100.48	110.30
1	A	1299	VAL	N-CA-CB	-5.17	100.14	111.50
2	B	284	ILE	CG1-CB-CG2	-5.17	100.04	111.40
6	H	106	GLU	CB-CA-C	5.17	120.73	110.40
1	A	78	PRO	N-CD-CG	5.16	110.94	103.20
1	A	524	VAL	CG1-CB-CG2	-5.16	102.64	110.90
3	C	10	ILE	CB-CA-C	-5.16	101.27	111.60
1	A	705	LYS	CA-C-N	-5.16	105.84	117.20
10	L	59	ALA	CB-CA-C	-5.16	102.36	110.10
8	J	56	LEU	CD1-CG-CD2	-5.16	95.03	110.50
7	I	13	MET	N-CA-CB	-5.16	101.32	110.60
1	A	1028	THR	OG1-CB-CG2	-5.15	98.15	110.00
2	B	787	VAL	N-CA-CB	-5.15	100.16	111.50
6	H	41	ASP	OD1-CG-OD2	-5.15	113.52	123.30
7	I	109	ILE	CA-CB-CG1	5.15	120.79	111.00
1	A	897	TYR	CG-CD2-CE2	-5.15	117.18	121.30
4	E	207	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
1	A	461	LYS	CD-CE-NZ	-5.14	99.87	111.70
1	A	898	ARG	NH1-CZ-NH2	-5.14	113.74	119.40
2	B	1060	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	1077	THR	O-C-N	-5.14	114.47	122.70
2	B	621	GLU	CG-CD-OE1	-5.14	108.02	118.30
1	A	927	VAL	CA-CB-CG2	-5.14	103.19	110.90
2	B	1005	GLY	N-CA-C	5.14	125.95	113.10
1	A	351	THR	CA-CB-CG2	-5.14	105.21	112.40
1	A	814	PHE	CB-CG-CD2	5.14	124.40	120.80
1	A	1275	GLY	CA-C-N	-5.13	105.90	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1417	GLU	N-CA-C	-5.13	97.14	111.00
1	A	831	THR	CA-CB-CG2	-5.13	105.21	112.40
2	B	1131	GLY	N-CA-C	5.13	125.93	113.10
2	B	935	ARG	NE-CZ-NH1	5.13	122.87	120.30
4	E	200	ARG	CG-CD-NE	-5.13	101.03	111.80
4	E	28	TYR	CB-CG-CD2	5.13	124.08	121.00
4	E	28	TYR	N-CA-C	-5.13	97.15	111.00
1	A	49	LYS	CD-CE-NZ	5.13	123.50	111.70
1	A	1148	ILE	CG1-CB-CG2	-5.13	100.12	111.40
1	A	400	PRO	N-CD-CG	5.13	110.89	103.20
2	B	1020	ARG	NH1-CZ-NH2	-5.13	113.76	119.40
1	A	968	GLN	CB-CA-C	-5.12	100.15	110.40
2	B	412	LEU	N-CA-CB	5.12	120.65	110.40
1	A	4	GLN	CB-CA-C	5.12	120.64	110.40
2	B	522	VAL	CA-CB-CG2	-5.12	103.22	110.90
3	C	132	PRO	CA-C-O	-5.12	107.91	120.20
6	H	91	ASP	CA-C-O	5.12	130.85	120.10
2	B	806	THR	N-CA-CB	-5.12	100.58	110.30
2	B	90	ILE	N-CA-C	5.12	124.81	111.00
6	H	77	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	B	362	PRO	CA-C-O	-5.11	107.93	120.20
2	B	945	GLU	CG-CD-OE2	-5.11	108.07	118.30
3	C	105	GLY	N-CA-C	-5.11	100.32	113.10
9	K	42	LEU	CB-CA-C	-5.11	100.48	110.20
3	C	72	LEU	CB-CG-CD1	-5.11	102.31	111.00
6	H	45	GLU	CG-CD-OE2	-5.11	108.08	118.30
10	L	54	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	980	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	1158	PRO	CA-C-O	-5.11	107.94	120.20
2	B	1168	LEU	CB-CG-CD2	-5.11	102.32	111.00
2	B	586	TRP	CB-CA-C	5.10	120.60	110.40
1	A	804	TYR	CG-CD2-CE2	5.10	125.38	121.30
2	B	395	GLN	N-CA-CB	5.10	119.77	110.60
3	C	125	MET	CB-CG-SD	5.10	127.69	112.40
10	L	50	ASP	N-CA-CB	5.10	119.77	110.60
1	A	1101	LEU	CB-CA-C	5.10	119.88	110.20
7	I	45	ARG	CA-CB-CG	5.10	124.61	113.40
1	A	795	GLU	CB-CG-CD	5.09	127.96	114.20
1	A	1326	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	A	1365	TYR	CG-CD1-CE1	-5.09	117.23	121.30
8	J	28	ASP	CB-CA-C	-5.09	100.22	110.40
7	I	28	GLU	CA-CB-CG	5.09	124.59	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	975	HIS	N-CA-CB	-5.09	101.44	110.60
7	I	45	ARG	CG-CD-NE	5.08	122.47	111.80
1	A	65	LEU	CB-CG-CD2	5.08	119.63	111.00
9	K	64	GLU	CG-CD-OE1	5.08	128.46	118.30
1	A	32	VAL	N-CA-CB	-5.08	100.33	111.50
3	C	89	GLU	OE1-CD-OE2	-5.08	117.21	123.30
2	B	567	GLU	CB-CA-C	5.07	120.55	110.40
1	A	793	SER	N-CA-CB	-5.07	102.89	110.50
2	B	1220	ARG	CG-CD-NE	5.07	122.44	111.80
2	B	279	ASP	CB-CG-OD1	5.07	122.86	118.30
4	E	103	LYS	CD-CE-NZ	5.07	123.35	111.70
9	K	39	ASP	CB-CG-OD2	5.07	122.86	118.30
2	B	684	LEU	CB-CG-CD2	5.06	119.61	111.00
3	C	240	VAL	CB-CA-C	-5.06	101.78	111.40
6	H	89	LEU	CA-C-N	5.06	128.34	117.20
1	A	840	ARG	CG-CD-NE	-5.06	101.18	111.80
2	B	1053	GLU	N-CA-CB	5.06	119.71	110.60
3	C	193	TYR	CB-CG-CD2	5.06	124.04	121.00
8	J	29	GLU	OE1-CD-OE2	5.05	129.36	123.30
2	B	1161	HIS	CB-CA-C	5.05	120.50	110.40
4	E	177	ARG	NE-CZ-NH2	5.05	122.83	120.30
7	I	75	CYS	N-CA-CB	5.05	119.69	110.60
1	A	644	LYS	CB-CA-C	-5.05	100.30	110.40
2	B	100	PRO	CA-N-CD	-5.05	104.43	111.50
3	C	267	GLN	N-CA-C	5.05	124.63	111.00
6	H	7	ASP	OD1-CG-OD2	-5.04	113.72	123.30
8	J	39	LEU	CB-CG-CD1	5.04	119.58	111.00
3	C	155	LEU	CB-CG-CD2	-5.04	102.42	111.00
1	A	932	GLU	CB-CG-CD	5.04	127.81	114.20
6	H	139	ASN	N-CA-C	-5.04	97.39	111.00
1	A	912	LEU	N-CA-CB	5.04	120.48	110.40
2	B	446	LEU	CB-CG-CD1	5.04	119.57	111.00
1	A	1374	VAL	CA-CB-CG2	-5.04	103.34	110.90
3	C	182	PRO	N-CD-CG	-5.04	95.65	103.20
10	L	61	THR	CA-CB-CG2	5.03	119.45	112.40
1	A	1233	ASP	CB-CG-OD2	5.03	122.83	118.30
4	E	152	LYS	CD-CE-NZ	-5.03	100.13	111.70
1	A	806	ARG	CB-CA-C	-5.03	100.34	110.40
2	B	486	TYR	CB-CG-CD2	-5.03	117.98	121.00
5	F	132	LEU	CA-CB-CG	5.03	126.86	115.30
2	B	1052	VAL	CG1-CB-CG2	-5.03	102.86	110.90
10	L	31	CYS	CB-CA-C	-5.03	100.35	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1004	ASN	N-CA-CB	-5.02	101.56	110.60
1	A	1221	LYS	N-CA-CB	5.02	119.64	110.60
2	B	1202	LEU	CA-CB-CG	-5.02	103.75	115.30
10	L	38	LEU	CB-CG-CD2	5.02	119.53	111.00
1	A	1135	ARG	CG-CD-NE	-5.02	101.26	111.80
4	E	12	LEU	CB-CG-CD2	5.02	119.53	111.00
10	L	40	LEU	CB-CG-CD1	5.02	119.53	111.00
1	A	350	ARG	NE-CZ-NH1	5.01	122.81	120.30
4	E	207	ARG	CB-CG-CD	5.01	124.64	111.60
1	A	656	TRP	CD1-NE1-CE2	-5.01	104.49	109.00
6	H	111	LEU	CB-CG-CD1	5.01	119.52	111.00
1	A	788	SER	CA-CB-OG	-5.01	97.67	111.20
1	A	1170	ILE	N-CA-C	-5.01	97.47	111.00
1	A	1376	THR	CA-CB-CG2	5.01	119.42	112.40
2	B	485	ARG	CD-NE-CZ	5.01	130.62	123.60
2	B	978	ASP	CB-CG-OD2	5.01	122.81	118.30
4	E	140	LEU	CB-CG-CD2	-5.01	102.48	111.00
1	A	887	GLY	C-N-CA	-5.01	111.78	122.30
2	B	624	LEU	CB-CG-CD1	5.01	119.52	111.00
1	A	962	ARG	O-C-N	-5.01	114.69	122.70
2	B	1222	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	1043	ASP	OD1-CG-OD2	-5.00	113.79	123.30
1	A	495	GLU	CB-CA-C	5.00	120.40	110.40
1	A	917	SER	CA-CB-OG	-5.00	97.70	111.20
3	C	4	GLU	N-CA-C	5.00	124.50	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	204	THR	CB

All (102) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1046	LEU	Mainchain
1	A	1093	LYS	Peptide
1	A	1111	MET	Mainchain
1	A	1119	TYR	Sidechain
1	A	1155	ASP	Mainchain,Peptide
1	A	1220	PHE	Peptide
1	A	1232	ASN	Peptide
1	A	1301	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	1366	ARG	Sidechain
1	A	1384	VAL	Peptide
1	A	1434	ALA	Mainchain
1	A	31	SER	Peptide
1	A	399	HIS	Peptide
1	A	434	ARG	Sidechain
1	A	44	THR	Peptide
1	A	464	PRO	Peptide
1	A	465	TYR	Sidechain
1	A	555	ASP	Peptide
1	A	60	SER	Peptide
1	A	659	HIS	Sidechain
1	A	70	CYS	Peptide
1	A	705	LYS	Peptide
1	A	706	HIS	Peptide
1	A	74	MET	Peptide
1	A	741	ASN	Mainchain
1	A	821	ARG	Sidechain
1	A	936	LEU	Mainchain
2	B	1025	HIS	Sidechain
2	B	104	GLU	Peptide
2	B	107	GLY	Peptide
2	B	1097	HIS	Sidechain
2	B	1101	ASP	Peptide
2	B	1102	LYS	Peptide
2	B	1109	GLY	Peptide
2	B	1141	HIS	Sidechain
2	B	1152	MET	Peptide
2	B	1153	GLU	Peptide
2	B	1155	SER	Peptide
2	B	1221	SER	Peptide
2	B	1222	ARG	Peptide
2	B	238	ALA	Mainchain
2	B	244	LEU	Peptide
2	B	248	SER	Peptide
2	B	369	GLY	Peptide
2	B	431	TYR	Peptide
2	B	518	HIS	Sidechain
2	B	642	ASP	Peptide
2	B	643	ASP	Peptide
2	B	644	GLU	Peptide
2	B	667	GLN	Peptide

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Mol	Chain	Res	Type	Group
2	B	732	SER	Peptide
2	B	868	MET	Peptide
2	B	882	THR	Peptide
2	B	884	ARG	Peptide
2	B	905	VAL	Peptide
2	B	956	THR	Peptide
2	B	963	PHE	Mainchain
2	B	968	VAL	Mainchain
2	B	98	THR	Peptide
3	C	103	ALA	Mainchain
3	C	155	LEU	Mainchain,Peptide
3	C	156	THR	Mainchain
3	C	184	ASN	Peptide
3	C	190	ASP	Peptide
3	C	238	ILE	Mainchain
3	C	240	VAL	Mainchain
3	C	261	ALA	Peptide
3	C	267	GLN	Peptide
3	C	34	ARG	Sidechain
3	C	35	ARG	Sidechain
3	C	4	GLU	Peptide
4	E	119	SER	Peptide
4	E	125	PRO	Peptide
4	E	128	PRO	Peptide
4	E	153	HIS	Sidechain
4	E	207	ARG	Mainchain
4	E	212	ARG	Sidechain
4	E	77	SER	Peptide
6	H	102	TYR	Peptide
6	H	103	LYS	Peptide
6	H	127	GLY	Peptide
6	H	131	ASN	Peptide
6	H	135	LEU	Peptide
6	H	136	LYS	Peptide
6	H	17	PRO	Peptide
6	H	26	ILE	Peptide
6	H	61	SER	Peptide
6	H	62	SER	Peptide
6	H	86	ASP	Peptide
6	H	87	ARG	Peptide
6	H	94	ASP	Peptide
7	I	3	THR	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
7	I	43	VAL	Mainchain
9	K	6	ARG	Sidechain
9	K	70	ARG	Mainchain
10	L	27	LEU	Peptide
10	L	34	CYS	Peptide
10	L	35	SER	Peptide
10	L	59	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10625	0	10693	807	0
2	B	8690	0	8713	507	0
3	C	2095	0	2051	140	0
4	E	1760	0	1788	125	0
5	F	670	0	690	48	0
6	H	1068	0	1040	155	0
7	I	990	0	949	70	0
8	J	525	0	535	39	0
9	K	919	0	929	64	0
10	L	364	0	386	51	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	0	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	2	0	0	0	0
13	B	32	0	11	8	0
14	A	11	0	0	3	0
14	B	11	0	0	4	0
14	F	1	0	0	0	0
14	L	1	0	0	1	0
All	All	27772	0	27785	1880	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 34.

All (1880) 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:61:ILE:CB	1:A:61:ILE:CA	1.75	1.64
10:L:61:THR:CG2	10:L:61:THR:CB	1.75	1.64
1:A:941:LYS:CG	1:A:941:LYS:CD	1.74	1.64
5:F:72:LYS:CE	5:F:72:LYS:CD	1.76	1.64
1:A:1405:THR:CA	1:A:1405:THR:CB	1.77	1.62
1:A:1132:LYS:CB	1:A:1132:LYS:CG	1.75	1.62
4:E:161:LYS:CD	4:E:161:LYS:CE	1.76	1.61
1:A:1055:ARG:CD	1:A:1055:ARG:CG	1.76	1.61
1:A:46:THR:CA	1:A:46:THR:CB	1.77	1.61
1:A:571:LEU:CD2	1:A:571:LEU:CG	1.78	1.61
2:B:227:LYS:CD	2:B:227:LYS:CG	1.74	1.61
1:A:1081:LEU:CG	1:A:1081:LEU:CD2	1.76	1.60
2:B:531:GLN:CG	2:B:531:GLN:CB	1.77	1.60
3:C:7:GLN:CG	3:C:7:GLN:CB	1.77	1.60
1:A:1215:ARG:CG	1:A:1215:ARG:CB	1.75	1.60
1:A:518:LYS:CD	1:A:518:LYS:CE	1.77	1.60
4:E:54:GLN:CG	4:E:54:GLN:CB	1.78	1.60
7:I:3:THR:CG2	7:I:3:THR:CB	1.75	1.60
1:A:973:ILE:CG2	1:A:973:ILE:CB	1.75	1.60
2:B:115:GLN:CB	2:B:115:GLN:CG	1.76	1.60
1:A:1102:LYS:CD	1:A:1102:LYS:CE	1.77	1.59
1:A:1261:LYS:CD	1:A:1261:LYS:CE	1.76	1.59
1:A:1385:THR:CB	1:A:1385:THR:CG2	1.75	1.59
1:A:368:LYS:CD	1:A:368:LYS:CG	1.75	1.59
7:I:120:GLN:CG	7:I:120:GLN:CB	1.74	1.59
2:B:434:ARG:CG	2:B:434:ARG:CD	1.78	1.59
1:A:274:ILE:CA	1:A:274:ILE:CB	1.78	1.59
1:A:1262:LYS:CD	1:A:1262:LYS:CG	1.75	1.59
4:E:131:THR:CA	4:E:131:THR:CB	1.74	1.59
1:A:1080:THR:CB	1:A:1080:THR:CA	1.75	1.59
2:B:436:VAL:CA	2:B:436:VAL:CB	1.78	1.59
10:L:26:THR:CG2	10:L:26:THR:CB	1.75	1.59
8:J:42:LYS:CD	8:J:42:LYS:CE	1.79	1.58
1:A:566:ILE:CB	1:A:566:ILE:CG2	1.75	1.58
4:E:98:ILE:CA	4:E:98:ILE:CB	1.79	1.58
9:K:20:LYS:CD	9:K:20:LYS:CG	1.77	1.58
1:A:843:LYS:CE	1:A:843:LYS:CD	1.76	1.58
6:H:77:ARG:CB	6:H:77:ARG:CG	1.81	1.58
1:A:1286:LYS:CG	1:A:1286:LYS:CB	1.77	1.58
10:L:54:ARG:CG	10:L:54:ARG:CD	1.76	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:37:LEU:CD1	4:E:37:LEU:CG	1.81	1.58
1:A:1112:LYS:CB	1:A:1112:LYS:CG	1.82	1.58
2:B:305:VAL:CB	2:B:305:VAL:CG1	1.79	1.58
2:B:1057:LYS:CD	2:B:1057:LYS:CG	1.74	1.57
2:B:775:LYS:CB	2:B:775:LYS:CG	1.81	1.57
3:C:9:LYS:CG	3:C:9:LYS:CD	1.82	1.57
1:A:1132:LYS:CD	1:A:1132:LYS:CG	1.80	1.57
2:B:958:GLN:CB	2:B:958:GLN:CG	1.76	1.57
1:A:1093:LYS:CG	1:A:1093:LYS:CB	1.76	1.57
1:A:977:LYS:CG	1:A:977:LYS:CB	1.75	1.57
1:A:1162:VAL:CG1	1:A:1162:VAL:CB	1.80	1.57
2:B:620:ARG:CG	2:B:620:ARG:CD	1.77	1.57
3:C:199:LYS:CE	3:C:199:LYS:CD	1.76	1.57
1:A:1109:LYS:CG	1:A:1109:LYS:CD	1.79	1.57
1:A:1272:THR:CB	1:A:1272:THR:CG2	1.76	1.57
1:A:44:THR:CB	1:A:44:THR:CA	1.77	1.56
1:A:74:MET:CG	1:A:74:MET:CB	1.78	1.56
6:H:9:ILE:CB	6:H:9:ILE:CA	1.76	1.56
1:A:237:THR:CB	1:A:237:THR:CG2	1.82	1.56
2:B:164:LYS:CE	2:B:164:LYS:CD	1.82	1.56
7:I:45:ARG:CD	7:I:45:ARG:CG	1.82	1.56
2:B:1097:HIS:CB	2:B:1097:HIS:CA	1.79	1.56
3:C:252:GLN:CG	3:C:252:GLN:CB	1.74	1.56
1:A:295:LEU:CG	1:A:295:LEU:CD2	1.77	1.56
2:B:230:ALA:CA	2:B:230:ALA:CB	1.77	1.56
2:B:415:GLN:CB	2:B:415:GLN:CG	1.82	1.56
4:E:152:LYS:CG	4:E:152:LYS:CD	1.82	1.56
1:A:1130:GLN:CG	1:A:1130:GLN:CD	1.74	1.56
2:B:191:LYS:CG	2:B:191:LYS:CB	1.81	1.56
4:E:129:PRO:CD	4:E:129:PRO:CG	1.75	1.55
1:A:1135:ARG:CD	1:A:1135:ARG:CG	1.78	1.55
1:A:840:ARG:CD	1:A:840:ARG:CG	1.75	1.55
1:A:1187:GLN:CG	1:A:1187:GLN:CB	1.84	1.55
3:C:116:LYS:CE	3:C:116:LYS:CD	1.79	1.55
1:A:1003:LYS:CG	1:A:1003:LYS:CB	1.78	1.55
1:A:66:LYS:CB	1:A:66:LYS:CG	1.78	1.55
3:C:102:GLN:CG	3:C:102:GLN:CB	1.78	1.55
2:B:434:ARG:CG	2:B:434:ARG:CB	1.78	1.55
2:B:646:LEU:CD1	2:B:646:LEU:CG	1.81	1.55
1:A:1445:ILE:CG2	1:A:1445:ILE:CB	1.83	1.55
9:K:26:LYS:CG	9:K:26:LYS:CD	1.77	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:509:ALA:CA	2:B:509:ALA:CB	1.84	1.55
2:B:959:ASP:CG	2:B:959:ASP:CB	1.74	1.55
2:B:246:LYS:C	2:B:246:LYS:CA	1.76	1.54
5:F:123:LYS:CE	5:F:123:LYS:NZ	1.67	1.54
2:B:1102:LYS:CG	2:B:1102:LYS:CB	1.78	1.54
1:A:1171:GLN:CD	1:A:1171:GLN:CG	1.76	1.54
2:B:233:PRO:CB	2:B:233:PRO:CG	1.76	1.54
1:A:1350:LYS:CD	1:A:1350:LYS:CG	1.78	1.54
2:B:227:LYS:CE	2:B:227:LYS:NZ	1.70	1.54
1:A:601:LYS:CD	1:A:601:LYS:CE	1.82	1.54
6:H:52:GLN:CD	6:H:52:GLN:CG	1.74	1.54
1:A:1109:LYS:CG	1:A:1109:LYS:CB	1.79	1.54
2:B:646:LEU:CD2	2:B:646:LEU:CG	1.81	1.54
2:B:962:LYS:CE	2:B:962:LYS:CD	1.82	1.53
1:A:1222:ASN:CG	1:A:1222:ASN:CB	1.76	1.53
2:B:477:ALA:CA	2:B:477:ALA:CB	1.85	1.53
1:A:720:ARG:CG	1:A:720:ARG:CD	1.79	1.53
2:B:598:GLU:CD	2:B:598:GLU:CG	1.76	1.53
2:B:723:VAL:CB	2:B:723:VAL:CA	1.84	1.53
10:L:43:THR:CG2	10:L:43:THR:CB	1.76	1.53
1:A:1419:ASP:CG	1:A:1419:ASP:CB	1.75	1.53
1:A:830:LYS:CD	1:A:830:LYS:CE	1.81	1.53
2:B:723:VAL:CB	2:B:723:VAL:CG1	1.82	1.53
1:A:5:GLN:CG	1:A:5:GLN:CB	1.80	1.53
2:B:346:GLU:CG	2:B:346:GLU:CD	1.77	1.53
3:C:154:LYS:CG	3:C:154:LYS:CD	1.82	1.53
1:A:941:LYS:CE	1:A:941:LYS:NZ	1.70	1.53
1:A:1235:LYS:CE	1:A:1235:LYS:NZ	1.69	1.53
2:B:962:LYS:CG	2:B:962:LYS:CD	1.87	1.52
9:K:111:LEU:CD1	9:K:111:LEU:CG	1.86	1.52
1:A:1110:ASN:CB	1:A:1110:ASN:CG	1.78	1.52
1:A:544:ASP:CB	1:A:544:ASP:CG	1.77	1.52
4:E:162:ARG:CB	4:E:162:ARG:CG	1.86	1.52
1:A:934:LYS:CE	1:A:934:LYS:CD	1.87	1.52
3:C:94:LYS:CE	3:C:94:LYS:NZ	1.67	1.52
1:A:423:ASP:CG	1:A:423:ASP:CB	1.76	1.52
10:L:28:LYS:CA	10:L:28:LYS:C	1.77	1.52
2:B:347:LYS:CD	2:B:347:LYS:CE	1.76	1.52
2:B:706:GLN:CG	2:B:706:GLN:CB	1.84	1.51
2:B:986:GLN:CG	2:B:986:GLN:CD	1.75	1.51
2:B:1154:ALA:CA	2:B:1154:ALA:CB	1.87	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:41:ASP:CB	4:E:41:ASP:CG	1.77	1.51
3:C:50:GLU:CD	3:C:50:GLU:CG	1.77	1.51
10:L:48:CYS:CA	10:L:48:CYS:C	1.77	1.51
1:A:795:GLU:CD	1:A:795:GLU:CG	1.76	1.51
2:B:1101:ASP:CB	2:B:1101:ASP:CG	1.77	1.51
2:B:622:LYS:NZ	2:B:622:LYS:CE	1.70	1.51
4:E:191:LYS:CE	4:E:191:LYS:NZ	1.72	1.51
1:A:695:LYS:CD	1:A:695:LYS:CE	1.88	1.51
1:A:728:LYS:CE	1:A:728:LYS:NZ	1.70	1.51
2:B:115:GLN:CD	2:B:115:GLN:CG	1.78	1.51
1:A:597:LEU:CG	1:A:597:LEU:CD1	1.87	1.50
1:A:620:LYS:CE	1:A:620:LYS:CD	1.86	1.50
4:E:180:ARG:CG	4:E:180:ARG:CD	1.87	1.50
1:A:830:LYS:CD	1:A:830:LYS:CG	1.87	1.50
1:A:481:ASP:CG	1:A:481:ASP:CB	1.76	1.50
2:B:951:GLN:CD	2:B:951:GLN:CG	1.74	1.50
1:A:895:LYS:CD	1:A:895:LYS:CE	1.85	1.50
2:B:870:ILE:CA	2:B:870:ILE:CB	1.87	1.50
4:E:152:LYS:CE	4:E:152:LYS:CD	1.86	1.50
1:A:843:LYS:CD	1:A:843:LYS:CG	1.87	1.49
10:L:26:THR:CB	10:L:26:THR:CA	1.89	1.49
1:A:555:ASP:CG	1:A:555:ASP:CB	1.78	1.49
1:A:69:THR:CA	1:A:69:THR:C	1.74	1.49
2:B:315:LYS:CE	2:B:315:LYS:NZ	1.72	1.49
1:A:1132:LYS:CE	1:A:1132:LYS:NZ	1.74	1.49
2:B:41:LYS:CE	2:B:41:LYS:NZ	1.72	1.49
3:C:15:LYS:CG	3:C:15:LYS:CD	1.90	1.49
1:A:1204:ASP:CB	1:A:1204:ASP:CG	1.79	1.48
2:B:641:GLU:CD	2:B:641:GLU:CG	1.79	1.48
1:A:978:PRO:CB	1:A:978:PRO:CG	1.78	1.48
1:A:941:LYS:CD	1:A:941:LYS:CE	1.88	1.48
2:B:199:MET:SD	2:B:199:MET:CE	2.02	1.48
2:B:231:PRO:CB	2:B:231:PRO:CG	1.85	1.47
4:E:53:PRO:CB	4:E:53:PRO:CG	1.74	1.47
5:F:129:LYS:NZ	5:F:129:LYS:CE	1.72	1.47
6:H:104:PHE:C	6:H:104:PHE:CA	1.82	1.47
4:E:50:MET:CG	4:E:50:MET:SD	2.02	1.47
2:B:432:MET:SD	2:B:432:MET:CE	2.03	1.46
4:E:106:GLN:CD	4:E:106:GLN:CG	1.79	1.46
7:I:17:ARG:CG	7:I:17:ARG:CD	1.91	1.46
4:E:93:MET:SD	4:E:93:MET:CG	2.02	1.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:201:LYS:CG	4:E:201:LYS:CD	1.93	1.45
1:A:705:LYS:CG	1:A:705:LYS:CB	1.90	1.45
1:A:676:MET:CE	1:A:676:MET:SD	2.05	1.45
1:A:41:MET:SD	1:A:41:MET:CE	2.05	1.45
2:B:789:MET:SD	2:B:789:MET:CE	2.05	1.45
1:A:676:MET:CG	1:A:676:MET:SD	2.04	1.44
2:B:999:MET:CG	2:B:999:MET:SD	2.05	1.44
6:H:139:ASN:CB	6:H:139:ASN:CG	1.86	1.44
1:A:346:ASP:CB	1:A:346:ASP:CG	1.86	1.44
1:A:56:PRO:O	1:A:57:ARG:CD	1.66	1.44
3:C:265:MET:SD	3:C:265:MET:CE	2.05	1.44
1:A:938:LYS:CE	1:A:938:LYS:CD	1.95	1.44
2:B:1169:MET:CE	2:B:1169:MET:SD	2.05	1.44
1:A:248:PRO:CG	1:A:248:PRO:CB	1.78	1.43
1:A:1350:LYS:NZ	1:A:1350:LYS:CE	1.75	1.43
1:A:1111:MET:CG	1:A:1111:MET:SD	2.05	1.43
1:A:728:LYS:CD	1:A:728:LYS:CG	1.92	1.43
2:B:987:LYS:NZ	2:B:987:LYS:CE	1.81	1.43
2:B:593:PRO:CG	2:B:593:PRO:CB	1.86	1.43
1:A:1290:LYS:NZ	1:A:1290:LYS:CE	1.80	1.43
2:B:531:GLN:CG	2:B:531:GLN:CD	1.88	1.42
7:I:1:MET:CE	7:I:1:MET:SD	2.07	1.42
2:B:736:THR:CG2	2:B:736:THR:CB	1.96	1.42
13:B:3008:GTP:C1'	13:B:3008:GTP:N9	1.81	1.42
10:L:68:GLU:CD	10:L:68:GLU:CG	1.85	1.41
2:B:382:ILE:CD1	2:B:382:ILE:CG1	1.95	1.41
3:C:154:LYS:CD	3:C:154:LYS:CE	1.98	1.41
1:A:1259:MET:CG	1:A:1259:MET:SD	2.09	1.41
2:B:347:LYS:CD	2:B:347:LYS:CG	1.98	1.41
8:J:1:MET:CE	8:J:1:MET:SD	2.07	1.40
4:E:93:MET:SD	4:E:93:MET:CE	2.08	1.40
1:A:1232:ASN:CG	1:A:1232:ASN:CB	1.89	1.40
6:H:19:ARG:CD	6:H:19:ARG:CG	1.98	1.40
4:E:121:MET:CE	4:E:121:MET:SD	2.08	1.40
1:A:620:LYS:CE	1:A:620:LYS:NZ	1.85	1.40
3:C:29:MET:SD	3:C:29:MET:CE	2.10	1.40
1:A:1302:PRO:CB	1:A:1302:PRO:CG	1.95	1.39
4:E:131:THR:CG2	4:E:131:THR:CB	1.99	1.39
4:E:20:LYS:CE	4:E:20:LYS:NZ	1.84	1.38
1:A:74:MET:SD	1:A:74:MET:CE	2.09	1.38
4:E:162:ARG:CG	4:E:162:ARG:CD	2.01	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:1:MET:CG	7:I:1:MET:SD	2.13	1.35
1:A:1444:MET:SD	1:A:1444:MET:CE	2.14	1.35
7:I:55:THR:CG2	7:I:55:THR:CB	2.05	1.35
2:B:1097:HIS:ND1	2:B:1097:HIS:HA	1.37	1.35
4:E:121:MET:SD	4:E:121:MET:CG	2.13	1.34
6:H:104:PHE:O	6:H:106:GLU:N	1.63	1.32
1:A:728:LYS:CE	1:A:728:LYS:CD	2.09	1.31
1:A:172:PRO:CG	1:A:185:TRP:CE2	2.11	1.31
1:A:1259:MET:CE	1:A:1259:MET:SD	2.18	1.30
1:A:437:MET:CE	1:A:437:MET:SD	2.18	1.30
2:B:999:MET:SD	2:B:999:MET:CE	1.20	1.30
4:E:1:MET:CE	4:E:1:MET:SD	2.21	1.29
1:A:156:ASP:O	1:A:158:PRO:CD	1.80	1.28
2:B:705:MET:CE	2:B:705:MET:SD	1.18	1.28
1:A:172:PRO:CD	1:A:185:TRP:CE2	2.18	1.26
1:A:304:MET:CE	1:A:304:MET:SD	2.25	1.24
3:C:75:MET:SD	3:C:75:MET:CE	2.25	1.24
1:A:172:PRO:CG	1:A:185:TRP:CZ2	2.18	1.24
1:A:186:LYS:HE2	1:A:197:PRO:CD	1.66	1.24
1:A:172:PRO:CD	1:A:185:TRP:NE1	2.01	1.24
3:C:165:LYS:NZ	3:C:165:LYS:CE	2.01	1.24
1:A:56:PRO:O	1:A:57:ARG:HD2	1.11	1.23
3:C:125:MET:SD	3:C:125:MET:CE	2.27	1.23
1:A:172:PRO:HG2	1:A:185:TRP:CZ2	1.71	1.22
1:A:156:ASP:O	1:A:158:PRO:HD2	1.07	1.21
1:A:369:SER:OG	9:K:2:ASN:ND2	1.73	1.20
1:A:153:PRO:HD3	1:A:161:LEU:CD2	1.71	1.20
1:A:605:MET:CE	1:A:607:ILE:HD11	1.71	1.19
2:B:999:MET:HE3	2:B:999:MET:SD	1.77	1.19
1:A:487:MET:SD	1:A:487:MET:CE	1.09	1.19
2:B:662:MET:CE	2:B:662:MET:SD	2.31	1.18
1:A:535:THR:HG21	1:A:617:VAL:H	1.07	1.16
10:L:68:GLU:OE1	14:L:3006:HOH:O	1.63	1.16
9:K:1:MET:SD	9:K:1:MET:CE	2.35	1.15
5:F:103:MET:CE	5:F:103:MET:SD	2.33	1.15
2:B:999:MET:HE1	2:B:999:MET:SD	1.77	1.14
2:B:999:MET:SD	2:B:999:MET:HE2	1.77	1.14
1:A:172:PRO:HD3	1:A:185:TRP:CD1	1.82	1.14
1:A:172:PRO:HD2	1:A:185:TRP:NE1	1.60	1.14
1:A:42:ASP:OD2	1:A:47:ARG:N	1.81	1.14
2:B:101:MET:SD	2:B:101:MET:CE	2.35	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:THR:HG21	14:A:3013:HOH:O	1.45	1.13
1:A:172:PRO:HG3	1:A:185:TRP:CE2	1.80	1.13
2:B:705:MET:HE3	2:B:705:MET:SD	1.76	1.13
1:A:487:MET:CE	1:A:487:MET:CG	2.25	1.12
2:B:846:ILE:HD11	2:B:974:PRO:HB2	1.13	1.12
1:A:708:MET:SD	1:A:708:MET:CE	2.37	1.12
1:A:518:LYS:CD	1:A:518:LYS:NZ	2.11	1.11
2:B:705:MET:HE1	2:B:705:MET:SD	1.76	1.11
7:I:45:ARG:HH11	7:I:45:ARG:HG2	1.10	1.11
2:B:705:MET:CE	2:B:705:MET:CG	2.28	1.10
1:A:186:LYS:HE2	1:A:197:PRO:HD3	1.22	1.10
1:A:605:MET:HE2	1:A:607:ILE:CD1	1.80	1.10
6:H:128:ASN:O	6:H:131:ASN:ND2	1.85	1.09
2:B:130:VAL:HG22	2:B:167:ILE:HD11	1.30	1.09
3:C:54:ASN:OD1	3:C:56:THR:HB	1.53	1.09
1:A:487:MET:SD	1:A:487:MET:HE2	1.68	1.09
1:A:107:CYS:HB2	1:A:148:CYS:SG	1.93	1.08
1:A:487:MET:HE3	1:A:487:MET:SD	1.68	1.08
1:A:567:LYS:HB3	6:H:96:VAL:H	1.16	1.08
2:B:792:MET:CE	2:B:792:MET:SD	2.42	1.08
6:H:138:GLU:O	6:H:139:ASN:C	1.92	1.07
1:A:487:MET:HE1	1:A:487:MET:SD	1.68	1.07
7:I:16:PRO:O	7:I:17:ARG:HD3	1.53	1.06
2:B:1097:HIS:ND1	2:B:1097:HIS:CA	2.12	1.06
1:A:172:PRO:HG3	1:A:185:TRP:CD2	1.88	1.05
2:B:705:MET:SD	2:B:705:MET:HE2	1.76	1.05
7:I:45:ARG:HH11	7:I:45:ARG:CG	1.69	1.05
7:I:4:PHE:HE1	7:I:13:MET:HE2	1.19	1.05
2:B:999:MET:CG	2:B:999:MET:CE	2.35	1.04
1:A:1233:ASP:O	1:A:1234:GLU:HB3	1.55	1.03
1:A:1285:MET:SD	1:A:1285:MET:CE	2.46	1.03
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.40	1.03
8:J:14:VAL:HG13	8:J:50:ILE:HD11	1.41	1.03
9:K:110:ASN:O	9:K:112:GLN:N	1.92	1.03
2:B:955:THR:HG22	10:L:54:ARG:O	1.57	1.03
4:E:12:LEU:HD21	4:E:58:MET:SD	1.99	1.03
6:H:63:LEU:C	6:H:90:ALA:HB3	1.77	1.03
4:E:57:MET:SD	4:E:57:MET:CE	2.47	1.02
2:B:552:MET:SD	2:B:552:MET:CG	2.48	1.02
6:H:106:GLU:O	6:H:107:VAL:C	1.98	1.02
1:A:1134:ILE:O	1:A:1138:ILE:HG13	1.58	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ILE:HD11	1:A:732:LEU:HB2	1.42	1.01
1:A:1079:MET:SD	1:A:1359:ASP:OD2	2.19	1.01
1:A:187:LYS:HB2	1:A:194:ALA:HB3	1.44	1.00
1:A:567:LYS:HD3	6:H:95:TYR:CG	1.95	0.99
1:A:567:LYS:HB3	6:H:96:VAL:N	1.78	0.99
1:A:89:PRO:HB2	1:A:204:THR:HG21	1.39	0.99
1:A:72:GLU:OE2	2:B:1175:LEU:HD11	1.63	0.98
1:A:153:PRO:HD3	1:A:161:LEU:HD22	1.43	0.97
1:A:119:ASN:O	1:A:120:GLU:HB2	1.63	0.97
2:B:643:ASP:O	2:B:644:GLU:HB2	1.63	0.96
1:A:107:CYS:CB	1:A:148:CYS:SG	2.53	0.96
1:A:172:PRO:HD3	1:A:185:TRP:NE1	1.77	0.96
1:A:186:LYS:CE	1:A:197:PRO:HD3	1.95	0.96
1:A:153:PRO:HD3	1:A:161:LEU:HD23	1.48	0.95
2:B:885:MET:CE	2:B:885:MET:SD	2.54	0.95
1:A:186:LYS:HE2	1:A:197:PRO:HD2	1.45	0.95
7:I:78:CYS:SG	7:I:103:CYS:SG	2.64	0.95
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.29	0.95
8:J:2:ILE:N	8:J:2:ILE:HD13	1.80	0.95
1:A:567:LYS:HD2	1:A:568:PRO:HD3	1.48	0.95
1:A:1081:LEU:HG	1:A:1081:LEU:CD2	1.97	0.94
2:B:552:MET:SD	2:B:552:MET:CE	2.55	0.94
1:A:186:LYS:NZ	1:A:195:ASP:HA	1.82	0.94
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.33	0.94
1:A:1364:ASN:ND2	1:A:1366:ARG:HD2	1.83	0.94
4:E:63:ASN:O	4:E:64:PRO:O	1.86	0.93
1:A:325:ILE:C	1:A:327:ALA:H	1.68	0.93
1:A:605:MET:HE2	1:A:607:ILE:HD11	0.95	0.93
2:B:555:ILE:CD1	2:B:587:HIS:CE1	2.51	0.93
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.03	0.92
1:A:487:MET:HE2	1:A:487:MET:CG	1.92	0.92
1:A:176:LYS:NZ	1:A:178:GLY:O	2.01	0.92
1:A:775:ILE:CD1	1:A:775:ILE:CG1	2.48	0.92
2:B:1190:ASP:O	2:B:1191:ILE:HG13	1.68	0.92
5:F:77:ASP:O	5:F:78:GLN:HB2	1.66	0.92
7:I:116:ASN:HD21	7:I:118:ARG:HB2	1.35	0.92
2:B:846:ILE:CD1	2:B:974:PRO:HB2	2.00	0.92
1:A:531:ILE:HD11	1:A:578:LEU:CD2	2.00	0.91
1:A:1055:ARG:CG	1:A:1055:ARG:NE	2.33	0.91
1:A:1079:MET:HG2	1:A:1359:ASP:OD2	1.71	0.91
2:B:130:VAL:H	2:B:167:ILE:HD11	1.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:81:THR:CG2	5:F:136:ARG:HH11	1.83	0.91
1:A:1236:LEU:O	1:A:1237:ILE:HD12	1.71	0.91
2:B:846:ILE:HD11	2:B:974:PRO:CB	1.98	0.91
1:A:535:THR:CG2	1:A:617:VAL:H	1.84	0.90
6:H:55:LEU:HD22	6:H:144:ILE:HD12	1.53	0.90
7:I:4:PHE:HE1	7:I:13:MET:CE	1.83	0.90
1:A:605:MET:CE	1:A:607:ILE:CD1	2.43	0.90
1:A:1134:ILE:O	1:A:1138:ILE:CG1	2.19	0.89
2:B:58:THR:O	2:B:62:ILE:HG12	1.71	0.89
2:B:1097:HIS:CA	2:B:1097:HIS:CG	2.55	0.89
2:B:620:ARG:NE	2:B:620:ARG:CG	2.36	0.89
4:E:117:THR:O	4:E:119:SER:N	2.06	0.89
8:J:1:MET:CE	8:J:1:MET:CG	2.51	0.89
1:A:369:SER:H	9:K:2:ASN:HD21	1.21	0.89
2:B:846:ILE:HD11	2:B:974:PRO:O	1.73	0.88
2:B:775:LYS:CD	2:B:775:LYS:CB	2.51	0.88
6:H:89:LEU:O	6:H:91:ASP:N	2.06	0.88
7:I:45:ARG:NH1	7:I:45:ARG:HG2	1.88	0.88
1:A:795:GLU:HG2	2:B:731:VAL:HG21	1.54	0.88
1:A:1341:ILE:HD12	1:A:1379:GLY:HA2	1.54	0.88
3:C:167:HIS:HD2	3:C:169:LYS:H	1.22	0.88
1:A:1286:LYS:CD	1:A:1286:LYS:CB	2.51	0.88
1:A:1166:ASP:HB3	1:A:1169:ILE:CG2	2.05	0.88
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.02	0.88
1:A:567:LYS:HD3	6:H:95:TYR:HA	1.54	0.88
4:E:147:HIS:HD2	4:E:149:LEU:H	1.17	0.87
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.02	0.87
1:A:56:PRO:O	1:A:57:ARG:HD3	1.69	0.87
2:B:555:ILE:HD12	2:B:587:HIS:CE1	2.09	0.87
5:F:93:ILE:CD1	5:F:134:ILE:HD11	2.04	0.87
1:A:567:LYS:CB	6:H:96:VAL:H	1.87	0.87
1:A:1079:MET:CG	1:A:1359:ASP:OD2	2.22	0.87
2:B:1025:HIS:HE1	2:B:1090:THR:HG21	1.41	0.86
3:C:167:HIS:HE1	10:L:70:ARG:O	1.58	0.86
1:A:172:PRO:HD3	1:A:185:TRP:CE2	2.10	0.86
2:B:846:ILE:CD1	2:B:974:PRO:O	2.24	0.86
6:H:104:PHE:O	6:H:105:GLU:C	2.10	0.86
6:H:57:VAL:HG22	6:H:144:ILE:HD11	1.57	0.86
4:E:79:TRP:HB2	4:E:105:PHE:CE1	2.10	0.86
1:A:1134:ILE:CG2	1:A:1138:ILE:HD11	2.06	0.86
1:A:567:LYS:CD	6:H:95:TYR:HA	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:2:ILE:CD1	8:J:2:ILE:N	2.37	0.85
1:A:567:LYS:CG	1:A:568:PRO:CD	2.54	0.85
1:A:567:LYS:HD3	6:H:95:TYR:CA	2.05	0.85
7:I:4:PHE:CE1	7:I:13:MET:HE2	2.10	0.85
5:F:123:LYS:NZ	5:F:123:LYS:CD	2.39	0.85
1:A:1166:ASP:HB3	1:A:1169:ILE:HG21	1.59	0.85
1:A:64:ASN:OD1	1:A:64:ASN:O	1.93	0.85
1:A:172:PRO:HG3	1:A:185:TRP:CE3	2.10	0.85
1:A:164:ARG:O	1:A:166:GLY:N	2.08	0.85
1:A:679:ILE:HD12	1:A:729:ALA:HA	1.58	0.85
2:B:104:GLU:OE1	10:L:54:ARG:NE	2.10	0.85
6:H:106:GLU:O	6:H:107:VAL:O	1.94	0.84
1:A:55:ASP:OD1	1:A:55:ASP:O	1.94	0.84
3:C:46:ILE:HD12	3:C:72:LEU:HD11	1.59	0.84
7:I:32:CYS:HB2	7:I:34:TYR:H	1.43	0.83
10:L:48:CYS:HA	10:L:48:CYS:C	1.98	0.83
1:A:61:ILE:CB	1:A:61:ILE:HA	2.04	0.83
2:B:1220:ARG:O	2:B:1222:ARG:HD3	1.77	0.83
2:B:542:MET:HG3	2:B:747:MET:CE	2.07	0.83
2:B:477:ALA:CB	2:B:477:ALA:HA	2.08	0.83
4:E:98:ILE:HA	4:E:98:ILE:CB	2.03	0.83
1:A:679:ILE:HD13	1:A:732:LEU:HD12	1.59	0.83
1:A:31:SER:CB	1:A:83:HIS:HD2	1.91	0.83
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.58	0.83
2:B:431:TYR:O	2:B:431:TYR:CD2	2.31	0.83
1:A:108:MET:H	1:A:171:GLN:HE22	1.23	0.82
13:B:3008:GTP:C8	13:B:3008:GTP:C1'	2.61	0.82
4:E:2:ASP:HB3	4:E:6:GLU:HB2	1.61	0.82
1:A:1233:ASP:O	1:A:1234:GLU:CB	2.26	0.82
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.93	0.82
2:B:561:TRP:O	2:B:590:HIS:HE1	1.61	0.82
1:A:1003:LYS:CG	1:A:1003:LYS:CA	2.56	0.82
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.59	0.82
7:I:4:PHE:CE1	7:I:13:MET:CE	2.62	0.82
1:A:325:ILE:O	1:A:327:ALA:N	2.12	0.82
10:L:28:LYS:HA	10:L:28:LYS:C	1.98	0.82
2:B:25:ILE:HD11	2:B:651:LEU:HD12	1.62	0.81
6:H:63:LEU:C	6:H:90:ALA:CB	2.49	0.81
2:B:644:GLU:OE1	2:B:646:LEU:HB2	1.79	0.81
1:A:531:ILE:HD12	1:A:617:VAL:HB	1.62	0.81
1:A:55:ASP:N	1:A:56:PRO:CD	2.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.63	0.81
2:B:515:HIS:H	2:B:518:HIS:CD2	1.99	0.81
1:A:347:PHE:H	2:B:1107:ALA:HA	1.46	0.81
1:A:1111:MET:CG	1:A:1111:MET:CE	2.58	0.81
1:A:901:LEU:H	1:A:926:GLN:NE2	1.77	0.81
1:A:265:LYS:CD	1:A:302:THR:HG22	2.11	0.81
6:H:138:GLU:O	6:H:140:ALA:N	2.14	0.80
1:A:535:THR:HG21	1:A:617:VAL:N	1.93	0.80
7:I:45:ARG:NH1	7:I:45:ARG:CG	2.45	0.80
2:B:542:MET:HG3	2:B:747:MET:HE3	1.63	0.80
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.10	0.80
1:A:172:PRO:HD3	1:A:185:TRP:CG	2.15	0.80
1:A:567:LYS:CD	1:A:568:PRO:HD3	2.11	0.80
1:A:982:THR:HG22	1:A:985:ASP:H	1.47	0.80
2:B:515:HIS:H	2:B:518:HIS:HD2	1.25	0.80
6:H:103:LYS:HB3	6:H:105:GLU:OE1	1.82	0.80
2:B:417:PHE:CD2	2:B:417:PHE:O	2.36	0.79
2:B:90:ILE:HA	2:B:133:LYS:O	1.83	0.79
5:F:77:ASP:O	5:F:78:GLN:CB	2.28	0.79
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.17	0.79
1:A:265:LYS:NZ	1:A:302:THR:HG21	1.98	0.79
2:B:114:PRO:HD3	2:B:124:TYR:CE1	2.17	0.79
2:B:643:ASP:O	2:B:644:GLU:CB	2.31	0.79
1:A:55:ASP:O	1:A:57:ARG:N	2.15	0.79
2:B:130:VAL:HG22	2:B:167:ILE:CD1	2.10	0.79
4:E:50:MET:CE	4:E:50:MET:SD	2.70	0.79
1:A:1364:ASN:HD22	1:A:1366:ARG:H	1.29	0.78
1:A:596:THR:HG22	1:A:597:LEU:H	1.47	0.78
3:C:260:LEU:O	3:C:260:LEU:HD12	1.82	0.78
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.13	0.78
1:A:869:GLY:O	4:E:204:THR:HG21	1.84	0.78
1:A:571:LEU:HG	1:A:571:LEU:CD2	2.08	0.78
1:A:711:ARG:HE	7:I:95:THR:HG22	1.48	0.78
1:A:134:ARG:O	1:A:138:ILE:HG23	1.84	0.78
1:A:69:THR:C	1:A:69:THR:HA	2.03	0.78
1:A:941:LYS:CD	1:A:941:LYS:NZ	2.47	0.78
2:B:754:SER:O	2:B:806:THR:HG21	1.84	0.78
1:A:46:THR:HB	1:A:46:THR:CA	2.10	0.77
2:B:281:PRO:HB2	2:B:284:ILE:HD13	1.63	0.77
1:A:481:ASP:CG	1:A:481:ASP:CA	2.50	0.77
2:B:1128:LEU:HD12	2:B:1128:LEU:C	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:ARG:CB	1:A:1055:ARG:CD	2.62	0.77
1:A:1151:GLU:CG	7:I:45:ARG:HD2	2.14	0.77
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.16	0.77
2:B:431:TYR:CE1	2:B:447:ALA:HB1	2.19	0.77
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.82	0.77
2:B:431:TYR:O	2:B:431:TYR:HD2	1.66	0.77
6:H:104:PHE:O	6:H:106:GLU:CA	2.32	0.77
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.65	0.77
1:A:909:ASP:OD1	1:A:911:SER:N	2.17	0.77
4:E:98:ILE:CA	4:E:98:ILE:HB	2.12	0.77
6:H:77:ARG:O	6:H:78:SER:O	2.03	0.77
1:A:325:ILE:C	1:A:327:ALA:N	2.37	0.76
1:A:587:HIS:HD2	1:A:966:ASN:OD1	1.69	0.76
6:H:84:ALA:O	6:H:88:SER:OG	2.02	0.76
6:H:91:ASP:O	6:H:91:ASP:OD1	2.01	0.76
2:B:305:VAL:CG1	2:B:305:VAL:CA	2.62	0.76
9:K:111:LEU:CB	9:K:111:LEU:CD1	2.62	0.76
2:B:29:ASP:HB3	2:B:658:ILE:HD12	1.68	0.76
1:A:327:ALA:O	2:B:1206:GLU:OE1	2.03	0.76
1:A:1118:VAL:HB	1:A:1327:ILE:HD12	1.66	0.76
1:A:156:ASP:C	1:A:158:PRO:CD	2.53	0.76
3:C:73:GLN:HE21	3:C:75:MET:H	1.33	0.76
1:A:567:LYS:CD	6:H:95:TYR:CG	2.69	0.75
2:B:680:THR:HG22	2:B:682:SER:H	1.50	0.75
1:A:172:PRO:HD2	1:A:185:TRP:HE1	1.48	0.75
1:A:941:LYS:CB	1:A:941:LYS:CD	2.62	0.75
2:B:549:THR:HG22	2:B:628:THR:HB	1.69	0.75
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.68	0.75
1:A:172:PRO:HG3	1:A:185:TRP:CH2	2.21	0.75
1:A:531:ILE:HD11	1:A:578:LEU:HD22	1.68	0.75
3:C:40:GLU:HA	3:C:163:ILE:HD12	1.69	0.75
1:A:1350:LYS:CB	1:A:1350:LYS:CD	2.65	0.75
1:A:172:PRO:CG	1:A:185:TRP:CH2	2.70	0.75
1:A:73:GLY:O	1:A:75:ASN:N	2.19	0.75
1:A:567:LYS:HD3	6:H:95:TYR:CD2	2.21	0.75
6:H:89:LEU:C	6:H:91:ASP:H	1.90	0.75
6:H:130:ARG:C	6:H:130:ARG:HD2	2.06	0.74
6:H:9:ILE:HA	6:H:9:ILE:CB	2.14	0.74
1:A:61:ILE:O	1:A:62:ASP:HB2	1.86	0.74
10:L:47:ARG:HG2	10:L:48:CYS:H	1.53	0.74
1:A:186:LYS:HZ1	1:A:195:ASP:HA	1.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.23	0.74
1:A:1259:MET:CB	1:A:1259:MET:SD	2.75	0.74
1:A:1445:ILE:CG2	1:A:1445:ILE:CA	2.65	0.74
8:J:1:MET:C	8:J:2:ILE:HD13	2.07	0.74
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.32	0.74
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.18	0.74
5:F:75:PRO:O	5:F:77:ASP:O	2.06	0.74
7:I:116:ASN:ND2	7:I:118:ARG:HB2	2.03	0.73
4:E:147:HIS:CD2	4:E:149:LEU:H	2.05	0.73
1:A:531:ILE:HD11	1:A:578:LEU:HD21	1.68	0.73
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.86	0.73
1:A:1151:GLU:OE2	7:I:45:ARG:HD3	1.88	0.73
1:A:1236:LEU:O	1:A:1237:ILE:CD1	2.36	0.73
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.36	0.73
2:B:723:VAL:CB	2:B:723:VAL:HA	2.16	0.73
3:C:33:LEU:HD13	3:C:248:ILE:HD13	1.70	0.73
4:E:29:PHE:O	4:E:30:ILE:HD13	1.87	0.73
10:L:34:CYS:SG	10:L:34:CYS:O	2.41	0.73
2:B:839:MET:HE3	2:B:1010:LEU:HD11	1.71	0.73
5:F:111:LEU:O	5:F:113:GLY:N	2.20	0.73
1:A:938:LYS:CG	1:A:938:LYS:CE	2.67	0.73
1:A:1134:ILE:HG22	1:A:1138:ILE:HD11	1.69	0.73
1:A:1341:ILE:HD11	1:A:1376:THR:O	1.88	0.73
1:A:328:ARG:HG3	1:A:329:LEU:H	1.53	0.73
1:A:368:LYS:CB	1:A:368:LYS:CD	2.66	0.73
2:B:1065:GLN:HE22	2:B:1067:ARG:HB2	1.53	0.73
1:A:156:ASP:OD2	1:A:156:ASP:N	2.21	0.73
1:A:172:PRO:HG3	1:A:185:TRP:CZ3	2.24	0.73
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.03	0.73
1:A:156:ASP:O	1:A:158:PRO:HD3	1.84	0.72
2:B:357:GLN:NE2	2:B:368:GLU:HG2	2.03	0.72
2:B:999:MET:CG	2:B:999:MET:HE3	2.17	0.72
6:H:27:GLU:OE1	6:H:39:THR:OG1	2.05	0.72
1:A:26:GLU:O	1:A:30:ILE:HD13	1.90	0.72
2:B:251:ILE:HG22	2:B:251:ILE:O	1.89	0.72
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.69	0.72
1:A:903:ASN:ND2	1:A:905:ASP:H	1.88	0.72
1:A:977:LYS:CA	1:A:977:LYS:CG	2.67	0.72
2:B:1162:ILE:CD1	2:B:1194:ILE:HG12	2.20	0.72
2:B:515:HIS:N	2:B:518:HIS:HD2	1.88	0.72
1:A:503:GLN:NE2	5:F:90:ARG:NH2	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ILE:CA	1:A:566:ILE:CG2	2.66	0.72
9:K:35:PHE:HE1	9:K:73:LEU:HD12	1.54	0.72
2:B:315:LYS:NZ	2:B:315:LYS:CD	2.50	0.72
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.19	0.72
1:A:1134:ILE:HG23	1:A:1138:ILE:HD11	1.70	0.72
1:A:172:PRO:CG	1:A:185:TRP:CD2	2.62	0.72
2:B:663:ALA:O	2:B:667:GLN:HG3	1.89	0.72
3:C:102:GLN:CA	3:C:102:GLN:CG	2.66	0.72
2:B:294:ASP:H	7:I:12:ASN:HD22	1.36	0.71
6:H:105:GLU:HG2	6:H:136:LYS:NZ	2.04	0.71
2:B:357:GLN:HE21	2:B:368:GLU:HG2	1.56	0.71
2:B:996:ARG:NH1	14:B:3012:HOH:O	2.22	0.71
1:A:154:SER:O	1:A:155:GLU:O	2.08	0.71
3:C:77:ILE:HD12	3:C:80:LEU:HB3	1.73	0.71
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.05	0.71
4:E:112:TYR:CG	4:E:116:ILE:HD11	2.25	0.71
1:A:23:SER:O	1:A:27:VAL:HG23	1.89	0.71
1:A:518:LYS:CD	1:A:518:LYS:HZ2	2.03	0.71
1:A:187:LYS:CB	1:A:194:ALA:HB3	2.19	0.71
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.25	0.71
6:H:6:PHE:CD2	6:H:7:ASP:N	2.59	0.71
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.88	0.71
1:A:531:ILE:O	1:A:535:THR:HB	1.90	0.71
1:A:265:LYS:HD3	1:A:302:THR:HG22	1.71	0.71
2:B:294:ASP:H	7:I:12:ASN:ND2	1.87	0.71
1:A:1385:THR:CA	1:A:1385:THR:CG2	2.68	0.71
8:J:1:MET:HB3	8:J:2:ILE:HD13	1.71	0.71
1:A:186:LYS:CE	1:A:197:PRO:CD	2.56	0.71
1:A:1080:THR:HB	1:A:1080:THR:CA	2.13	0.70
1:A:560:ILE:HD12	1:A:560:ILE:H	1.56	0.70
1:A:53:LEU:HD23	1:A:54:ASN:N	2.06	0.70
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.55	0.70
4:E:47:CYS:SG	4:E:52:ARG:O	2.50	0.70
1:A:261:ASP:N	1:A:261:ASP:OD1	2.24	0.70
2:B:242:SER:HG	2:B:363:HIS:HD1	1.35	0.70
2:B:877:PRO:O	2:B:878:GLN:HG2	1.92	0.70
3:C:8:VAL:HG12	3:C:9:LYS:H	1.56	0.70
1:A:107:CYS:SG	1:A:171:GLN:OE1	2.49	0.70
1:A:547:LEU:HB3	9:K:58:PHE:CE1	2.27	0.70
2:B:227:LYS:CE	2:B:227:LYS:CG	2.70	0.70
1:A:1162:VAL:CG1	1:A:1162:VAL:CA	2.69	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASP:OD2	1:A:47:ARG:CA	2.40	0.70
2:B:484:ASN:OD1	2:B:486:TYR:CE1	2.45	0.70
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.74	0.70
3:C:172:PRO:O	3:C:235:VAL:HG12	1.90	0.70
9:K:65:HIS:HD2	9:K:67:PHE:H	1.36	0.70
1:A:1135:ARG:CG	1:A:1135:ARG:NE	2.53	0.70
1:A:1405:THR:CA	1:A:1405:THR:HB	2.14	0.70
8:J:1:MET:C	8:J:2:ILE:CD1	2.60	0.70
1:A:369:SER:CB	9:K:2:ASN:ND2	2.54	0.70
1:A:1341:ILE:HD12	1:A:1379:GLY:CA	2.21	0.70
1:A:150:THR:HA	1:A:166:GLY:HA2	1.73	0.70
3:C:181:ASP:OD2	3:C:186:LEU:HB2	1.92	0.70
1:A:679:ILE:HD12	1:A:729:ALA:CA	2.21	0.69
1:A:32:VAL:HG23	1:A:33:ALA:H	1.57	0.69
1:A:567:LYS:CD	1:A:568:PRO:CD	2.70	0.69
2:B:1025:HIS:CE1	2:B:1090:THR:HG21	2.25	0.69
2:B:1166:CYS:O	2:B:1168:LEU:N	2.25	0.69
2:B:463:THR:HG21	2:B:465:ASN:OD1	1.91	0.69
2:B:645:SER:OG	2:B:646:LEU:N	2.23	0.69
2:B:119:LEU:O	2:B:965:LYS:NZ	2.24	0.69
2:B:1031:LEU:HB2	2:B:1055:ILE:CD1	2.22	0.69
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.05	0.69
1:A:608:ILE:HD12	1:A:613:ILE:HG13	1.74	0.69
2:B:1222:ARG:HH11	2:B:1222:ARG:HB2	1.57	0.69
3:C:209:TYR:H	3:C:209:TYR:HD1	1.41	0.69
1:A:46:THR:O	1:A:48:ALA:N	2.26	0.69
1:A:885:THR:CG2	14:A:3013:HOH:O	2.19	0.69
2:B:217:ARG:HD3	2:B:407:ASP:OD2	1.93	0.69
3:C:199:LYS:NZ	3:C:199:LYS:CD	2.56	0.69
3:C:50:GLU:HB3	10:L:64:LEU:HD13	1.73	0.69
7:I:120:GLN:O	7:I:121:PHE:HB2	1.91	0.69
8:J:2:ILE:HG22	8:J:3:VAL:N	2.07	0.69
1:A:523:ILE:HB	1:A:622:VAL:HG13	1.75	0.69
1:A:328:ARG:CG	1:A:329:LEU:H	2.03	0.69
1:A:849:MET:HE2	1:A:1061:GLY:HA2	1.75	0.69
1:A:282:ASN:C	1:A:283:GLY:O	2.28	0.69
1:A:679:ILE:CD1	1:A:729:ALA:HA	2.21	0.69
1:A:840:ARG:NE	1:A:840:ARG:CG	2.54	0.69
2:B:744:HIS:HD2	2:B:746:SER:H	1.41	0.69
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.74	0.69
4:E:100:ILE:HG22	4:E:101:GLN:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:839:MET:CE	2:B:1010:LEU:HD11	2.23	0.68
2:B:955:THR:CG2	10:L:54:ARG:O	2.39	0.68
1:A:166:GLY:O	1:A:167:CYS:HB3	1.92	0.68
2:B:1161:HIS:C	2:B:1162:ILE:HD12	2.13	0.68
1:A:351:THR:HG21	2:B:1103:ILE:HG12	1.75	0.68
6:H:103:LYS:O	6:H:115:TYR:HD1	1.76	0.68
5:F:76:LYS:O	5:F:79:ARG:HD2	1.93	0.68
1:A:587:HIS:CE1	1:A:969:GLN:HG2	2.28	0.68
6:H:105:GLU:HG2	6:H:136:LYS:HZ2	1.58	0.68
1:A:567:LYS:HE2	6:H:95:TYR:CE2	2.26	0.68
1:A:265:LYS:CE	1:A:302:THR:HG22	2.23	0.68
1:A:69:THR:HG22	2:B:1174:LYS:HE2	1.75	0.68
4:E:112:TYR:CD2	4:E:116:ILE:HD11	2.28	0.68
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.56	0.68
6:H:105:GLU:HB3	6:H:107:VAL:HG23	1.76	0.68
1:A:1161:THR:CG2	1:A:1163:ILE:H	2.06	0.68
4:E:98:ILE:O	4:E:101:GLN:HB3	1.93	0.68
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.28	0.68
1:A:679:ILE:HD13	1:A:732:LEU:CD1	2.24	0.68
2:B:531:GLN:H	2:B:531:GLN:CD	1.97	0.68
1:A:1385:THR:HG22	1:A:1385:THR:O	1.94	0.67
4:E:79:TRP:HB2	4:E:105:PHE:CD1	2.28	0.67
2:B:417:PHE:CD2	2:B:417:PHE:C	2.67	0.67
1:A:46:THR:C	1:A:46:THR:CB	2.63	0.67
1:A:834:THR:HG21	1:A:1077:THR:OG1	1.94	0.67
3:C:116:LYS:NZ	3:C:116:LYS:CD	2.56	0.67
1:A:351:THR:CG2	2:B:1103:ILE:HG12	2.24	0.67
1:A:567:LYS:CG	1:A:568:PRO:HD3	2.25	0.67
1:A:184:SER:HB2	1:A:199:LEU:HD23	1.75	0.67
1:A:912:LEU:N	1:A:912:LEU:HD23	2.10	0.67
2:B:1222:ARG:NH1	2:B:1222:ARG:HG2	2.09	0.67
2:B:435:THR:O	2:B:435:THR:HG22	1.95	0.67
2:B:654:ARG:H	2:B:657:HIS:HD2	1.42	0.67
1:A:567:LYS:CB	6:H:95:TYR:HA	2.25	0.67
2:B:1162:ILE:HD13	2:B:1194:ILE:HG12	1.77	0.67
2:B:227:LYS:CB	2:B:227:LYS:CD	2.70	0.67
2:B:487:THR:HG22	2:B:490:SER:H	1.58	0.67
2:B:51:PHE:CZ	2:B:172:ILE:HD13	2.30	0.67
1:A:503:GLN:NE2	5:F:90:ARG:HH21	1.93	0.67
1:A:63:ARG:HA	1:A:74:MET:HG2	1.77	0.67
2:B:90:ILE:HD13	2:B:134:LYS:HA	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:TYR:OH	3:C:188:HIS:ND1	2.26	0.67
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.60	0.67
1:A:172:PRO:HD3	1:A:185:TRP:CD2	2.30	0.67
1:A:46:THR:HB	1:A:46:THR:O	1.95	0.67
7:I:3:THR:CG2	7:I:3:THR:CA	2.70	0.67
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.25	0.66
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.75	0.66
1:A:328:ARG:HA	2:B:1206:GLU:OE1	1.95	0.66
9:K:20:LYS:CE	9:K:20:LYS:CG	2.73	0.66
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.25	0.66
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.26	0.66
6:H:123:MET:HE3	6:H:142:LEU:HD22	1.76	0.66
1:A:567:LYS:CG	6:H:96:VAL:H	2.09	0.66
1:A:1350:LYS:CG	1:A:1350:LYS:CE	2.74	0.66
1:A:351:THR:CG2	2:B:1103:ILE:CG1	2.74	0.66
1:A:369:SER:N	9:K:2:ASN:HD21	1.90	0.66
2:B:243:ALA:C	2:B:244:LEU:HG	2.14	0.66
2:B:291:ILE:HG22	2:B:297:ILE:HD13	1.76	0.66
2:B:206:ASN:OD1	2:B:458:LYS:CE	2.44	0.66
6:H:115:TYR:O	6:H:123:MET:O	2.13	0.66
1:A:265:LYS:NZ	1:A:302:THR:CG2	2.59	0.66
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.78	0.66
1:A:534:LEU:O	1:A:574:GLY:HA3	1.96	0.66
9:K:93:SER:O	9:K:97:LYS:HG3	1.95	0.66
1:A:172:PRO:CD	1:A:185:TRP:CD2	2.79	0.66
4:E:117:THR:O	4:E:118:PRO:C	2.34	0.66
1:A:99:ILE:HD13	1:A:235:ILE:HD13	1.77	0.66
4:E:36:GLU:O	4:E:37:LEU:C	2.30	0.66
6:H:131:ASN:HD22	6:H:131:ASN:H	1.42	0.66
1:A:172:PRO:HD2	1:A:185:TRP:CE2	2.11	0.65
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.31	0.65
1:A:57:ARG:HB3	1:A:68:GLN:HG2	1.75	0.65
1:A:537:ARG:NH2	1:A:600:PRO:O	2.29	0.65
2:B:1019:SER:CB	13:B:3008:GTP:O6	2.43	0.65
1:A:224:PHE:CG	1:A:231:PRO:HD3	2.31	0.65
8:J:53:HIS:HE1	8:J:55:ASP:HA	1.62	0.65
1:A:156:ASP:C	1:A:158:PRO:HD3	2.17	0.65
1:A:187:LYS:HB2	1:A:194:ALA:CB	2.21	0.65
1:A:919:ILE:HD13	1:A:983:ILE:HD13	1.79	0.65
3:C:7:GLN:CD	3:C:7:GLN:CB	2.63	0.65
2:B:228:LYS:O	2:B:261:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.78	0.65
9:K:24:ASP:OD1	9:K:74:ARG:NH1	2.29	0.65
3:C:167:HIS:CE1	10:L:70:ARG:O	2.47	0.65
2:B:191:LYS:CG	2:B:191:LYS:CA	2.74	0.65
2:B:341:LEU:HD12	2:B:342:GLY:H	1.60	0.65
1:A:960:ILE:O	1:A:964:ILE:HD13	1.97	0.65
2:B:246:LYS:C	2:B:246:LYS:HA	2.07	0.65
1:A:562:THR:CG2	6:H:98:TYR:CD2	2.80	0.65
1:A:1151:GLU:HG2	7:I:45:ARG:HD2	1.79	0.64
1:A:1298:TYR:O	1:A:1299:VAL:HG23	1.97	0.64
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.61	0.64
4:E:152:LYS:CB	4:E:152:LYS:CD	2.75	0.64
7:I:120:GLN:O	7:I:121:PHE:CB	2.45	0.64
1:A:934:LYS:NZ	1:A:934:LYS:CD	2.60	0.64
2:B:115:GLN:CA	2:B:115:GLN:CG	2.74	0.64
2:B:1222:ARG:HH11	2:B:1222:ARG:CG	2.10	0.64
5:F:109:VAL:CG1	5:F:110:ASP:N	2.60	0.64
6:H:89:LEU:HB3	6:H:91:ASP:OD1	1.98	0.64
7:I:4:PHE:CE1	7:I:13:MET:HE1	2.31	0.64
1:A:1272:THR:CA	1:A:1272:THR:CG2	2.72	0.64
2:B:1163:CYS:SG	2:B:1165:ILE:HG13	2.38	0.64
1:A:407:ARG:CD	1:A:413:ILE:HD11	2.27	0.64
2:B:291:ILE:O	2:B:297:ILE:HD11	1.97	0.64
3:C:41:ILE:N	3:C:163:ILE:HD11	2.13	0.64
4:E:115:ASN:O	4:E:116:ILE:HD13	1.96	0.64
5:F:105:ALA:HB1	5:F:106:PRO:HD2	1.77	0.64
3:C:77:ILE:CD1	3:C:80:LEU:HB3	2.28	0.64
6:H:47:PHE:CG	6:H:95:TYR:HD1	2.16	0.64
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.62	0.64
1:A:1172:LEU:O	1:A:1173:HIS:CD2	2.49	0.64
1:A:265:LYS:HZ2	1:A:302:THR:HG21	1.62	0.64
1:A:1155:ASP:O	1:A:1241:ARG:NH2	2.31	0.64
2:B:841:MET:HB2	2:B:990:ILE:HD12	1.78	0.64
3:C:77:ILE:HD12	3:C:77:ILE:O	1.98	0.64
6:H:105:GLU:H	6:H:105:GLU:CD	2.01	0.64
1:A:894:GLU:HB2	1:A:933:TYR:OH	1.98	0.64
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.01	0.64
8:J:1:MET:CE	8:J:1:MET:CB	2.76	0.64
1:A:446:ARG:HH11	1:A:446:ARG:HG2	1.62	0.63
1:A:84:ILE:HD12	1:A:270:LEU:HD13	1.80	0.63
2:B:94:LYS:HG2	2:B:96:TYR:CE1	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:GLU:HA	3:C:163:ILE:CD1	2.28	0.63
1:A:709:THR:HG22	1:A:712:GLU:H	1.63	0.63
2:B:393:LYS:NZ	2:B:621:GLU:OE2	2.23	0.63
2:B:120:ARG:NH2	2:B:956:THR:O	2.29	0.63
4:E:117:THR:OG1	4:E:120:ALA:CB	2.47	0.63
10:L:26:THR:HB	10:L:26:THR:CA	2.19	0.63
2:B:127:GLY:HA2	2:B:168:GLY:O	1.98	0.63
4:E:152:LYS:NZ	4:E:152:LYS:CD	2.62	0.63
8:J:53:HIS:HE1	8:J:55:ASP:CA	2.10	0.63
9:K:55:LYS:HB2	9:K:81:TYR:CD1	2.34	0.63
3:C:18:VAL:HG23	3:C:240:VAL:CG1	2.29	0.63
3:C:99:LEU:HD12	3:C:99:LEU:N	2.14	0.63
1:A:1265:ASN:O	1:A:1266:THR:C	2.35	0.63
1:A:579:SER:HA	1:A:582:ILE:HD12	1.80	0.63
1:A:589:GLN:HB2	1:A:961:ARG:HH22	1.63	0.63
1:A:11:LEU:HD11	2:B:1195:HIS:CD2	2.34	0.63
6:H:76:THR:HG22	6:H:76:THR:O	1.99	0.63
1:A:531:ILE:CD1	1:A:578:LEU:HD22	2.29	0.63
2:B:1222:ARG:NH1	2:B:1222:ARG:CG	2.59	0.63
6:H:32:THR:CG2	6:H:33:GLN:OE1	2.47	0.63
6:H:93:TYR:HB3	6:H:144:ILE:O	1.98	0.63
1:A:31:SER:HB3	1:A:83:HIS:HD2	1.62	0.63
4:E:161:LYS:CG	4:E:161:LYS:CE	2.69	0.63
1:A:1162:VAL:HG12	1:A:1162:VAL:O	1.98	0.62
1:A:224:PHE:CD2	1:A:231:PRO:HD3	2.34	0.62
2:B:531:GLN:CG	2:B:531:GLN:CA	2.71	0.62
9:K:55:LYS:CB	9:K:81:TYR:CD1	2.82	0.62
1:A:164:ARG:C	1:A:166:GLY:H	2.02	0.62
5:F:81:THR:HG23	5:F:136:ARG:HH11	1.62	0.62
6:H:96:VAL:HG22	6:H:143:LEU:HD23	1.80	0.62
2:B:955:THR:HG23	10:L:55:ILE:HA	1.80	0.62
1:A:237:THR:CA	1:A:237:THR:CG2	2.73	0.62
2:B:436:VAL:CA	2:B:436:VAL:HB	2.16	0.62
1:A:901:LEU:H	1:A:926:GLN:HE22	1.47	0.62
2:B:100:PRO:HD2	2:B:180:TYR:CZ	2.35	0.62
10:L:58:LYS:O	10:L:59:ALA:HB3	2.00	0.62
2:B:899:ILE:HD12	2:B:911:ILE:HG13	1.80	0.62
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.12	0.62
6:H:63:LEU:HB2	6:H:90:ALA:HB2	1.81	0.62
1:A:1111:MET:CG	1:A:1111:MET:HE2	2.29	0.62
2:B:1084:GLN:HE22	3:C:192:TRP:N	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:884:ARG:HG2	2:B:884:ARG:NH1	2.13	0.62
1:A:186:LYS:CD	1:A:197:PRO:HD3	2.29	0.62
1:A:518:LYS:CG	1:A:518:LYS:CE	2.75	0.62
2:B:531:GLN:NE2	2:B:532:ALA:H	1.97	0.62
2:B:787:VAL:O	2:B:787:VAL:CG1	2.47	0.62
6:H:57:VAL:HG22	6:H:144:ILE:CD1	2.30	0.62
1:A:55:ASP:N	1:A:56:PRO:HD3	2.12	0.62
2:B:1077:THR:HG22	2:B:1079:LYS:N	2.12	0.62
3:C:255:VAL:HG12	3:C:255:VAL:O	1.99	0.62
1:A:751:SER:O	1:A:752:LYS:HB2	1.99	0.62
1:A:84:ILE:HD12	1:A:270:LEU:CD1	2.30	0.62
1:A:837:ILE:HD11	1:A:1102:LYS:HG2	1.81	0.61
1:A:328:ARG:HH11	1:A:1405:THR:HG22	1.65	0.61
3:C:46:ILE:CD1	3:C:72:LEU:HD11	2.29	0.61
2:B:843:GLN:NE2	2:B:846:ILE:CG2	2.62	0.61
1:A:1259:MET:HB2	1:A:1259:MET:SD	2.40	0.61
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.98	0.61
2:B:130:VAL:CG2	2:B:167:ILE:HD11	2.20	0.61
2:B:498:THR:CG2	2:B:537:LYS:HB2	2.30	0.61
9:K:110:ASN:C	9:K:112:GLN:H	2.00	0.61
1:A:1436:ILE:HD12	1:A:1436:ILE:O	2.00	0.61
1:A:636:GLU:OE2	1:A:962:ARG:HD2	2.01	0.61
2:B:251:ILE:O	2:B:251:ILE:CG2	2.48	0.61
1:A:1118:VAL:HB	1:A:1327:ILE:CD1	2.30	0.61
1:A:44:THR:CB	1:A:44:THR:C	2.67	0.61
1:A:567:LYS:CE	6:H:95:TYR:CE2	2.83	0.61
1:A:596:THR:HG22	1:A:597:LEU:N	2.11	0.61
2:B:118:ARG:HH22	2:B:194:GLU:CG	2.12	0.61
7:I:4:PHE:CZ	7:I:13:MET:HE1	2.34	0.61
1:A:1323:ASP:OD1	1:A:1325:THR:HB	1.99	0.61
2:B:1002:THR:HG21	2:B:1006:ILE:HB	1.83	0.61
6:H:47:PHE:CZ	6:H:146:ARG:HD2	2.36	0.61
5:F:81:THR:HG23	5:F:136:ARG:NH1	2.16	0.61
8:J:2:ILE:HG22	8:J:3:VAL:H	1.65	0.61
9:K:12:LEU:N	9:K:12:LEU:HD12	2.15	0.61
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.40	0.61
2:B:128:LEU:O	2:B:167:ILE:HD12	2.00	0.61
4:E:129:PRO:CD	4:E:130:ALA:H	2.13	0.61
5:F:73:ALA:HB2	5:F:143:PHE:CZ	2.35	0.61
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.81	0.61
1:A:1318:THR:HG23	4:E:11:ARG:HH12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:191:LYS:CD	4:E:191:LYS:NZ	2.64	0.61
6:H:114:VAL:HG11	6:H:134:ASN:HD22	1.66	0.61
6:H:8:ASP:OD2	6:H:9:ILE:N	2.27	0.61
1:A:567:LYS:CB	1:A:568:PRO:CD	2.79	0.60
4:E:65:THR:O	4:E:69:ILE:HG13	2.01	0.60
8:J:53:HIS:CE1	8:J:54:VAL:C	2.74	0.60
1:A:1266:THR:O	1:A:1267:MET:C	2.39	0.60
1:A:72:GLU:OE2	2:B:1175:LEU:CD1	2.45	0.60
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.01	0.60
2:B:995:ARG:HD2	2:B:997:GLU:OE2	2.01	0.60
3:C:242:GLN:NE2	3:C:246:ARG:HE	1.98	0.60
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.65	0.60
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.31	0.60
7:I:16:PRO:HG3	7:I:27:PHE:CE2	2.37	0.60
1:A:595:THR:HG22	1:A:596:THR:N	2.16	0.60
2:B:879:ARG:NH2	2:B:885:MET:CE	2.65	0.60
1:A:571:LEU:CD2	1:A:571:LEU:CD1	2.73	0.60
1:A:369:SER:CB	9:K:2:ASN:HD21	2.12	0.60
1:A:1236:LEU:C	1:A:1237:ILE:CD1	2.70	0.60
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.01	0.60
6:H:130:ARG:O	6:H:130:ARG:HD2	2.01	0.60
8:J:14:VAL:CG1	8:J:50:ILE:HD11	2.23	0.60
1:A:658:LEU:HD12	1:A:658:LEU:O	2.01	0.60
1:A:895:LYS:CD	1:A:895:LYS:NZ	2.62	0.60
2:B:249:ARG:CZ	2:B:415:GLN:HG3	2.32	0.60
2:B:775:LYS:CB	2:B:775:LYS:HD2	2.31	0.60
1:A:562:THR:HG22	6:H:98:TYR:CD2	2.36	0.60
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.84	0.60
4:E:153:HIS:CE1	4:E:184:VAL:HG11	2.36	0.60
1:A:1146:VAL:O	1:A:1146:VAL:CG1	2.50	0.60
1:A:1172:LEU:O	1:A:1173:HIS:CG	2.55	0.60
1:A:172:PRO:CD	1:A:185:TRP:CD1	2.59	0.60
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.02	0.60
2:B:1166:CYS:O	2:B:1167:GLY:C	2.40	0.60
2:B:885:MET:HB3	2:B:885:MET:CE	2.31	0.60
3:C:252:GLN:HE22	9:K:99:GLY:N	2.00	0.60
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.01	0.59
2:B:787:VAL:O	2:B:787:VAL:HG12	2.02	0.59
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.38	0.59
3:C:55:THR:O	3:C:55:THR:HG22	2.01	0.59
6:H:11:GLN:NE2	6:H:52:GLN:HG2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:680:THR:HG22	2:B:682:SER:N	2.14	0.59
2:B:879:ARG:NH2	2:B:885:MET:HE2	2.17	0.59
2:B:916:THR:N	2:B:935:ARG:O	2.34	0.59
4:E:37:LEU:HD23	4:E:42:PHE:HB2	1.84	0.59
1:A:353:ILE:HD12	1:A:482:PHE:CE2	2.38	0.59
1:A:42:ASP:OD2	1:A:46:THR:C	2.39	0.59
1:A:265:LYS:CE	1:A:302:THR:CG2	2.80	0.59
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.83	0.59
4:E:78:LEU:HD11	4:E:109:ILE:HD12	1.84	0.59
9:K:55:LYS:CB	9:K:81:TYR:HD1	2.15	0.59
1:A:804:TYR:O	2:B:761:HIS:ND1	2.35	0.59
2:B:862:GLN:HE22	2:B:961:LEU:HD13	1.67	0.59
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.02	0.59
1:A:189:ARG:HG2	1:A:189:ARG:O	2.03	0.59
1:A:679:ILE:CD1	1:A:732:LEU:HD12	2.32	0.59
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.84	0.59
3:C:40:GLU:C	3:C:163:ILE:HD11	2.22	0.59
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.03	0.59
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.02	0.59
1:A:567:LYS:HB2	6:H:95:TYR:HA	1.83	0.59
1:A:744:LYS:HD3	1:A:748:MET:SD	2.43	0.59
2:B:843:GLN:NE2	2:B:846:ILE:HG22	2.16	0.59
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.35	0.59
6:H:9:ILE:C	6:H:9:ILE:CB	2.68	0.59
1:A:3:GLY:CA	1:A:76:GLU:HG2	2.33	0.59
1:A:679:ILE:HD11	1:A:729:ALA:O	2.02	0.59
1:A:903:ASN:ND2	1:A:905:ASP:N	2.50	0.59
2:B:1222:ARG:HH11	2:B:1222:ARG:CB	2.15	0.59
2:B:282:ILE:HD11	2:B:317:CYS:HB3	1.85	0.59
3:C:94:LYS:CD	3:C:94:LYS:NZ	2.59	0.59
4:E:131:THR:HA	4:E:131:THR:CB	2.17	0.59
8:J:53:HIS:ND1	8:J:54:VAL:N	2.50	0.59
1:A:1077:THR:HG22	1:A:1078:GLN:NE2	2.17	0.59
1:A:122:MET:O	1:A:122:MET:HG3	2.02	0.59
6:H:103:LYS:HE3	6:H:135:LEU:O	2.03	0.59
9:K:65:HIS:CD2	9:K:67:PHE:H	2.19	0.59
2:B:1097:HIS:CE1	2:B:1102:LYS:HG3	2.38	0.58
3:C:120:ILE:H	3:C:120:ILE:HD12	1.68	0.58
6:H:32:THR:HB	6:H:33:GLN:OE1	2.03	0.58
1:A:535:THR:O	1:A:575:LYS:HE2	2.03	0.58
2:B:1221:SER:OG	5:F:72:LYS:HD2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:531:GLN:HE21	2:B:532:ALA:H	1.49	0.58
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.27	0.58
1:A:683:ILE:HD13	1:A:725:ALA:HB1	1.85	0.58
3:C:239:PRO:O	3:C:242:GLN:HB2	2.03	0.58
1:A:770:VAL:HG23	1:A:775:ILE:HD13	1.85	0.58
2:B:705:MET:HB3	2:B:706:GLN:HE21	1.67	0.58
2:B:870:ILE:HA	2:B:870:ILE:CB	2.17	0.58
4:E:131:THR:C	4:E:131:THR:CB	2.65	0.58
1:A:1325:THR:O	4:E:148:GLU:HG2	2.02	0.58
7:I:7:CYS:SG	7:I:32:CYS:SG	3.00	0.58
1:A:40:THR:HG23	1:A:54:ASN:ND2	2.18	0.58
2:B:1097:HIS:CG	2:B:1097:HIS:HA	2.22	0.58
2:B:1154:ALA:HA	2:B:1154:ALA:CB	2.19	0.58
4:E:83:CYS:O	4:E:113:GLN:NE2	2.35	0.58
1:A:280:GLU:HG3	1:A:289:ILE:HD12	1.86	0.58
1:A:464:PRO:O	1:A:465:TYR:O	2.22	0.58
2:B:134:LYS:O	2:B:135:ARG:HG3	2.03	0.58
6:H:123:MET:CE	6:H:142:LEU:HD22	2.33	0.58
6:H:89:LEU:C	6:H:91:ASP:N	2.49	0.58
1:A:107:CYS:SG	1:A:148:CYS:CB	2.92	0.58
1:A:247:ARG:HH11	1:A:263:THR:HG23	1.69	0.58
1:A:533:LYS:NZ	1:A:745:GLN:HE22	2.01	0.58
1:A:56:PRO:O	1:A:57:ARG:CG	2.50	0.58
2:B:103:ASN:HB2	2:B:169:ARG:HH22	1.69	0.58
2:B:555:ILE:CD1	2:B:587:HIS:NE2	2.67	0.58
5:F:123:LYS:HD2	5:F:123:LYS:NZ	2.16	0.58
6:H:113:ALA:CB	6:H:124:ARG:HH21	2.17	0.58
7:I:111:THR:HG21	7:I:113:ASP:HB2	1.86	0.58
1:A:555:ASP:OD1	9:K:26:LYS:NZ	2.37	0.58
2:B:51:PHE:HZ	2:B:172:ILE:HD13	1.68	0.58
2:B:561:TRP:O	2:B:590:HIS:CE1	2.51	0.58
10:L:38:LEU:HG	10:L:39:SER:H	1.67	0.58
2:B:1152:MET:CE	2:B:1152:MET:HA	2.34	0.58
10:L:47:ARG:HG2	10:L:48:CYS:N	2.18	0.58
1:A:1166:ASP:CB	1:A:1169:ILE:CG2	2.82	0.57
6:H:130:ARG:HB2	6:H:133:ASN:CB	2.33	0.57
7:I:3:THR:CG2	7:I:3:THR:OG1	2.47	0.57
8:J:3:VAL:HA	8:J:53:HIS:CD2	2.39	0.57
9:K:26:LYS:CB	9:K:26:LYS:CD	2.81	0.57
2:B:914:LYS:H	2:B:938:SER:HB2	1.69	0.57
9:K:35:PHE:CE1	9:K:73:LEU:HD12	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.04	0.57
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.25	0.57
3:C:80:LEU:HD22	3:C:129:ILE:CD1	2.34	0.57
5:F:74:ILE:HD12	5:F:144:GLU:HG2	1.86	0.57
3:C:252:GLN:HE22	9:K:99:GLY:CA	2.18	0.57
3:C:55:THR:HB	3:C:152:GLU:H	1.69	0.57
3:C:10:ILE:HD12	9:K:108:GLU:O	2.04	0.57
1:A:1080:THR:CB	1:A:1080:THR:N	2.64	0.57
1:A:231:PRO:O	1:A:234:MET:HG3	2.05	0.57
5:F:89:GLU:HG2	5:F:134:ILE:HD13	1.85	0.57
6:H:32:THR:HG22	6:H:33:GLN:CD	2.25	0.57
10:L:34:CYS:SG	10:L:36:SER:OG	2.63	0.57
1:A:61:ILE:CG1	1:A:61:ILE:CA	2.78	0.57
1:A:587:HIS:NE2	1:A:969:GLN:HG2	2.19	0.57
2:B:890:TYR:OH	2:B:936:ASP:OD1	2.19	0.57
6:H:114:VAL:HG11	6:H:134:ASN:ND2	2.18	0.57
6:H:47:PHE:CB	6:H:95:TYR:CD1	2.88	0.57
7:I:16:PRO:O	7:I:17:ARG:CD	2.42	0.57
1:A:351:THR:HG21	2:B:1103:ILE:CG1	2.35	0.57
9:K:18:LYS:HE3	9:K:38:GLU:HG2	1.85	0.57
2:B:167:ILE:HG22	2:B:167:ILE:O	2.05	0.57
2:B:516:ASN:H	2:B:516:ASN:HD22	1.51	0.57
4:E:169:ARG:HD3	5:F:140:ASP:OD2	2.05	0.57
8:J:14:VAL:HG13	8:J:50:ILE:CD1	2.27	0.57
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.86	0.56
2:B:555:ILE:HD13	2:B:587:HIS:CE1	2.37	0.56
2:B:95:ILE:HG22	2:B:96:TYR:N	2.20	0.56
1:A:903:ASN:HD21	1:A:905:ASP:HB2	1.70	0.56
1:A:982:THR:HB	1:A:985:ASP:OD2	2.05	0.56
6:H:118:PHE:O	6:H:119:GLY:C	2.44	0.56
6:H:6:PHE:CG	6:H:7:ASP:N	2.73	0.56
3:C:102:GLN:N	3:C:102:GLN:CG	2.68	0.56
3:C:133:ILE:O	3:C:134:ILE:HD13	2.05	0.56
1:A:155:GLU:HB2	1:A:156:ASP:OD2	2.06	0.56
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.40	0.56
5:F:114:GLU:HB2	5:F:120:ILE:HD13	1.88	0.56
1:A:1385:THR:C	1:A:1385:THR:CG2	2.74	0.56
2:B:705:MET:HE3	2:B:705:MET:CG	2.24	0.56
1:A:843:LYS:NZ	1:A:843:LYS:CD	2.67	0.56
3:C:209:TYR:CD1	3:C:209:TYR:N	2.73	0.56
1:A:846:GLU:HA	1:A:1066:VAL:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:HG2	1:A:123:ARG:HH22	1.70	0.56
1:A:385:ILE:HD13	1:A:385:ILE:O	2.06	0.56
2:B:566:LEU:HD13	2:B:588:GLY:HA2	1.87	0.56
3:C:33:LEU:CD1	3:C:248:ILE:HD13	2.36	0.56
4:E:117:THR:OG1	4:E:120:ALA:HB3	2.06	0.56
4:E:129:PRO:HD2	4:E:130:ALA:H	1.70	0.56
6:H:55:LEU:HD22	6:H:144:ILE:CD1	2.33	0.56
1:A:844:ALA:CB	1:A:1384:VAL:HG12	2.35	0.56
2:B:864:LYS:HD2	2:B:871:THR:OG1	2.05	0.56
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.71	0.56
1:A:44:THR:HB	1:A:44:THR:CA	2.18	0.56
1:A:567:LYS:CB	1:A:568:PRO:HD3	2.35	0.56
3:C:8:VAL:HG12	3:C:9:LYS:N	2.21	0.56
6:H:104:PHE:C	6:H:104:PHE:HA	2.10	0.56
6:H:127:GLY:O	6:H:128:ASN:HB2	2.05	0.56
1:A:1127:ASP:HB3	1:A:1130:GLN:H	1.70	0.55
1:A:567:LYS:HD3	6:H:95:TYR:CB	2.34	0.55
1:A:84:ILE:CG2	1:A:241:VAL:CG2	2.84	0.55
2:B:605:ARG:NE	2:B:639:ILE:HD11	2.21	0.55
1:A:679:ILE:HD12	1:A:729:ALA:CB	2.36	0.55
1:A:1215:ARG:CA	1:A:1215:ARG:CG	2.79	0.55
1:A:50:ILE:HG22	1:A:52:GLY:N	2.20	0.55
2:B:1162:ILE:HD11	2:B:1194:ILE:HG12	1.87	0.55
2:B:436:VAL:CB	2:B:436:VAL:HA	2.20	0.55
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.71	0.55
2:B:280:ILE:HD12	2:B:280:ILE:N	2.21	0.55
3:C:265:MET:CE	3:C:265:MET:CG	2.84	0.55
7:I:64:SER:O	7:I:66:PRO:HD3	2.07	0.55
10:L:61:THR:CG2	10:L:61:THR:OG1	2.48	0.55
10:L:51:CYS:SG	10:L:53:HIS:HB2	2.47	0.55
9:K:18:LYS:CE	9:K:38:GLU:OE2	2.55	0.55
1:A:135:PHE:CE1	1:A:222:LEU:HD22	2.42	0.55
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.42	0.55
2:B:620:ARG:CG	2:B:620:ARG:HE	2.18	0.55
2:B:68:THR:HG23	2:B:91:SER:HB3	1.89	0.55
1:A:1105:LEU:O	1:A:1383:SER:OG	2.23	0.55
1:A:41:MET:O	1:A:50:ILE:HD11	2.06	0.55
1:A:834:THR:HG21	1:A:1077:THR:CA	2.37	0.55
1:A:1146:VAL:O	1:A:1146:VAL:HG13	2.07	0.55
1:A:1445:ILE:CG2	1:A:1445:ILE:HA	2.37	0.55
1:A:903:ASN:C	1:A:903:ASN:HD22	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:ARG:CB	1:A:840:ARG:CD	2.79	0.55
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.42	0.55
3:C:15:LYS:CB	3:C:15:LYS:CD	2.84	0.55
3:C:29:MET:HB2	3:C:29:MET:CE	2.37	0.55
6:H:106:GLU:O	6:H:108:SER:N	2.40	0.55
6:H:47:PHE:CG	6:H:95:TYR:CD1	2.95	0.55
1:A:3:GLY:HA3	1:A:76:GLU:HG2	1.90	0.54
2:B:98:THR:HB	2:B:99:LYS:O	2.08	0.54
4:E:147:HIS:CD2	4:E:149:LEU:HB2	2.43	0.54
6:H:32:THR:CB	6:H:33:GLN:OE1	2.55	0.54
1:A:1261:LYS:CD	1:A:1261:LYS:NZ	2.67	0.54
1:A:597:LEU:HG	1:A:597:LEU:CD1	2.21	0.54
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.42	0.54
3:C:102:GLN:HG2	3:C:102:GLN:N	2.21	0.54
3:C:116:LYS:CE	3:C:116:LYS:CG	2.81	0.54
6:H:138:GLU:O	6:H:139:ASN:O	2.25	0.54
1:A:567:LYS:CD	6:H:95:TYR:CD1	2.91	0.54
7:I:98:VAL:HG22	7:I:99:LEU:N	2.20	0.54
1:A:1169:ILE:HD11	1:A:1227:ILE:HD12	1.89	0.54
1:A:540:PHE:O	1:A:541:ILE:HD13	2.07	0.54
2:B:526:GLU:HG2	2:B:538:ASN:ND2	2.23	0.54
6:H:4:THR:O	6:H:5:LEU:HD23	2.08	0.54
10:L:28:LYS:O	10:L:59:ALA:HB3	2.07	0.54
1:A:295:LEU:CD1	1:A:295:LEU:CD2	2.79	0.54
1:A:679:ILE:CD1	1:A:732:LEU:HB2	2.25	0.54
2:B:203:PHE:HB3	2:B:205:ILE:CD1	2.36	0.54
3:C:252:GLN:CD	3:C:252:GLN:CB	2.72	0.54
6:H:103:LYS:CB	6:H:105:GLU:OE1	2.54	0.54
1:A:237:THR:HB	1:A:237:THR:CG2	2.19	0.54
1:A:53:LEU:HD23	1:A:54:ASN:H	1.70	0.54
1:A:1151:GLU:CG	7:I:45:ARG:CD	2.85	0.54
8:J:42:LYS:CG	8:J:42:LYS:CE	2.83	0.54
2:B:1006:ILE:HD11	8:J:43:ARG:HB2	1.90	0.54
4:E:154:ILE:HD13	4:E:199:ILE:HD12	1.90	0.54
1:A:1172:LEU:C	1:A:1173:HIS:CD2	2.81	0.54
1:A:1226:VAL:HG12	1:A:1227:ILE:N	2.20	0.54
2:B:98:THR:OG1	2:B:127:GLY:O	2.25	0.54
2:B:864:LYS:HG3	2:B:865:LYS:N	2.21	0.54
7:I:35:VAL:HG23	7:I:35:VAL:O	2.06	0.54
1:A:605:MET:HE3	1:A:607:ILE:CD1	2.32	0.54
1:A:31:SER:CB	1:A:83:HIS:CD2	2.83	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1166:ASP:CA	1:A:1169:ILE:HG22	2.37	0.54
1:A:369:SER:H	9:K:2:ASN:ND2	2.00	0.54
1:A:903:ASN:HD22	1:A:905:ASP:N	2.05	0.54
2:B:26:THR:O	2:B:27:ALA:C	2.45	0.54
2:B:899:ILE:HG22	2:B:900:ALA:H	1.72	0.54
2:B:983:ARG:HD3	14:B:3009:HOH:O	2.08	0.54
3:C:43:THR:CG2	3:C:44:LEU:N	2.71	0.54
1:A:446:ARG:CG	1:A:446:ARG:HH11	2.19	0.53
2:B:841:MET:CE	2:B:990:ILE:HD11	2.37	0.53
6:H:59:ILE:HG22	6:H:60:ALA:N	2.23	0.53
4:E:117:THR:OG1	4:E:120:ALA:HB2	2.09	0.53
1:A:268:ASP:HB3	1:A:299:HIS:CD2	2.44	0.53
2:B:102:VAL:O	2:B:109:THR:HA	2.09	0.53
2:B:906:SER:O	2:B:907:GLY:C	2.46	0.53
3:C:80:LEU:HD12	3:C:94:LYS:O	2.08	0.53
1:A:134:ARG:O	1:A:138:ILE:CG2	2.55	0.53
1:A:189:ARG:O	1:A:190:ALA:CB	2.55	0.53
1:A:518:LYS:HD3	1:A:518:LYS:NZ	2.14	0.53
1:A:601:LYS:CD	1:A:601:LYS:NZ	2.70	0.53
1:A:84:ILE:HG22	1:A:241:VAL:CG2	2.38	0.53
1:A:913:LEU:HD11	1:A:981:LEU:O	2.08	0.53
3:C:80:LEU:HD22	3:C:129:ILE:HD13	1.91	0.53
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.42	0.53
5:F:109:VAL:HG22	5:F:127:GLU:OE1	2.09	0.53
6:H:91:ASP:C	6:H:91:ASP:OD1	2.45	0.53
9:K:88:LYS:O	9:K:89:ASN:C	2.45	0.53
1:A:172:PRO:HG2	1:A:185:TRP:CH2	2.31	0.53
1:A:636:GLU:OE2	1:A:962:ARG:CD	2.56	0.53
2:B:999:MET:HB3	2:B:1000:PRO:HD2	1.89	0.53
3:C:70:ILE:HD11	3:C:144:ILE:HD12	1.90	0.53
3:C:8:VAL:CG1	3:C:9:LYS:H	2.22	0.53
6:H:95:TYR:CD2	6:H:95:TYR:C	2.82	0.53
2:B:620:ARG:HG2	7:I:62:ILE:CD1	2.38	0.53
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.56	0.53
1:A:1130:GLN:NE2	1:A:1130:GLN:CG	2.65	0.53
1:A:154:SER:O	1:A:155:GLU:C	2.47	0.53
1:A:93:VAL:HA	1:A:96:ILE:CD1	2.39	0.53
2:B:249:ARG:NH1	2:B:418:LYS:NZ	2.57	0.53
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.37	0.53
6:H:62:SER:O	6:H:63:LEU:O	2.26	0.53
1:A:704:ALA:HB1	1:A:708:MET:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.24	0.53
2:B:1152:MET:HE2	2:B:1152:MET:HA	1.90	0.53
5:F:72:LYS:CG	5:F:72:LYS:CE	2.85	0.53
10:L:58:LYS:O	10:L:59:ALA:CB	2.54	0.53
1:A:106:VAL:HG21	1:A:214:ILE:HG12	1.90	0.53
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.43	0.53
4:E:93:MET:HE3	4:E:116:ILE:HG21	1.91	0.53
6:H:37:LYS:O	6:H:125:LEU:HA	2.09	0.53
1:A:1151:GLU:HG2	7:I:45:ARG:CD	2.39	0.53
7:I:49:ILE:HG22	7:I:49:ILE:O	2.09	0.53
3:C:169:LYS:NZ	10:L:69:ALA:O	2.41	0.53
1:A:535:THR:HG23	1:A:616:VAL:HA	1.91	0.52
1:A:63:ARG:HA	1:A:74:MET:SD	2.49	0.52
1:A:741:ASN:C	1:A:741:ASN:HD22	2.12	0.52
2:B:313:MET:CE	2:B:386:LEU:HD22	2.39	0.52
4:E:37:LEU:CD1	4:E:37:LEU:HG	2.20	0.52
1:A:693:VAL:HG21	1:A:721:PHE:CE1	2.42	0.52
1:A:752:LYS:HD2	2:B:1015:HIS:O	2.09	0.52
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.56	0.52
2:B:431:TYR:CE1	2:B:447:ALA:CB	2.91	0.52
1:A:541:ILE:HD11	1:A:656:TRP:HE1	1.73	0.52
6:H:9:ILE:CG2	6:H:9:ILE:CA	2.81	0.52
1:A:1262:LYS:CE	1:A:1262:LYS:CG	2.82	0.52
1:A:407:ARG:O	1:A:408:ASP:C	2.48	0.52
1:A:588:LEU:C	1:A:588:LEU:HD23	2.29	0.52
1:A:964:ILE:N	1:A:964:ILE:CD1	2.72	0.52
4:E:127:ILE:N	4:E:128:PRO:CD	2.72	0.52
1:A:351:THR:HG23	2:B:1103:ILE:CG1	2.40	0.52
2:B:424:LEU:O	2:B:428:ILE:HG13	2.08	0.52
1:A:1318:THR:CG2	4:E:11:ARG:HH12	2.22	0.52
6:H:55:LEU:CD2	6:H:144:ILE:HD12	2.33	0.52
1:A:120:GLU:HG2	1:A:123:ARG:NH2	2.25	0.52
1:A:1341:ILE:HD13	4:E:212:ARG:NH2	2.24	0.52
1:A:186:LYS:HZ3	1:A:195:ASP:HA	1.69	0.52
1:A:98:LYS:HB3	1:A:234:MET:CE	2.39	0.52
3:C:114:TYR:HB3	3:C:140:ASN:O	2.10	0.52
3:C:148:ARG:O	3:C:149:LYS:C	2.48	0.52
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.44	0.52
1:A:42:ASP:OD2	1:A:47:ARG:CG	2.58	0.52
13:B:3008:GTP:C2'	13:B:3008:GTP:N9	2.68	0.52
2:B:789:MET:CG	2:B:789:MET:CE	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:ILE:CG2	1:A:973:ILE:CA	2.82	0.52
1:A:1035:TYR:O	1:A:1036:ARG:HB2	2.10	0.52
1:A:1256:GLU:HB3	1:A:1259:MET:HE2	1.92	0.52
1:A:973:ILE:CG2	1:A:973:ILE:CG1	2.81	0.52
2:B:775:LYS:CA	2:B:775:LYS:CG	2.82	0.52
2:B:59:LEU:HG	2:B:95:ILE:HD13	1.92	0.52
3:C:94:LYS:CG	3:C:94:LYS:NZ	2.72	0.52
7:I:43:VAL:O	7:I:43:VAL:HG12	2.09	0.52
1:A:1236:LEU:C	1:A:1237:ILE:HD13	2.31	0.51
1:A:186:LYS:HG3	1:A:197:PRO:HD3	1.92	0.51
2:B:757:PRO:HG2	2:B:984:HIS:HE1	1.75	0.51
3:C:178:PHE:C	3:C:178:PHE:CD2	2.84	0.51
4:E:52:ARG:HG3	4:E:53:PRO:HD3	1.91	0.51
10:L:68:GLU:O	10:L:69:ALA:HB3	2.10	0.51
1:A:1287:TYR:O	1:A:1302:PRO:HA	2.10	0.51
1:A:1341:ILE:CD1	1:A:1379:GLY:HA2	2.36	0.51
1:A:186:LYS:NZ	1:A:195:ASP:CA	2.67	0.51
2:B:864:LYS:HB2	2:B:871:THR:HA	1.92	0.51
3:C:73:GLN:HA	3:C:133:ILE:HD11	1.91	0.51
7:I:45:ARG:CD	7:I:45:ARG:CB	2.80	0.51
1:A:34:LYS:O	1:A:35:ILE:C	2.48	0.51
1:A:598:LEU:HD21	6:H:124:ARG:HB2	1.92	0.51
1:A:73:GLY:C	1:A:75:ASN:N	2.61	0.51
2:B:612:GLU:HG3	2:B:612:GLU:O	2.11	0.51
2:B:43:LEU:HD11	2:B:811:TYR:O	2.11	0.51
2:B:705:MET:CE	2:B:705:MET:HG3	2.36	0.51
2:B:843:GLN:HE22	2:B:846:ILE:HG21	1.75	0.51
3:C:209:TYR:N	3:C:209:TYR:HD1	2.08	0.51
7:I:10:CYS:SG	7:I:32:CYS:SG	3.09	0.51
1:A:274:ILE:C	1:A:274:ILE:CB	2.70	0.51
1:A:689:LYS:O	1:A:693:VAL:HG23	2.10	0.51
6:H:113:ALA:HB2	6:H:124:ARG:NH2	2.25	0.51
1:A:551:TYR:CD2	9:K:62:LYS:HD3	2.46	0.51
2:B:1019:SER:HB2	13:B:3008:GTP:N7	2.26	0.51
2:B:744:HIS:CD2	2:B:746:SER:H	2.24	0.51
2:B:792:MET:SD	2:B:857:ARG:NH2	2.84	0.51
4:E:162:ARG:CG	4:E:162:ARG:CA	2.86	0.51
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.92	0.51
1:A:110:CYS:SG	1:A:167:CYS:SG	3.09	0.51
1:A:229:SER:O	1:A:229:SER:OG	2.25	0.51
9:K:18:LYS:HE2	9:K:38:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.71	0.51
6:H:44:VAL:HG13	6:H:44:VAL:O	2.11	0.51
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.75	0.51
1:A:189:ARG:O	1:A:190:ALA:HB3	2.11	0.51
1:A:55:ASP:C	1:A:57:ARG:H	2.09	0.51
2:B:884:ARG:HG2	2:B:884:ARG:HH11	1.76	0.51
4:E:176:PRO:O	4:E:212:ARG:HA	2.11	0.51
6:H:130:ARG:HB2	6:H:133:ASN:HB3	1.92	0.51
6:H:135:LEU:HD13	6:H:139:ASN:O	2.11	0.51
6:H:6:PHE:C	6:H:6:PHE:CD2	2.84	0.51
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.40	0.51
2:B:900:ALA:O	2:B:901:PRO:C	2.48	0.51
3:C:196:ASP:HB3	3:C:199:LYS:HG3	1.91	0.51
3:C:214:ASN:O	3:C:217:ASP:HB2	2.11	0.51
6:H:142:LEU:HG	6:H:143:LEU:N	2.26	0.51
1:A:328:ARG:NH1	1:A:1405:THR:HG22	2.24	0.50
2:B:1051:THR:CG2	2:B:1053:GLU:H	2.14	0.50
2:B:486:TYR:CZ	2:B:1096:ARG:NH2	2.79	0.50
1:A:279:LEU:H	1:A:281:HIS:H	1.59	0.50
1:A:35:ILE:HD13	1:A:241:VAL:HG11	1.93	0.50
2:B:435:THR:O	2:B:435:THR:CG2	2.59	0.50
2:B:436:VAL:CA	2:B:436:VAL:CG2	2.79	0.50
2:B:662:MET:CE	2:B:662:MET:CG	2.90	0.50
3:C:252:GLN:NE2	9:K:99:GLY:H	2.09	0.50
3:C:41:ILE:C	3:C:163:ILE:HD11	2.32	0.50
9:K:111:LEU:N	9:K:111:LEU:HD23	2.27	0.50
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.94	0.50
2:B:435:THR:HG23	2:B:437:GLU:HB2	1.93	0.50
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.46	0.50
3:C:29:MET:HE2	3:C:29:MET:HB2	1.92	0.50
6:H:77:ARG:HB2	6:H:77:ARG:HH11	1.76	0.50
1:A:1134:ILE:O	1:A:1138:ILE:CD1	2.59	0.50
1:A:121:LEU:HB3	1:A:141:LEU:HD21	1.94	0.50
1:A:365:GLY:HA2	1:A:461:LYS:O	2.11	0.50
1:A:679:ILE:HD12	1:A:729:ALA:HB1	1.94	0.50
2:B:167:ILE:N	2:B:167:ILE:HD12	2.26	0.50
2:B:846:ILE:HD11	2:B:974:PRO:C	2.31	0.50
5:F:109:VAL:HG12	5:F:110:ASP:N	2.24	0.50
1:A:1449:SER:HB2	5:F:149:GLU:OE2	2.11	0.50
9:K:46:ILE:O	9:K:47:ARG:C	2.40	0.50
1:A:664:THR:HG22	1:A:742:ASN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HA	1:A:96:ILE:HD13	1.94	0.50
1:A:587:HIS:CD2	1:A:966:ASN:OD1	2.58	0.50
1:A:466:SER:CB	2:B:1103:ILE:HD11	2.41	0.50
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.47	0.50
2:B:458:LYS:NZ	2:B:958:GLN:NE2	2.59	0.50
2:B:1097:HIS:CB	2:B:1097:HIS:N	2.66	0.50
2:B:436:VAL:CB	2:B:436:VAL:N	2.69	0.50
1:A:1112:LYS:CA	1:A:1112:LYS:CG	2.81	0.50
8:J:4:PRO:HD3	8:J:53:HIS:HD2	1.77	0.50
1:A:89:PRO:CB	1:A:204:THR:HG21	2.28	0.50
1:A:63:ARG:HA	1:A:74:MET:CG	2.40	0.50
2:B:512:ARG:HB2	14:B:3017:HOH:O	2.12	0.50
2:B:843:GLN:NE2	2:B:846:ILE:HG21	2.27	0.50
1:A:1081:LEU:CD1	1:A:1081:LEU:CD2	2.81	0.49
1:A:328:ARG:NH1	1:A:1405:THR:CG2	2.75	0.49
1:A:55:ASP:N	1:A:56:PRO:HD2	2.25	0.49
2:B:516:ASN:ND2	2:B:516:ASN:H	2.10	0.49
2:B:956:THR:HA	2:B:961:LEU:O	2.12	0.49
7:I:16:PRO:HG3	7:I:27:PHE:HE2	1.76	0.49
1:A:1224:LEU:HG	1:A:1225:PHE:N	2.27	0.49
1:A:913:LEU:HD12	1:A:914:GLU:N	2.27	0.49
1:A:69:THR:CG2	2:B:1174:LYS:HE2	2.42	0.49
3:C:252:GLN:NE2	9:K:99:GLY:N	2.60	0.49
6:H:77:ARG:C	6:H:78:SER:O	2.49	0.49
10:L:48:CYS:HB3	10:L:51:CYS:O	2.13	0.49
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.93	0.49
1:A:853:ASP:O	1:A:854:ASN:HB2	2.12	0.49
1:A:867:ILE:HD12	1:A:1000:LEU:HD21	1.95	0.49
2:B:235:SER:OG	2:B:236:HIS:HD2	1.96	0.49
3:C:19:ASP:C	3:C:19:ASP:OD1	2.50	0.49
6:H:103:LYS:HG2	6:H:105:GLU:OE2	2.12	0.49
10:L:26:THR:CG2	10:L:27:LEU:H	2.26	0.49
2:B:1014:PRO:HA	2:B:1017:ILE:HD12	1.94	0.49
2:B:393:LYS:HZ1	2:B:621:GLU:CD	2.15	0.49
2:B:365:THR:HG22	2:B:367:LEU:H	1.76	0.49
7:I:55:THR:CG2	7:I:55:THR:HB	2.29	0.49
10:L:30:ILE:HG22	10:L:31:CYS:N	2.27	0.49
10:L:32:ALA:HB2	10:L:55:ILE:HG22	1.93	0.49
1:A:1162:VAL:CG1	1:A:1162:VAL:O	2.61	0.49
2:B:237:VAL:HG12	2:B:238:ALA:N	2.28	0.49
2:B:360:PHE:O	2:B:361:LEU:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:19:ARG:HA	6:H:19:ARG:CD	2.43	0.49
7:I:65:ASP:C	7:I:65:ASP:OD1	2.50	0.49
8:J:1:MET:C	8:J:2:ILE:HD12	2.32	0.49
3:C:252:GLN:HE22	9:K:99:GLY:HA2	1.75	0.49
1:A:387:ARG:O	1:A:388:LEU:C	2.51	0.49
1:A:507:VAL:N	1:A:508:PRO:CD	2.75	0.49
1:A:560:ILE:N	1:A:560:ILE:HD12	2.26	0.49
1:A:983:ILE:HD12	1:A:983:ILE:N	2.28	0.49
2:B:284:ILE:HD11	2:B:321:GLY:HA2	1.94	0.49
2:B:453:ILE:HG22	2:B:454:THR:N	2.28	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.95	0.49
1:A:706:HIS:CE1	1:A:1135:ARG:HD3	2.48	0.49
1:A:1151:GLU:OE2	7:I:45:ARG:CD	2.59	0.49
1:A:156:ASP:C	1:A:158:PRO:HD2	2.10	0.49
2:B:531:GLN:HE21	2:B:532:ALA:N	2.10	0.49
6:H:103:LYS:CE	6:H:135:LEU:O	2.60	0.49
1:A:1166:ASP:CA	1:A:1169:ILE:CG2	2.91	0.49
1:A:1436:ILE:CD1	2:B:1144:ALA:HB2	2.42	0.49
1:A:741:ASN:ND2	1:A:741:ASN:C	2.67	0.49
2:B:121:ASN:HD21	2:B:965:LYS:NZ	2.10	0.49
2:B:821:GLN:OE1	2:B:850:LEU:HD12	2.12	0.49
7:I:71:SER:OG	7:I:83:ASN:ND2	2.45	0.49
1:A:1162:VAL:CG2	1:A:1162:VAL:CG1	2.81	0.48
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.95	0.48
10:L:38:LEU:O	10:L:39:SER:HB2	2.13	0.48
1:A:1111:MET:CB	1:A:1111:MET:SD	2.92	0.48
1:A:1161:THR:HG23	1:A:1163:ILE:H	1.77	0.48
1:A:44:THR:CB	1:A:44:THR:HA	2.21	0.48
1:A:531:ILE:O	1:A:531:ILE:HD13	2.13	0.48
1:A:768:GLN:NE2	1:A:816:HIS:HA	2.28	0.48
6:H:103:LYS:O	6:H:115:TYR:CD1	2.63	0.48
1:A:144:THR:HG22	1:A:145:LYS:N	2.28	0.48
1:A:278:THR:HG22	1:A:278:THR:O	2.13	0.48
1:A:596:THR:HG22	1:A:597:LEU:HD12	1.94	0.48
2:B:1153:GLU:OE1	2:B:1153:GLU:HA	2.13	0.48
2:B:498:THR:HG21	2:B:537:LYS:HB2	1.95	0.48
1:A:1318:THR:HG23	4:E:11:ARG:NH1	2.28	0.48
4:E:65:THR:O	4:E:69:ILE:CG1	2.60	0.48
7:I:29:CYS:SG	7:I:31:THR:HB	2.54	0.48
2:B:1006:ILE:HD11	8:J:43:ARG:CB	2.43	0.48
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:HIS:CD2	1:A:786:HIS:N	2.81	0.48
8:J:1:MET:CE	8:J:1:MET:HG3	2.43	0.48
10:L:47:ARG:CG	10:L:48:CYS:N	2.75	0.48
1:A:187:LYS:HD2	1:A:194:ALA:HB2	1.94	0.48
1:A:295:LEU:CD2	1:A:295:LEU:HG	2.19	0.48
1:A:66:LYS:CB	1:A:66:LYS:CD	2.84	0.48
3:C:183:TRP:NE1	3:C:207:CYS:HB3	2.28	0.48
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.61	0.48
6:H:4:THR:C	6:H:5:LEU:HD23	2.33	0.48
6:H:9:ILE:CG1	6:H:9:ILE:CA	2.83	0.48
1:A:901:LEU:CD2	1:A:919:ILE:HD12	2.43	0.48
2:B:213:ILE:HD13	2:B:481:GLN:HG3	1.95	0.48
2:B:350:GLN:O	2:B:350:GLN:HG3	2.13	0.48
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.96	0.48
2:B:65:GLU:HG2	2:B:66:ASP:N	2.27	0.48
2:B:999:MET:HE3	2:B:999:MET:HG2	1.93	0.48
4:E:5:ASN:O	4:E:9:ILE:HG13	2.13	0.48
6:H:100:THR:O	6:H:116:TYR:HA	2.13	0.48
6:H:5:LEU:O	6:H:133:ASN:ND2	2.46	0.48
1:A:373:THR:O	1:A:373:THR:HG22	2.12	0.48
2:B:758:PHE:N	2:B:759:PRO:CD	2.76	0.48
4:E:93:MET:CE	4:E:116:ILE:HG21	2.43	0.48
7:I:58:VAL:HG11	7:I:109:ILE:HD11	1.96	0.48
9:K:10:PHE:HD1	9:K:11:LEU:HD13	1.78	0.48
1:A:1102:LYS:NZ	1:A:1102:LYS:CD	2.69	0.48
1:A:153:PRO:CD	1:A:161:LEU:CD2	2.66	0.48
1:A:466:SER:HB3	2:B:1103:ILE:HD11	1.94	0.48
1:A:476:SER:N	1:A:477:PRO:HD2	2.29	0.48
1:A:518:LYS:CD	1:A:518:LYS:HZ3	2.20	0.48
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.40	0.48
1:A:901:LEU:HD21	1:A:919:ILE:HD12	1.95	0.48
2:B:1128:LEU:O	2:B:1128:LEU:HG	2.14	0.48
1:A:92:HIS:HD2	1:A:94:GLY:N	2.12	0.48
2:B:1220:ARG:O	2:B:1222:ARG:CD	2.57	0.48
4:E:63:ASN:O	4:E:64:PRO:C	2.44	0.48
6:H:40:LEU:HD12	6:H:41:ASP:H	1.78	0.48
1:A:472:LEU:O	1:A:475:THR:HB	2.14	0.48
1:A:55:ASP:H	1:A:56:PRO:HD3	1.77	0.48
1:A:664:THR:HG21	1:A:746:MET:CE	2.44	0.48
2:B:121:ASN:HD22	2:B:121:ASN:N	2.11	0.48
2:B:185:THR:HG23	2:B:188:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:PHE:HB3	2:B:205:ILE:HD11	1.96	0.48
2:B:498:THR:HG22	2:B:537:LYS:HB2	1.95	0.48
3:C:94:LYS:HG2	3:C:94:LYS:NZ	2.28	0.48
9:K:18:LYS:HE3	9:K:38:GLU:CG	2.44	0.48
9:K:82:ASP:OD1	9:K:83:PRO:HG2	2.14	0.48
5:F:109:VAL:HG13	5:F:110:ASP:N	2.29	0.47
1:A:1232:ASN:ND2	1:A:1232:ASN:CB	2.73	0.47
1:A:670:ILE:HD13	2:B:1067:ARG:CZ	2.43	0.47
2:B:117:ALA:O	2:B:207:GLY:HA2	2.14	0.47
3:C:73:GLN:HE21	3:C:75:MET:N	2.08	0.47
4:E:37:LEU:C	4:E:38:PRO:O	2.50	0.47
1:A:1291:VAL:HG12	1:A:1291:VAL:O	2.10	0.47
1:A:274:ILE:CA	1:A:274:ILE:CG1	2.84	0.47
2:B:864:LYS:O	2:B:961:LEU:CD2	2.62	0.47
2:B:899:ILE:HD12	2:B:911:ILE:HA	1.97	0.47
4:E:61:GLN:HG3	4:E:62:ALA:N	2.29	0.47
9:K:65:HIS:CD2	9:K:66:PRO:HD2	2.49	0.47
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.14	0.47
1:A:1436:ILE:HD12	2:B:1144:ALA:HB2	1.97	0.47
1:A:399:HIS:HE1	1:A:436:ILE:O	1.97	0.47
1:A:64:ASN:O	1:A:66:LYS:N	2.46	0.47
1:A:720:ARG:O	1:A:724:GLU:HB3	2.14	0.47
4:E:117:THR:C	4:E:119:SER:N	2.67	0.47
6:H:105:GLU:C	6:H:107:VAL:N	2.63	0.47
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.28	0.47
1:A:138:ILE:HD12	1:A:142:CYS:SG	2.54	0.47
1:A:84:ILE:HG22	1:A:241:VAL:HG21	1.96	0.47
1:A:913:LEU:HD12	1:A:913:LEU:C	2.30	0.47
2:B:1177:HIS:HB2	2:B:1179:GLN:NE2	2.29	0.47
10:L:47:ARG:CG	10:L:48:CYS:H	2.18	0.47
2:B:101:MET:HA	2:B:110:HIS:O	2.14	0.47
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.96	0.47
2:B:724:ASP:O	2:B:725:PRO:C	2.51	0.47
2:B:727:LYS:HE2	2:B:1049:ASP:CG	2.35	0.47
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.49	0.47
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.96	0.47
1:A:752:LYS:CD	2:B:1015:HIS:O	2.62	0.47
6:H:37:LYS:O	6:H:125:LEU:HD23	2.14	0.47
6:H:76:THR:CG2	6:H:76:THR:O	2.61	0.47
1:A:1150:SER:OG	7:I:46:HIS:HB3	2.15	0.47
1:A:1134:ILE:HG22	1:A:1306:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:HG2	1:A:83:HIS:HE1	1.80	0.47
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.15	0.47
2:B:169:ARG:O	2:B:457:LEU:HD12	2.14	0.47
2:B:259:TYR:HB2	2:B:268:THR:HG22	1.97	0.47
2:B:864:LYS:O	2:B:961:LEU:HD23	2.13	0.47
1:A:605:MET:HG3	1:A:607:ILE:HD12	1.97	0.47
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.44	0.47
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.80	0.47
2:B:616:ILE:HD13	2:B:696:GLU:HG3	1.97	0.47
6:H:113:ALA:HA	6:H:125:LEU:O	2.15	0.47
1:A:1143:LEU:O	1:A:1144:LYS:C	2.53	0.47
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.97	0.47
3:C:120:ILE:N	3:C:120:ILE:HD12	2.29	0.47
2:B:955:THR:CG2	10:L:55:ILE:HA	2.45	0.47
1:A:237:THR:C	1:A:237:THR:CG2	2.82	0.47
2:B:755:ILE:HG22	2:B:755:ILE:O	2.14	0.47
1:A:555:ASP:OD1	9:K:26:LYS:CE	2.63	0.47
1:A:1445:ILE:HD13	1:A:1445:ILE:N	2.30	0.46
1:A:413:ILE:HD12	1:A:413:ILE:N	2.30	0.46
2:B:916:THR:HG22	2:B:916:THR:O	2.14	0.46
6:H:9:ILE:HB	6:H:9:ILE:CA	2.20	0.46
3:C:52:GLU:HA	10:L:64:LEU:HD21	1.97	0.46
2:B:827:ILE:HG12	2:B:1012:ILE:HD11	1.96	0.46
2:B:1027:ILE:HD13	2:B:1027:ILE:HG21	1.56	0.46
2:B:755:ILE:HD12	2:B:814:PHE:CD1	2.51	0.46
1:A:1154:TYR:CZ	1:A:1156:PRO:HB3	2.51	0.46
1:A:119:ASN:O	1:A:120:GLU:CB	2.45	0.46
1:A:110:CYS:SG	1:A:167:CYS:CB	3.04	0.46
2:B:566:LEU:HA	2:B:566:LEU:HD12	1.78	0.46
2:B:844:SER:O	2:B:847:ASP:HB2	2.15	0.46
3:C:66:ARG:O	3:C:67:LEU:C	2.53	0.46
1:A:1127:ASP:OD2	1:A:1130:GLN:HB2	2.15	0.46
1:A:26:GLU:HA	1:A:29:ALA:HB3	1.96	0.46
2:B:134:LYS:HB2	2:B:134:LYS:HE3	1.74	0.46
2:B:820:GLY:HA3	2:B:1091:TYR:CZ	2.51	0.46
6:H:101:ALA:HA	6:H:116:TYR:H	1.81	0.46
2:B:1058:LEU:O	2:B:1062:HIS:HD2	1.98	0.46
2:B:65:GLU:O	2:B:67:SER:N	2.49	0.46
1:A:153:PRO:CD	1:A:161:LEU:HD22	2.30	0.46
1:A:523:ILE:HB	1:A:622:VAL:CG1	2.45	0.46
1:A:567:LYS:HG2	6:H:96:VAL:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ASN:OD1	1:A:64:ASN:C	2.53	0.46
1:A:901:LEU:HD11	1:A:919:ILE:HD12	1.98	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.97	0.46
1:A:1055:ARG:HG3	1:A:1055:ARG:NE	2.25	0.46
1:A:551:TYR:CE2	9:K:62:LYS:HD3	2.50	0.46
1:A:595:THR:CG2	1:A:596:THR:N	2.77	0.46
1:A:80:HIS:O	1:A:243:PRO:HD3	2.16	0.46
1:A:956:LEU:HB3	1:A:957:PRO:HD2	1.97	0.46
2:B:515:HIS:CB	2:B:518:HIS:CD2	2.98	0.46
4:E:41:ASP:O	4:E:42:PHE:C	2.53	0.46
6:H:106:GLU:HB2	6:H:113:ALA:HB3	1.96	0.46
1:A:328:ARG:HH11	1:A:1405:THR:CG2	2.28	0.46
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.43	0.46
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.80	0.46
2:B:261:ARG:O	2:B:264:SER:N	2.48	0.46
4:E:44:ALA:O	4:E:46:TYR:N	2.49	0.46
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.81	0.46
9:K:78:THR:HG22	9:K:79:GLU:H	1.81	0.46
10:L:26:THR:OG1	10:L:26:THR:CG2	2.57	0.46
1:A:34:LYS:HG2	1:A:83:HIS:CE1	2.51	0.46
2:B:622:LYS:NZ	2:B:622:LYS:CD	2.70	0.46
4:E:55:ARG:O	4:E:58:MET:HB2	2.16	0.46
8:J:53:HIS:HD1	8:J:54:VAL:N	2.13	0.46
1:A:919:ILE:HD13	1:A:983:ILE:CD1	2.45	0.46
1:A:920:LEU:HD22	1:A:921:GLY:N	2.31	0.46
2:B:227:LYS:NZ	2:B:236:HIS:HE1	2.13	0.46
4:E:161:LYS:CE	4:E:172:GLU:OE2	2.64	0.46
5:F:89:GLU:CG	5:F:134:ILE:HD13	2.45	0.46
6:H:113:ALA:CB	6:H:124:ARG:NH2	2.79	0.46
6:H:113:ALA:HB2	6:H:124:ARG:HH21	1.81	0.46
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.98	0.45
1:A:535:THR:CG2	1:A:617:VAL:N	2.66	0.45
4:E:117:THR:C	4:E:119:SER:H	2.19	0.45
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.98	0.45
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.29	0.45
1:A:195:ASP:O	1:A:196:GLU:CB	2.64	0.45
1:A:265:LYS:HZ3	1:A:302:THR:HG21	1.77	0.45
2:B:723:VAL:HB	2:B:723:VAL:CA	2.23	0.45
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.76	0.45
4:E:12:LEU:CD2	4:E:58:MET:SD	2.88	0.45
5:F:128:LYS:NZ	5:F:151:LEU:O	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:123:MET:HE3	6:H:142:LEU:HD13	1.97	0.45
6:H:48:PRO:C	6:H:49:VAL:HG23	2.36	0.45
1:A:436:ILE:HD13	1:A:436:ILE:HG21	1.63	0.45
1:A:92:HIS:HD2	1:A:94:GLY:H	1.64	0.45
3:C:15:LYS:O	3:C:240:VAL:CG2	2.64	0.45
8:J:42:LYS:HG3	8:J:43:ARG:N	2.32	0.45
1:A:98:LYS:O	1:A:102:VAL:HG23	2.15	0.45
1:A:1055:ARG:HE	1:A:1055:ARG:CG	2.27	0.45
1:A:1256:GLU:CB	1:A:1259:MET:HE2	2.46	0.45
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.52	0.45
1:A:264:PHE:O	1:A:267:ALA:HB3	2.17	0.45
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.98	0.45
1:A:1109:LYS:CG	1:A:1109:LYS:CA	2.80	0.45
1:A:605:MET:CE	1:A:607:ILE:CG1	2.95	0.45
2:B:121:ASN:H	2:B:121:ASN:HD22	1.63	0.45
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.57	0.45
2:B:417:PHE:C	2:B:417:PHE:HD2	2.16	0.45
2:B:642:ASP:HA	2:B:643:ASP:HA	1.29	0.45
7:I:43:VAL:O	7:I:43:VAL:CG1	2.64	0.45
9:K:102:LYS:O	9:K:106:GLU:HB2	2.17	0.45
1:A:1166:ASP:O	1:A:1169:ILE:HG23	2.16	0.45
1:A:1385:THR:HB	1:A:1385:THR:CG2	2.19	0.45
1:A:98:LYS:HB3	1:A:234:MET:HE1	1.99	0.45
1:A:523:ILE:CB	1:A:622:VAL:HG13	2.45	0.45
1:A:925:LEU:HA	1:A:925:LEU:HD23	1.82	0.45
2:B:206:ASN:OD1	2:B:458:LYS:HE3	2.15	0.45
2:B:215:GLN:HE22	2:B:499:ASN:HD22	1.65	0.45
2:B:916:THR:HB	2:B:935:ARG:HB2	1.98	0.45
4:E:39:LEU:O	4:E:42:PHE:HB3	2.17	0.45
1:A:1192:LEU:HD11	1:A:1239:ARG:HB2	1.99	0.45
1:A:511:ILE:HD13	1:A:646:PHE:HE1	1.81	0.45
1:A:597:LEU:H	1:A:597:LEU:HD12	1.81	0.45
1:A:908:LEU:HD23	1:A:908:LEU:HA	1.77	0.45
2:B:246:LYS:CA	2:B:247:GLY:N	2.66	0.45
2:B:841:MET:HE1	2:B:990:ILE:HD11	1.97	0.45
3:C:56:THR:CG2	3:C:58:LEU:H	2.29	0.45
5:F:128:LYS:HA	5:F:128:LYS:HD3	1.76	0.45
8:J:53:HIS:CE1	8:J:55:ASP:N	2.85	0.45
8:J:62:ARG:HE	8:J:62:ARG:HB3	1.29	0.45
1:A:61:ILE:CA	1:A:61:ILE:CG2	2.86	0.45
2:B:345:LYS:O	2:B:346:GLU:C	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:455:SER:O	2:B:459:TYR:HB3	2.16	0.45
3:C:218:PRO:O	3:C:219:PHE:C	2.55	0.45
1:A:1111:MET:HE1	1:A:1331:SER:HA	1.99	0.45
1:A:858:ASN:HD22	1:A:858:ASN:C	2.20	0.45
2:B:859:TYR:CD1	2:B:859:TYR:N	2.85	0.45
4:E:63:ASN:C	4:E:64:PRO:O	2.55	0.45
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.99	0.45
3:C:80:LEU:HD12	3:C:80:LEU:HA	1.58	0.45
4:E:129:PRO:CD	4:E:130:ALA:N	2.78	0.45
7:I:51:ASN:HB2	7:I:118:ARG:CZ	2.46	0.45
1:A:566:ILE:CG2	1:A:566:ILE:HB	2.20	0.44
2:B:1019:SER:OG	13:B:3008:GTP:C6	2.57	0.44
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.99	0.44
2:B:210:LYS:HE3	2:B:461:LEU:O	2.17	0.44
4:E:131:THR:N	4:E:131:THR:CB	2.67	0.44
4:E:31:THR:O	4:E:32:GLN:C	2.55	0.44
4:E:80:VAL:HG12	4:E:81:GLU:N	2.32	0.44
5:F:107:VAL:HG12	5:F:109:VAL:H	1.81	0.44
7:I:75:CYS:HB3	7:I:110:PHE:CE2	2.52	0.44
1:A:515:GLN:OE1	14:A:3018:HOH:O	2.21	0.44
1:A:941:LYS:HD3	1:A:941:LYS:NZ	2.30	0.44
2:B:806:THR:HG23	2:B:808:ALA:H	1.82	0.44
3:C:196:ASP:CG	3:C:199:LYS:HG3	2.38	0.44
1:A:1157:ASP:O	1:A:1160:SER:O	2.36	0.44
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.31	0.44
1:A:481:ASP:CG	1:A:481:ASP:N	2.70	0.44
1:A:543:LEU:HG	1:A:543:LEU:O	2.15	0.44
4:E:116:ILE:HG22	4:E:120:ALA:HB3	2.00	0.44
6:H:40:LEU:HD12	6:H:41:ASP:N	2.31	0.44
7:I:120:GLN:O	7:I:121:PHE:CD1	2.71	0.44
1:A:328:ARG:NH1	1:A:1405:THR:HB	2.32	0.44
1:A:356:ASP:OD2	1:A:469:ARG:HD3	2.17	0.44
1:A:58:LEU:O	1:A:59:GLY:O	2.34	0.44
1:A:809:THR:HB	1:A:810:PRO:CD	2.47	0.44
1:A:896:ARG:HD3	1:A:897:TYR:CZ	2.52	0.44
2:B:249:ARG:NH1	2:B:418:LYS:HZ2	2.15	0.44
6:H:93:TYR:CD1	6:H:93:TYR:N	2.86	0.44
8:J:53:HIS:C	8:J:53:HIS:ND1	2.70	0.44
1:A:596:THR:CG2	1:A:597:LEU:N	2.77	0.44
1:A:531:ILE:CD1	1:A:617:VAL:HB	2.39	0.44
1:A:843:LYS:CE	1:A:843:LYS:CG	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:LEU:CD1	1:A:919:ILE:HD12	2.48	0.44
1:A:982:THR:O	1:A:985:ASP:HB2	2.18	0.44
2:B:1190:ASP:C	2:B:1191:ILE:HG13	2.36	0.44
2:B:1019:SER:CB	13:B:3008:GTP:N7	2.81	0.44
2:B:983:ARG:CD	14:B:3009:HOH:O	2.66	0.44
4:E:213:ILE:O	4:E:213:ILE:HG23	2.17	0.44
4:E:36:GLU:O	4:E:38:PRO:N	2.50	0.44
1:A:503:GLN:HE21	5:F:90:ARG:NH2	2.12	0.44
2:B:56:ASP:N	2:B:56:ASP:OD1	2.45	0.44
2:B:755:ILE:CG2	2:B:755:ILE:O	2.66	0.44
3:C:255:VAL:CG1	3:C:255:VAL:O	2.65	0.44
3:C:260:LEU:CD1	3:C:260:LEU:O	2.59	0.44
3:C:54:ASN:OD1	3:C:56:THR:CB	2.44	0.44
7:I:91:ARG:HD3	7:I:91:ARG:HA	1.77	0.44
10:L:48:CYS:CA	10:L:49:LYS:N	2.66	0.44
1:A:1111:MET:CB	1:A:1111:MET:CE	2.96	0.44
1:A:599:SER:O	1:A:600:PRO:C	2.56	0.44
2:B:284:ILE:CD1	2:B:321:GLY:HA2	2.48	0.44
6:H:10:PHE:HA	6:H:29:ALA:O	2.18	0.44
6:H:82:PRO:O	6:H:83:GLN:HB2	2.18	0.44
1:A:555:ASP:OD1	9:K:26:LYS:HE3	2.17	0.44
10:L:38:LEU:HD13	10:L:48:CYS:HA	1.99	0.44
10:L:38:LEU:HG	10:L:39:SER:N	2.32	0.44
1:A:1333:ILE:HD12	1:A:1333:ILE:N	2.33	0.44
2:B:114:PRO:HD3	2:B:124:TYR:HE1	1.78	0.44
2:B:130:VAL:H	2:B:167:ILE:CD1	2.17	0.44
4:E:36:GLU:O	4:E:38:PRO:HD3	2.18	0.44
1:A:1166:ASP:HA	1:A:1169:ILE:HG22	1.98	0.44
2:B:969:ARG:HH11	2:B:969:ARG:HD3	1.43	0.44
3:C:252:GLN:HB3	3:C:252:GLN:CG	2.20	0.44
3:C:262:LEU:HA	3:C:262:LEU:HD23	1.78	0.44
4:E:116:ILE:HG22	4:E:120:ALA:CB	2.48	0.44
6:H:89:LEU:O	6:H:90:ALA:C	2.50	0.44
6:H:95:TYR:CE2	6:H:97:MET:HG3	2.53	0.44
1:A:1151:GLU:HG3	7:I:45:ARG:HD2	1.95	0.44
1:A:145:LYS:HE2	1:A:149:GLU:OE1	2.18	0.43
2:B:555:ILE:HD12	2:B:587:HIS:HE1	1.75	0.43
1:A:834:THR:HG21	1:A:1077:THR:N	2.33	0.43
1:A:587:HIS:CE1	1:A:609:ASP:H	2.36	0.43
1:A:882:SER:CB	1:A:953:ASN:OD1	2.66	0.43
1:A:979:SER:OG	1:A:981:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:999:MET:CE	2:B:1011:ILE:HD11	2.48	0.43
2:B:1202:LEU:HA	2:B:1202:LEU:HD23	1.88	0.43
2:B:118:ARG:NH2	2:B:194:GLU:CG	2.80	0.43
2:B:276:ILE:HG23	2:B:276:ILE:HD12	1.71	0.43
2:B:323:VAL:O	2:B:323:VAL:CG1	2.65	0.43
2:B:654:ARG:N	2:B:657:HIS:HD2	2.14	0.43
2:B:789:MET:CE	2:B:965:LYS:HB3	2.48	0.43
3:C:47:ASP:CG	3:C:47:ASP:O	2.56	0.43
1:A:605:MET:HE3	1:A:607:ILE:HG13	2.00	0.43
2:B:620:ARG:CB	2:B:620:ARG:CD	2.82	0.43
4:E:78:LEU:HG	4:E:79:TRP:N	2.33	0.43
6:H:27:GLU:OE1	6:H:39:THR:CG2	2.66	0.43
6:H:96:VAL:HA	6:H:142:LEU:O	2.18	0.43
1:A:11:LEU:O	1:A:12:ARG:HG2	2.18	0.43
1:A:1242:VAL:HG11	1:A:1259:MET:CE	2.48	0.43
1:A:353:ILE:HD12	1:A:482:PHE:CD2	2.54	0.43
1:A:666:ILE:HD13	1:A:666:ILE:O	2.19	0.43
1:A:676:MET:CB	1:A:676:MET:SD	2.98	0.43
1:A:977:LYS:HA	1:A:977:LYS:CG	2.49	0.43
1:A:1438:THR:HB	2:B:1142:GLY:O	2.18	0.43
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.76	0.43
2:B:387:LEU:HD12	2:B:387:LEU:HA	1.55	0.43
2:B:25:ILE:CD1	2:B:651:LEU:HD12	2.41	0.43
3:C:179:GLU:CG	3:C:180:TYR:N	2.81	0.43
3:C:196:ASP:CB	3:C:199:LYS:HG3	2.49	0.43
3:C:74:SER:HB2	3:C:238:ILE:HD12	2.01	0.43
6:H:98:TYR:C	6:H:118:PHE:HD2	2.21	0.43
2:B:293:PRO:HA	7:I:12:ASN:HD21	1.83	0.43
1:A:1339:LEU:HA	1:A:1339:LEU:HD23	1.77	0.43
1:A:243:PRO:CB	1:A:245:PRO:HD2	2.46	0.43
1:A:901:LEU:HB2	1:A:926:GLN:HE21	1.83	0.43
2:B:1150:ARG:HD2	2:B:1150:ARG:HH11	1.45	0.43
2:B:870:ILE:CA	2:B:870:ILE:HB	2.24	0.43
4:E:115:ASN:C	4:E:116:ILE:HD13	2.38	0.43
5:F:81:THR:HG22	5:F:136:ARG:NH1	2.32	0.43
1:A:567:LYS:CD	6:H:95:TYR:CD2	2.97	0.43
1:A:483:ASP:O	2:B:987:LYS:NZ	2.37	0.43
2:B:705:MET:CG	2:B:705:MET:HE2	2.31	0.43
3:C:131:HIS:O	3:C:132:PRO:C	2.57	0.43
1:A:503:GLN:HE22	5:F:90:ARG:NH2	2.14	0.43
2:B:896:ASP:OD2	10:L:29:TYR:OH	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:GLU:HG2	3:C:5:GLY:H	1.84	0.43
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.54	0.43
5:F:114:GLU:CB	5:F:120:ILE:HD13	2.49	0.43
7:I:55:THR:HG21	7:I:121:PHE:O	2.19	0.43
7:I:10:CYS:SG	7:I:31:THR:HG22	2.58	0.43
8:J:43:ARG:O	8:J:47:ARG:HG3	2.19	0.43
1:A:1383:SER:OG	1:A:1384:VAL:N	2.51	0.43
1:A:34:LYS:CG	1:A:83:HIS:CE1	3.02	0.43
1:A:359:LEU:HA	1:A:359:LEU:HD23	1.75	0.43
1:A:886:ILE:HD12	1:A:943:LEU:HB3	2.01	0.43
2:B:169:ARG:HB2	2:B:454:THR:CG2	2.41	0.43
2:B:451:LYS:HA	2:B:454:THR:HB	2.00	0.43
2:B:529:GLU:O	2:B:531:GLN:NE2	2.52	0.43
2:B:863:GLU:OE1	2:B:962:LYS:HD3	2.18	0.43
2:B:986:GLN:CG	2:B:986:GLN:OE1	2.53	0.43
3:C:163:ILE:HA	3:C:163:ILE:HD13	1.43	0.43
4:E:78:LEU:HD11	4:E:109:ILE:CD1	2.49	0.43
6:H:13:SER:O	6:H:14:GLU:HG3	2.19	0.43
6:H:81:PRO:C	6:H:82:PRO:O	2.55	0.43
1:A:593:GLU:HG2	1:A:593:GLU:O	2.18	0.43
1:A:597:LEU:CB	1:A:597:LEU:CD1	2.86	0.43
1:A:700:ASN:O	7:I:115:LYS:HE3	2.19	0.43
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.48	0.43
2:B:542:MET:CE	2:B:747:MET:HG3	2.49	0.43
1:A:562:THR:HG21	6:H:98:TYR:CD2	2.53	0.43
1:A:1169:ILE:HD11	1:A:1227:ILE:CD1	2.48	0.43
1:A:295:LEU:CB	1:A:295:LEU:CD2	2.82	0.43
1:A:853:ASP:OD2	1:A:857:ARG:NH2	2.50	0.43
2:B:118:ARG:HG3	2:B:204:ILE:CD1	2.47	0.43
2:B:542:MET:HE2	2:B:747:MET:HG3	1.99	0.43
3:C:180:TYR:CD1	3:C:180:TYR:C	2.93	0.43
3:C:77:ILE:HD11	3:C:80:LEU:HD23	2.00	0.43
6:H:33:GLN:C	6:H:35:GLN:H	2.22	0.43
9:K:18:LYS:HE3	9:K:38:GLU:OE2	2.19	0.43
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.11	0.42
1:A:186:LYS:CG	1:A:197:PRO:HD3	2.48	0.42
1:A:563:PRO:HB3	1:A:572:TRP:CD2	2.53	0.42
2:B:132:VAL:HG12	2:B:133:LYS:N	2.34	0.42
2:B:461:LEU:HD12	2:B:461:LEU:N	2.34	0.42
2:B:885:MET:HB3	2:B:885:MET:HE3	1.99	0.42
2:B:914:LYS:N	2:B:938:SER:HB2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:THR:HG23	3:C:44:LEU:N	2.33	0.42
6:H:95:TYR:HD2	6:H:95:TYR:C	2.22	0.42
1:A:1165:GLU:HG2	1:A:1165:GLU:H	1.56	0.42
1:A:391:LEU:CD2	1:A:400:PRO:HB2	2.50	0.42
1:A:560:ILE:H	1:A:560:ILE:CD1	2.30	0.42
2:B:1194:ILE:O	2:B:1194:ILE:HG13	2.19	0.42
2:B:51:PHE:CE2	2:B:172:ILE:HD13	2.54	0.42
2:B:213:ILE:CD1	2:B:481:GLN:CD	2.88	0.42
6:H:32:THR:CG2	6:H:33:GLN:CD	2.87	0.42
8:J:6:ARG:HD2	8:J:11:GLY:O	2.18	0.42
1:A:157:ASP:O	1:A:160:GLN:HG3	2.19	0.42
1:A:868:TYR:CE1	1:A:1064:VAL:HG13	2.54	0.42
2:B:1169:MET:CE	2:B:1204:PHE:HB2	2.49	0.42
4:E:147:HIS:HD2	4:E:149:LEU:HB2	1.84	0.42
6:H:32:THR:HG22	6:H:33:GLN:OE1	2.17	0.42
7:I:17:ARG:HG3	7:I:28:GLU:OE1	2.19	0.42
1:A:664:THR:HG21	1:A:746:MET:HE1	2.00	0.42
1:A:744:LYS:HD3	1:A:748:MET:CE	2.49	0.42
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.20	0.42
2:B:554:ILE:H	2:B:554:ILE:HD12	1.84	0.42
3:C:240:VAL:C	3:C:242:GLN:N	2.70	0.42
4:E:37:LEU:CB	4:E:37:LEU:CD1	2.84	0.42
4:E:59:SER:O	4:E:60:PHE:HB3	2.20	0.42
5:F:74:ILE:CD1	5:F:144:GLU:HG2	2.49	0.42
6:H:105:GLU:N	6:H:105:GLU:CD	2.69	0.42
6:H:95:TYR:HE2	6:H:97:MET:HG3	1.85	0.42
9:K:12:LEU:HD12	9:K:12:LEU:H	1.85	0.42
1:A:599:SER:HB2	1:A:602:ASP:H	1.85	0.42
1:A:722:LEU:HA	1:A:722:LEU:HD23	1.90	0.42
1:A:913:LEU:HD12	1:A:913:LEU:HA	1.61	0.42
2:B:509:ALA:C	2:B:511:PRO:HD3	2.39	0.42
2:B:554:ILE:HD12	2:B:554:ILE:N	2.34	0.42
2:B:996:ARG:HH11	2:B:996:ARG:HD3	1.53	0.42
3:C:7:GLN:CG	3:C:7:GLN:CA	2.87	0.42
6:H:44:VAL:O	6:H:44:VAL:CG1	2.67	0.42
9:K:111:LEU:H	9:K:111:LEU:HD23	1.85	0.42
10:L:34:CYS:HB3	10:L:51:CYS:HB3	2.02	0.42
1:A:195:ASP:O	1:A:196:GLU:HB3	2.20	0.42
1:A:922:ASP:OD1	1:A:922:ASP:C	2.58	0.42
2:B:976:ILE:O	2:B:1099:VAL:HG21	2.19	0.42
2:B:646:LEU:CD2	2:B:646:LEU:CD1	2.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ILE:HD12	2:B:70:ILE:N	2.34	0.42
2:B:121:ASN:ND2	2:B:965:LYS:NZ	2.68	0.42
1:A:1336:MET:HE2	1:A:1381:LEU:H	1.85	0.42
2:B:1002:THR:O	2:B:1005:GLY:N	2.42	0.42
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.20	0.42
2:B:286:PHE:CB	2:B:297:ILE:HD12	2.40	0.42
2:B:773:MET:O	2:B:774:GLY:C	2.55	0.42
4:E:43:LYS:O	4:E:47:CYS:CB	2.68	0.42
1:A:709:THR:HG22	1:A:711:ARG:N	2.35	0.42
1:A:786:HIS:CD2	1:A:786:HIS:H	2.36	0.42
2:B:199:MET:HE1	2:B:488:TYR:CE1	2.55	0.42
4:E:79:TRP:HE1	4:E:81:GLU:HB2	1.84	0.42
6:H:138:GLU:C	6:H:140:ALA:N	2.67	0.42
10:L:49:LYS:O	10:L:50:ASP:HB2	2.20	0.42
1:A:1102:LYS:CG	1:A:1102:LYS:CE	2.87	0.42
1:A:1146:VAL:HG12	1:A:1197:LEU:HD22	2.02	0.42
1:A:1385:THR:CG2	1:A:1385:THR:O	2.66	0.42
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.20	0.42
1:A:830:LYS:CD	1:A:830:LYS:CB	2.84	0.42
2:B:104:GLU:HB2	2:B:108:VAL:HA	2.02	0.42
2:B:757:PRO:HD2	2:B:984:HIS:HE1	1.85	0.42
2:B:95:ILE:HG22	2:B:96:TYR:O	2.20	0.42
8:J:16:ASP:OD1	8:J:17:LYS:HG3	2.19	0.42
2:B:1006:ILE:CD1	8:J:43:ARG:HD2	2.50	0.42
2:B:902:GLY:O	10:L:65:VAL:HG11	2.19	0.42
1:A:230:ARG:NH1	1:A:232:GLU:OE2	2.52	0.41
1:A:93:VAL:HG13	1:A:301:ALA:HB1	2.01	0.41
2:B:282:ILE:HD11	2:B:317:CYS:CB	2.50	0.41
2:B:274:PRO:HG3	2:B:359:GLU:O	2.20	0.41
1:A:1134:ILE:O	1:A:1138:ILE:HD11	2.21	0.41
1:A:492:PRO:HB2	1:A:497:THR:CG2	2.48	0.41
1:A:70:CYS:HB3	2:B:1172:ILE:HG23	2.02	0.41
3:C:214:ASN:O	3:C:217:ASP:N	2.54	0.41
3:C:7:GLN:OE1	9:K:104:ASN:ND2	2.54	0.41
4:E:61:GLN:HB2	4:E:79:TRP:CE3	2.56	0.41
6:H:47:PHE:HB2	6:H:95:TYR:HD1	1.83	0.41
7:I:40:SER:CB	7:I:41:PRO:CD	2.97	0.41
1:A:1170:ILE:HD13	1:A:1170:ILE:HA	1.96	0.41
1:A:145:LYS:HE2	1:A:149:GLU:CD	2.40	0.41
1:A:807:GLY:CA	2:B:761:HIS:CE1	3.04	0.41
2:B:879:ARG:HH21	2:B:885:MET:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1322:ILE:HD12	1:A:1322:ILE:C	2.41	0.41
1:A:446:ARG:CG	1:A:446:ARG:NH1	2.83	0.41
2:B:1195:HIS:C	2:B:1196:ILE:HG23	2.40	0.41
4:E:168:TYR:O	4:E:169:ARG:HB2	2.20	0.41
4:E:154:ILE:CD1	4:E:199:ILE:HD12	2.50	0.41
7:I:71:SER:O	7:I:83:ASN:ND2	2.53	0.41
1:A:973:ILE:CD1	1:A:1038:THR:HG23	2.51	0.41
1:A:1166:ASP:CB	1:A:1169:ILE:HG21	2.39	0.41
1:A:1237:ILE:HD12	1:A:1237:ILE:HA	1.75	0.41
1:A:138:ILE:HG13	1:A:139:TRP:N	2.35	0.41
1:A:96:ILE:HG21	1:A:176:LYS:HE2	2.03	0.41
1:A:557:ASP:O	1:A:559:VAL:N	2.53	0.41
1:A:666:ILE:HD12	2:B:1052:VAL:HG11	2.02	0.41
1:A:752:LYS:HE2	13:B:3008:GTP:N1	2.35	0.41
1:A:95:PHE:O	1:A:99:ILE:HG13	2.21	0.41
2:B:1189:ILE:N	2:B:1189:ILE:HD12	2.35	0.41
2:B:28:GLU:OE1	2:B:807:ARG:NH2	2.54	0.41
4:E:98:ILE:CA	4:E:98:ILE:CG2	2.88	0.41
7:I:103:CYS:SG	7:I:106:CYS:SG	3.18	0.41
2:B:900:ALA:HA	10:L:58:LYS:HD2	2.02	0.41
1:A:846:GLU:HA	1:A:1066:VAL:CG2	2.50	0.41
2:B:280:ILE:HD12	2:B:280:ILE:H	1.86	0.41
4:E:79:TRP:NE1	4:E:81:GLU:HB2	2.36	0.41
5:F:128:LYS:NZ	5:F:149:GLU:O	2.48	0.41
6:H:138:GLU:HG2	6:H:139:ASN:N	2.36	0.41
8:J:14:VAL:CG1	8:J:50:ILE:CD1	2.95	0.41
9:K:47:ARG:C	9:K:47:ARG:HD2	2.41	0.41
1:A:834:THR:CG2	1:A:1077:THR:OG1	2.66	0.41
1:A:571:LEU:HA	1:A:571:LEU:HD12	1.70	0.41
1:A:741:ASN:ND2	1:A:743:VAL:H	2.19	0.41
1:A:9:ALA:O	2:B:1193:GLN:OE1	2.39	0.41
1:A:351:THR:HG23	2:B:1103:ILE:HG12	1.98	0.41
2:B:780:VAL:HG21	8:J:56:LEU:HD11	2.03	0.41
2:B:914:LYS:HD2	2:B:937:ALA:HB3	2.02	0.41
2:B:939:THR:HA	2:B:940:PRO:HD3	1.93	0.41
3:C:44:LEU:HD22	3:C:129:ILE:HD12	2.03	0.41
4:E:161:LYS:NZ	4:E:172:GLU:OE2	2.51	0.41
6:H:145:ARG:HG2	6:H:145:ARG:NH1	2.36	0.41
1:A:1023:ARG:HD3	1:A:1023:ARG:HH21	1.66	0.41
1:A:516:SER:OG	1:A:1362:TYR:O	2.39	0.41
1:A:1207:LEU:HD23	1:A:1211:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1362:TYR:C	1:A:1362:TYR:CD2	2.93	0.41
1:A:269:ILE:CD1	1:A:300:VAL:HG22	2.50	0.41
2:B:1161:HIS:HA	2:B:1192:TYR:O	2.21	0.41
2:B:90:ILE:HD11	2:B:134:LYS:HE2	2.03	0.41
3:C:29:MET:CB	3:C:29:MET:CE	2.99	0.41
5:F:94:LEU:HD23	5:F:94:LEU:HA	1.85	0.41
8:J:1:MET:HG3	8:J:60:PHE:HE2	1.86	0.41
9:K:98:LEU:O	9:K:99:GLY:C	2.58	0.41
10:L:54:ARG:NE	10:L:54:ARG:CG	2.66	0.41
1:A:1258:HIS:O	1:A:1259:MET:C	2.59	0.41
1:A:1267:MET:HA	1:A:1271:ILE:HD13	2.03	0.41
1:A:186:LYS:HD2	1:A:197:PRO:HG3	2.03	0.41
1:A:541:ILE:HG22	1:A:546:VAL:HG23	2.03	0.41
1:A:582:ILE:HA	1:A:583:PRO:HD3	1.92	0.41
2:B:1179:GLN:HB2	2:B:1179:GLN:HE21	1.70	0.41
2:B:323:VAL:O	2:B:323:VAL:HG12	2.20	0.41
3:C:216:GLY:O	3:C:217:ASP:C	2.60	0.41
6:H:142:LEU:HD12	6:H:142:LEU:HA	1.76	0.41
1:A:1220:PHE:HB3	1:A:1224:LEU:HB3	2.03	0.41
1:A:93:VAL:HG22	1:A:301:ALA:HA	2.02	0.41
2:B:643:ASP:HB3	2:B:644:GLU:C	2.42	0.41
1:A:1025:ARG:HD3	1:A:1025:ARG:HA	1.88	0.40
1:A:1039:LYS:HG3	1:A:1039:LYS:O	2.21	0.40
1:A:1166:ASP:HB3	1:A:1169:ILE:HG23	1.97	0.40
1:A:210:ILE:HA	1:A:210:ILE:HD13	1.91	0.40
1:A:274:ILE:CA	1:A:274:ILE:HB	2.21	0.40
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.56	0.40
1:A:679:ILE:CD1	1:A:729:ALA:O	2.68	0.40
1:A:83:HIS:C	1:A:83:HIS:ND1	2.74	0.40
1:A:983:ILE:HD12	1:A:983:ILE:H	1.86	0.40
3:C:102:GLN:CD	3:C:102:GLN:CB	2.78	0.40
3:C:40:GLU:CD	3:C:254:LYS:NZ	2.75	0.40
4:E:55:ARG:O	4:E:56:LYS:C	2.59	0.40
5:F:93:ILE:HD12	5:F:134:ILE:HD11	1.98	0.40
6:H:101:ALA:HA	6:H:116:TYR:HA	2.01	0.40
9:K:27:ALA:HB1	9:K:28:PRO:CD	2.51	0.40
9:K:59:ALA:HA	9:K:74:ARG:O	2.21	0.40
1:A:1004:ASN:OD1	4:E:167:ARG:HG3	2.21	0.40
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.84	0.40
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.57	0.40
2:B:724:ASP:O	2:B:726:ALA:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:ILE:HD11	3:C:144:ILE:CD1	2.51	0.40
4:E:161:LYS:NZ	4:E:193:GLY:O	2.54	0.40
8:J:1:MET:HG3	8:J:1:MET:HE2	2.04	0.40
9:K:110:ASN:C	9:K:112:GLN:N	2.63	0.40
1:A:1166:ASP:O	1:A:1169:ILE:CG2	2.69	0.40
1:A:1209:MET:SD	1:A:1236:LEU:HD22	2.62	0.40
1:A:44:THR:CA	1:A:44:THR:CG2	2.86	0.40
1:A:599:SER:HA	1:A:600:PRO:HD2	1.82	0.40
2:B:1065:GLN:NE2	2:B:1067:ARG:HB2	2.28	0.40
1:A:497:THR:HG21	2:B:1149:GLU:OE1	2.20	0.40
2:B:361:LEU:N	2:B:362:PRO:CD	2.85	0.40
2:B:840:ILE:HB	2:B:1011:ILE:HB	2.03	0.40
3:C:11:ARG:NE	3:C:209:TYR:CE2	2.89	0.40
4:E:43:LYS:O	4:E:47:CYS:HB3	2.21	0.40
1:A:1003:LYS:CG	1:A:1003:LYS:HA	2.43	0.40
1:A:127:ALA:O	1:A:128:ILE:C	2.59	0.40
1:A:35:ILE:H	1:A:35:ILE:HG13	1.65	0.40
2:B:121:ASN:HD21	2:B:965:LYS:CE	2.35	0.40
2:B:165:VAL:O	2:B:165:VAL:HG12	2.20	0.40
3:C:29:MET:CB	3:C:29:MET:HE2	2.52	0.40
4:E:61:GLN:HE21	4:E:63:ASN:HD21	1.68	0.40
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.84	0.40
1:A:1259:MET:O	1:A:1260:LEU:C	2.58	0.40
1:A:35:ILE:HA	1:A:52:GLY:O	2.22	0.40
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.35	0.40
2:B:270:LYS:HB3	2:B:279:ASP:HB3	2.02	0.40
2:B:291:ILE:O	2:B:297:ILE:CD1	2.67	0.40
1:A:771:GLU:CD	2:B:510:LYS:HZ3	2.24	0.40
2:B:458:LYS:HZ1	2:B:958:GLN:NE2	2.18	0.40
4:E:76:GLY:HA3	4:E:106:GLN:HB3	2.02	0.40
4:E:28:TYR:CE1	4:E:75:MET:CE	3.04	0.40
7:I:10:CYS:SG	7:I:31:THR:CG2	3.10	0.40
8:J:53:HIS:C	8:J:53:HIS:HD1	2.24	0.40
3:C:248:ILE:HD12	9:K:101:LEU:HD12	2.03	0.40
9:K:42:LEU:HA	9:K:42:LEU:HD12	1.64	0.40
10:L:29:TYR:O	10:L:30:ILE:HG13	2.21	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 X-ray entries followed by that with respect to entries of similar resolution.

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	1334/1733 (77%)	1196 (90%)	84 (6%)	54 (4%)	3	17
2	B	1071/1224 (88%)	931 (87%)	104 (10%)	36 (3%)	3	20
3	C	264/318 (83%)	225 (85%)	30 (11%)	9 (3%)	3	20
4	E	213/215 (99%)	181 (85%)	20 (9%)	12 (6%)	2	10
5	F	81/155 (52%)	72 (89%)	8 (10%)	1 (1%)	13	48
6	H	129/146 (88%)	89 (69%)	17 (13%)	23 (18%)	0	0
7	I	119/122 (98%)	108 (91%)	10 (8%)	1 (1%)	19	57
8	J	62/70 (89%)	60 (97%)	2 (3%)	0	100	100
9	K	112/120 (93%)	99 (88%)	10 (9%)	3 (3%)	5	26
10	L	44/70 (63%)	25 (57%)	11 (25%)	8 (18%)	0	0
All	All	3429/4173 (82%)	2986 (87%)	296 (9%)	147 (4%)	2	15

All (147) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	45	GLN
1	A	47	ARG
1	A	59	GLY
1	A	62	ASP
1	A	65	LEU
1	A	69	THR
1	A	72	GLU
1	A	74	MET
1	A	120	GLU
1	A	155	GLU
1	A	156	ASP
1	A	157	ASP
1	A	165	GLY

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Mol	Chain	Res	Type
1	A	190	ALA
1	A	286	HIS
1	A	418	SER
1	A	465	TYR
1	A	567	LYS
1	A	707	GLY
1	A	752	LYS
1	A	885	THR
1	A	1080	THR
1	A	1221	LYS
1	A	1448	GLU
2	B	66	ASP
2	B	105	SER
2	B	108	VAL
2	B	109	THR
2	B	165	VAL
2	B	230	ALA
2	B	436	VAL
2	B	645	SER
2	B	646	LEU
2	B	733	HIS
2	B	864	LYS
2	B	879	ARG
2	B	957	ASN
2	B	1108	ARG
2	B	1128	LEU
2	B	1167	GLY
3	C	4	GLU
3	C	9	LYS
3	C	206	ASN
4	E	48	ASP
4	E	64	PRO
4	E	118	PRO
5	F	73	ALA
6	H	32	THR
6	H	52	GLN
6	H	53	ASP
6	H	78	SER
6	H	90	ALA
6	H	104	PHE
6	H	105	GLU
6	H	116	TYR

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Mol	Chain	Res	Type
6	H	136	LYS
7	I	4	PHE
9	K	111	LEU
10	L	28	LYS
10	L	45	ALA
10	L	50	ASP
1	A	56	PRO
1	A	57	ARG
1	A	158	PRO
1	A	167	CYS
1	A	279	LEU
1	A	326	ARG
1	A	464	PRO
1	A	672	ASP
1	A	975	HIS
1	A	1223	ASP
1	A	1359	ASP
2	B	266	ALA
2	B	432	MET
2	B	451	LYS
2	B	466	TRP
2	B	887	HIS
2	B	1097	HIS
2	B	1105	ALA
3	C	209	TYR
3	C	231	ASN
4	E	44	ALA
4	E	45	LYS
4	E	50	MET
4	E	126	SER
6	H	77	ARG
6	H	81	PRO
6	H	86	ASP
6	H	89	LEU
6	H	107	VAL
6	H	135	LEU
6	H	139	ASN
9	K	99	GLY
10	L	39	SER
10	L	58	LYS
1	A	38	PRO
1	A	60	SER

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Mol	Chain	Res	Type
1	A	278	THR
1	A	1002	GLY
1	A	1255	GLU
2	B	865	LYS
2	B	1155	SER
2	B	1190	ASP
3	C	267	GLN
4	E	74	ASP
6	H	82	PRO
6	H	83	GLN
6	H	128	ASN
9	K	50	LEU
10	L	41	SER
1	A	32	VAL
1	A	75	ASN
1	A	706	HIS
2	B	90	ILE
2	B	447	ALA
2	B	643	ASP
3	C	137	LYS
4	E	2	ASP
4	E	56	LYS
6	H	19	ARG
10	L	46	VAL
1	A	42	ASP
1	A	196	GLU
1	A	599	SER
1	A	958	VAL
1	A	1204	ASP
1	A	1280	GLU
2	B	19	GLU
2	B	137	TYR
2	B	424	LEU
2	B	831	SER
2	B	1189	ILE
4	E	59	SER
6	H	119	GLY
10	L	59	ALA
1	A	400	PRO
2	B	940	PRO
2	B	1017	ILE
3	C	217	ASP

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Mol	Chain	Res	Type
6	H	5	LEU
6	H	103	LYS
1	A	52	GLY
1	A	55	ASP
3	C	126	GLY
4	E	38	PRO
1	A	1123	GLY

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	1183/1520 (78%)	993 (84%)	190 (16%)	2	12
2	B	947/1061 (89%)	801 (85%)	146 (15%)	2	13
3	C	234/274 (85%)	194 (83%)	40 (17%)	2	10
4	E	197/197 (100%)	153 (78%)	44 (22%)	1	4
5	F	73/137 (53%)	62 (85%)	11 (15%)	3	14
6	H	117/128 (91%)	74 (63%)	43 (37%)	0	0
7	I	115/116 (99%)	93 (81%)	22 (19%)	1	8
8	J	59/65 (91%)	49 (83%)	10 (17%)	2	11
9	K	99/102 (97%)	83 (84%)	16 (16%)	2	12
10	L	40/57 (70%)	20 (50%)	20 (50%)	0	0
All	All	3064/3657 (84%)	2522 (82%)	542 (18%)	2	9

All (542) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	11	LEU
1	A	15	LYS
1	A	22	PHE
1	A	30	ILE
1	A	34	LYS

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Mol	Chain	Res	Type
1	A	36	ARG
1	A	39	GLU
1	A	44	THR
1	A	46	THR
1	A	49	LYS
1	A	58	LEU
1	A	60	SER
1	A	62	ASP
1	A	68	GLN
1	A	70	CYS
1	A	74	MET
1	A	81	PHE
1	A	84	ILE
1	A	90	VAL
1	A	93	VAL
1	A	98	LYS
1	A	106	VAL
1	A	110	CYS
1	A	112	LYS
1	A	114	LEU
1	A	120	GLU
1	A	121	LEU
1	A	122	MET
1	A	129	LYS
1	A	131	SER
1	A	138	ILE
1	A	144	THR
1	A	145	LYS
1	A	148	CYS
1	A	153	PRO
1	A	156	ASP
1	A	158	PRO
1	A	160	GLN
1	A	167	CYS
1	A	172	PRO
1	A	173	THR
1	A	176	LYS
1	A	191	THR
1	A	193	ASP
1	A	195	ASP
1	A	197	PRO
1	A	198	GLU

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Mol	Chain	Res	Type
1	A	206	GLU
1	A	215	SER
1	A	230	ARG
1	A	231	PRO
1	A	235	ILE
1	A	239	LEU
1	A	247	ARG
1	A	261	ASP
1	A	263	THR
1	A	265	LYS
1	A	268	ASP
1	A	269	ILE
1	A	270	LEU
1	A	275	SER
1	A	286	HIS
1	A	294	SER
1	A	328	ARG
1	A	329	LEU
1	A	346	ASP
1	A	351	THR
1	A	354	SER
1	A	368	LYS
1	A	385	ILE
1	A	409	SER
1	A	416	ARG
1	A	419	LYS
1	A	434	ARG
1	A	451	HIS
1	A	461	LYS
1	A	466	SER
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	493	GLN
1	A	495	GLU
1	A	498	ARG
1	A	504	LEU
1	A	508	PRO
1	A	513	SER
1	A	531	ILE
1	A	535	THR
1	A	537	ARG

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Mol	Chain	Res	Type
1	A	543	LEU
1	A	571	LEU
1	A	588	LEU
1	A	590	ARG
1	A	597	LEU
1	A	599	SER
1	A	618	GLU
1	A	622	VAL
1	A	626	ASN
1	A	636	GLU
1	A	666	ILE
1	A	679	ILE
1	A	681	GLU
1	A	683	ILE
1	A	688	LYS
1	A	702	LEU
1	A	703	THR
1	A	705	LYS
1	A	708	MET
1	A	709	THR
1	A	710	LEU
1	A	720	ARG
1	A	724	GLU
1	A	728	LYS
1	A	741	ASN
1	A	794	PRO
1	A	810	PRO
1	A	821	ARG
1	A	830	LYS
1	A	843	LYS
1	A	858	ASN
1	A	882	SER
1	A	885	THR
1	A	895	LYS
1	A	903	ASN
1	A	907	THR
1	A	909	ASP
1	A	918	GLU
1	A	920	LEU
1	A	940	ARG
1	A	964	ILE
1	A	973	ILE

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Mol	Chain	Res	Type
1	A	974	ASP
1	A	979	SER
1	A	982	THR
1	A	1003	LYS
1	A	1006	ILE
1	A	1015	VAL
1	A	1030	ARG
1	A	1064	VAL
1	A	1078	GLN
1	A	1081	LEU
1	A	1092	LYS
1	A	1093	LYS
1	A	1096	SER
1	A	1102	LYS
1	A	1109	LYS
1	A	1129	GLU
1	A	1138	ILE
1	A	1146	VAL
1	A	1161	THR
1	A	1165	GLU
1	A	1171	GLN
1	A	1172	LEU
1	A	1176	LEU
1	A	1187	GLN
1	A	1204	ASP
1	A	1208	THR
1	A	1217	LYS
1	A	1225	PHE
1	A	1230	GLU
1	A	1235	LYS
1	A	1236	LEU
1	A	1237	ILE
1	A	1239	ARG
1	A	1258	HIS
1	A	1259	MET
1	A	1267	MET
1	A	1269	GLU
1	A	1277	GLU
1	A	1281	ARG
1	A	1293	SER
1	A	1309	ASP
1	A	1317	MET

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Mol	Chain	Res	Type
1	A	1318	THR
1	A	1325	THR
1	A	1327	ILE
1	A	1335	ILE
1	A	1359	ASP
1	A	1361	SER
1	A	1366	ARG
1	A	1376	THR
1	A	1377	THR
1	A	1384	VAL
1	A	1405	THR
1	A	1426	GLU
1	A	1438	THR
1	A	1445	ILE
1	A	1448	GLU
1	A	1449	SER
2	B	18	PHE
2	B	20	ASP
2	B	25	ILE
2	B	46	GLN
2	B	65	GLU
2	B	68	THR
2	B	69	LEU
2	B	70	ILE
2	B	89	GLU
2	B	92	PHE
2	B	98	THR
2	B	102	VAL
2	B	106	ASP
2	B	128	LEU
2	B	130	VAL
2	B	133	LYS
2	B	134	LYS
2	B	136	THR
2	B	138	GLU
2	B	164	LYS
2	B	167	ILE
2	B	178	ASN
2	B	179	CYS
2	B	183	GLU
2	B	194	GLU
2	B	199	MET

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Mol	Chain	Res	Type
2	B	204	ILE
2	B	217	ARG
2	B	228	LYS
2	B	239	GLU
2	B	242	SER
2	B	244	LEU
2	B	248	SER
2	B	252	SER
2	B	261	ARG
2	B	264	SER
2	B	277	LYS
2	B	282	ILE
2	B	358	LYS
2	B	367	LEU
2	B	373	ARG
2	B	384	ARG
2	B	387	LEU
2	B	417	PHE
2	B	422	LYS
2	B	423	LYS
2	B	425	THR
2	B	434	ARG
2	B	435	THR
2	B	463	THR
2	B	466	TRP
2	B	485	ARG
2	B	487	THR
2	B	498	THR
2	B	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	524	PRO
2	B	531	GLN
2	B	547	VAL
2	B	549	THR
2	B	550	ASP
2	B	566	LEU
2	B	567	GLU
2	B	589	VAL
2	B	591	ARG
2	B	595	ARG
2	B	598	GLU

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Mol	Chain	Res	Type
2	B	606	LYS
2	B	614	SER
2	B	639	ILE
2	B	641	GLU
2	B	645	SER
2	B	648	HIS
2	B	650	GLU
2	B	653	VAL
2	B	666	TYR
2	B	680	THR
2	B	691	GLU
2	B	706	GLN
2	B	710	LEU
2	B	722	ASP
2	B	723	VAL
2	B	730	ARG
2	B	733	HIS
2	B	736	THR
2	B	775	LYS
2	B	788	ARG
2	B	806	THR
2	B	838	SER
2	B	846	ILE
2	B	857	ARG
2	B	863	GLU
2	B	864	LYS
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	879	ARG
2	B	881	ASN
2	B	882	THR
2	B	883	LEU
2	B	884	ARG
2	B	889	THR
2	B	895	ASP
2	B	896	ASP
2	B	908	GLU
2	B	914	LYS
2	B	933	SER
2	B	938	SER
2	B	955	THR

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Mol	Chain	Res	Type
2	B	956	THR
2	B	958	GLN
2	B	962	LYS
2	B	964	VAL
2	B	975	GLN
2	B	987	LYS
2	B	996	ARG
2	B	997	GLU
2	B	1007	VAL
2	B	1010	LEU
2	B	1055	ILE
2	B	1056	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1077	THR
2	B	1097	HIS
2	B	1099	VAL
2	B	1101	ASP
2	B	1106	ARG
2	B	1150	ARG
2	B	1152	MET
2	B	1155	SER
2	B	1156	ASP
2	B	1159	ARG
2	B	1165	ILE
2	B	1166	CYS
2	B	1174	LYS
2	B	1179	GLN
2	B	1182	CYS
2	B	1183	LYS
2	B	1185	CYS
2	B	1187	ASN
2	B	1211	ASN
2	B	1220	ARG
2	B	1222	ARG
2	B	1224	PHE
3	C	3	GLU
3	C	4	GLU
3	C	9	LYS
3	C	14	SER
3	C	23	SER
3	C	25	VAL

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Mol	Chain	Res	Type
3	C	26	ASP
3	C	29	MET
3	C	33	LEU
3	C	43	THR
3	C	56	THR
3	C	57	VAL
3	C	77	ILE
3	C	86	CYS
3	C	93	ASP
3	C	102	GLN
3	C	119	VAL
3	C	125	MET
3	C	127	ARG
3	C	132	PRO
3	C	137	LYS
3	C	154	LYS
3	C	163	ILE
3	C	178	PHE
3	C	184	ASN
3	C	185	LYS
3	C	186	LEU
3	C	197	SER
3	C	205	LYS
3	C	209	TYR
3	C	214	ASN
3	C	238	ILE
3	C	240	VAL
3	C	245	VAL
3	C	251	LEU
3	C	264	GLN
3	C	265	MET
3	C	266	ASP
3	C	267	GLN
3	C	268	ASP
4	E	3	GLN
4	E	10	SER
4	E	14	ARG
4	E	33	GLU
4	E	34	GLU
4	E	36	GLU
4	E	37	LEU
4	E	47	CYS

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Mol	Chain	Res	Type
4	E	49	SER
4	E	50	MET
4	E	52	ARG
4	E	57	MET
4	E	60	PHE
4	E	61	GLN
4	E	69	ILE
4	E	70	SER
4	E	72	PHE
4	E	74	ASP
4	E	78	LEU
4	E	81	GLU
4	E	82	PHE
4	E	84	ASP
4	E	91	LYS
4	E	92	THR
4	E	95	THR
4	E	101	GLN
4	E	103	LYS
4	E	107	THR
4	E	116	ILE
4	E	119	SER
4	E	121	MET
4	E	123	LEU
4	E	129	PRO
4	E	137	GLU
4	E	149	LEU
4	E	158	SER
4	E	159	ASP
4	E	161	LYS
4	E	162	ARG
4	E	171	LYS
4	E	192	ARG
4	E	200	ARG
4	E	204	THR
4	E	212	ARG
5	F	72	LYS
5	F	77	ASP
5	F	79	ARG
5	F	81	THR
5	F	82	THR
5	F	87	LYS

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Mol	Chain	Res	Type
5	F	97	ARG
5	F	110	ASP
5	F	111	LEU
5	F	117	PRO
5	F	119	ARG
6	H	4	THR
6	H	5	LEU
6	H	6	PHE
6	H	7	ASP
6	H	9	ILE
6	H	13	SER
6	H	27	GLU
6	H	34	ASP
6	H	35	GLN
6	H	36	CYS
6	H	40	LEU
6	H	42	ILE
6	H	45	GLU
6	H	46	LEU
6	H	52	GLN
6	H	53	ASP
6	H	54	SER
6	H	56	THR
6	H	63	LEU
6	H	77	ARG
6	H	78	SER
6	H	80	ARG
6	H	86	ASP
6	H	87	ARG
6	H	88	SER
6	H	89	LEU
6	H	91	ASP
6	H	92	ASP
6	H	93	TYR
6	H	105	GLU
6	H	106	GLU
6	H	108	SER
6	H	109	LYS
6	H	111	LEU
6	H	112	ILE
6	H	121	LEU
6	H	126	GLU

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Mol	Chain	Res	Type
6	H	129	TYR
6	H	130	ARG
6	H	131	ASN
6	H	136	LYS
6	H	144	ILE
6	H	145	ARG
7	I	1	MET
7	I	2	THR
7	I	4	PHE
7	I	10	CYS
7	I	18	GLU
7	I	31	THR
7	I	40	SER
7	I	45	ARG
7	I	46	HIS
7	I	55	THR
7	I	61	ASP
7	I	76	PRO
7	I	77	LYS
7	I	78	CYS
7	I	82	GLU
7	I	84	VAL
7	I	95	THR
7	I	116	ASN
7	I	117	LYS
7	I	118	ARG
7	I	119	THR
7	I	120	GLN
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	14	VAL
8	J	20	SER
8	J	28	ASP
8	J	38	ARG
8	J	48	ARG
8	J	62	ARG
8	J	64	ASN
9	K	1	MET
9	K	2	ASN
9	K	11	LEU
9	K	18	LYS

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Mol	Chain	Res	Type
9	K	20	LYS
9	K	31	VAL
9	K	42	LEU
9	K	47	ARG
9	K	63	VAL
9	K	73	LEU
9	K	75	ILE
9	K	78	THR
9	K	93	SER
9	K	112	GLN
9	K	113	THR
9	K	114	LEU
10	L	27	LEU
10	L	28	LYS
10	L	33	GLU
10	L	36	SER
10	L	42	ARG
10	L	44	ASP
10	L	46	VAL
10	L	47	ARG
10	L	48	CYS
10	L	49	LYS
10	L	50	ASP
10	L	51	CYS
10	L	54	ARG
10	L	58	LYS
10	L	60	ARG
10	L	61	THR
10	L	63	ARG
10	L	64	LEU
10	L	65	VAL
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	92	HIS
1	A	171	GLN
1	A	299	HIS
1	A	390	GLN
1	A	399	HIS

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Mol	Chain	Res	Type
1	A	451	HIS
1	A	479	ASN
1	A	503	GLN
1	A	515	GLN
1	A	517	ASN
1	A	587	HIS
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	768	GLN
1	A	786	HIS
1	A	854	ASN
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	994	GLN
1	A	1078	GLN
1	A	1124	HIS
1	A	1173	HIS
1	A	1364	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	325	GLN
2	B	357	GLN
2	B	366	GLN
2	B	383	ASN
2	B	433	GLN
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	538	ASN
2	B	587	HIS
2	B	590	HIS
2	B	657	HIS
2	B	706	GLN
2	B	744	HIS
2	B	843	GLN
2	B	862	GLN
2	B	878	GLN

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Mol	Chain	Res	Type
2	B	958	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1025	HIS
2	B	1062	HIS
2	B	1065	GLN
2	B	1084	GLN
2	B	1093	GLN
2	B	1161	HIS
2	B	1179	GLN
2	B	1187	ASN
3	C	73	GLN
3	C	112	ASN
3	C	167	HIS
3	C	242	GLN
3	C	252	GLN
4	E	5	ASN
4	E	61	GLN
4	E	113	GLN
4	E	147	HIS
6	H	11	GLN
6	H	131	ASN
6	H	133	ASN
7	I	12	ASN
7	I	83	ASN
7	I	116	ASN
8	J	53	HIS
9	K	2	ASN
9	K	65	HIS
9	K	76	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	GTP	B	3008	2,12	26,34,34	1.73	4 (15%)	33,54,54	3.87	10 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GTP	B	3008	2,12	1/1/7/7	8/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	3008	GTP	C8-N7	-4.67	1.26	1.34
13	B	3008	GTP	C4-N3	4.00	1.41	1.35
13	B	3008	GTP	C6-N1	3.88	1.39	1.33
13	B	3008	GTP	C6-C5	3.38	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	3008	GTP	C1'-N9-C4	18.32	158.82	126.64
13	B	3008	GTP	C5-C6-N1	-7.25	113.51	123.43
13	B	3008	GTP	C6-N1-C2	4.91	123.73	115.93
13	B	3008	GTP	O4'-C1'-C2'	4.26	113.16	106.93
13	B	3008	GTP	PA-O3A-PB	-3.55	120.63	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	3008	GTP	PB-O3B-PG	-3.43	121.06	132.83
13	B	3008	GTP	N2-C2-N1	-2.68	113.09	117.25
13	B	3008	GTP	C2'-C3'-C4'	2.37	107.25	102.64
13	B	3008	GTP	N2-C2-N3	2.33	121.58	117.79
13	B	3008	GTP	C4-C5-N7	2.26	111.76	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	B	3008	GTP	C1'

All (8) torsion outliers are listed below:

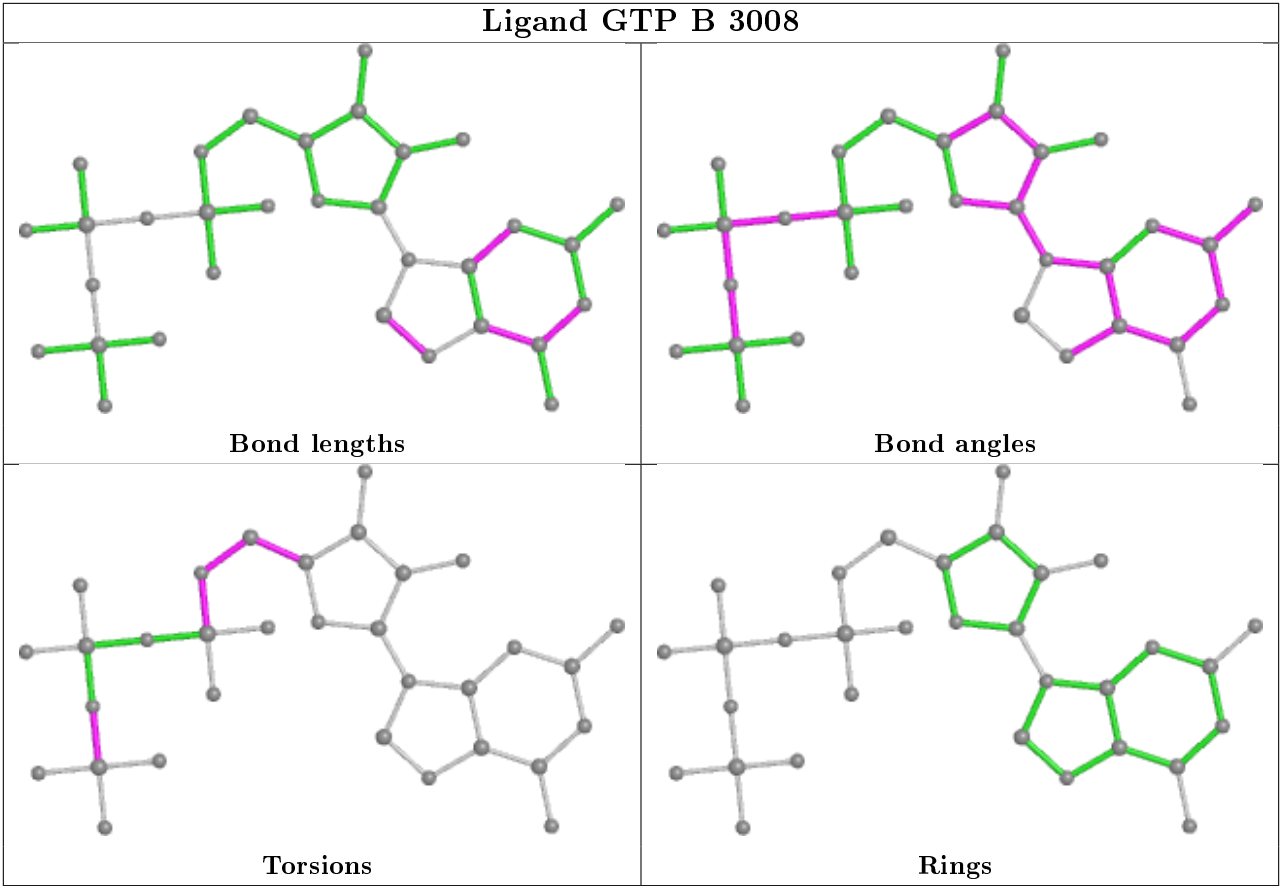
Mol	Chain	Res	Type	Atoms
13	B	3008	GTP	C5'-O5'-PA-O3A
13	B	3008	GTP	O4'-C4'-C5'-O5'
13	B	3008	GTP	C3'-C4'-C5'-O5'
13	B	3008	GTP	PB-O3B-PG-O2G
13	B	3008	GTP	C5'-O5'-PA-O2A
13	B	3008	GTP	C4'-C5'-O5'-PA
13	B	3008	GTP	PB-O3B-PG-O3G
13	B	3008	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	3008	GTP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	366:VAL	C	367:PRO	N	1.20

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1351/1733 (77%)	-0.44	23 (1%) 70 41	20, 46, 110, 159	0
2	B	1091/1224 (89%)	-0.34	37 (3%) 45 19	21, 44, 116, 146	0
3	C	266/318 (83%)	-0.51	2 (0%) 86 65	29, 50, 79, 131	0
4	E	215/215 (100%)	-0.35	5 (2%) 60 31	23, 60, 108, 138	0
5	F	83/155 (53%)	-0.50	0 100 100	24, 45, 71, 80	0
6	H	133/146 (91%)	0.06	4 (3%) 50 22	56, 88, 128, 135	0
7	I	121/122 (99%)	-0.44	1 (0%) 86 65	30, 50, 81, 111	0
8	J	64/70 (91%)	-0.59	0 100 100	31, 42, 71, 81	0
9	K	114/120 (95%)	-0.41	0 100 100	31, 58, 79, 86	0
10	L	46/70 (65%)	0.15	4 (8%) 10 3	49, 95, 122, 125	0
All	All	3484/4173 (83%)	-0.38	76 (2%) 62 33	20, 49, 113, 159	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1109	GLY	7.4
2	B	246	LYS	7.4
2	B	882	THR	7.0
1	A	44	THR	6.8
1	A	188	ASP	6.4
1	A	69	THR	6.0
2	B	870	ILE	5.6
1	A	248	PRO	5.5
2	B	1223	ASP	5.4
2	B	1110	PRO	5.3
6	H	85	GLY	5.2
2	B	1106	ARG	5.1
2	B	247	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	45	GLN	5.0
2	B	1105	ALA	4.9
1	A	1450	LEU	4.8
1	A	191	THR	4.8
3	C	268	ASP	4.5
6	H	132	LEU	4.1
2	B	734	HIS	3.9
10	L	25	ALA	3.7
1	A	190	ALA	3.6
2	B	1176	ASN	3.6
4	E	1	MET	3.6
2	B	1104	HIS	3.6
10	L	43	THR	3.5
2	B	245	GLU	3.4
2	B	869	SER	3.4
3	C	267	GLN	3.4
6	H	131	ASN	3.4
1	A	192	GLY	3.3
2	B	868	MET	3.2
2	B	883	LEU	3.2
1	A	43	GLU	3.2
2	B	137	TYR	3.1
2	B	888	GLY	3.1
2	B	89	GLU	3.1
2	B	733	HIS	3.0
1	A	189	ARG	3.0
1	A	1449	SER	2.9
4	E	2	ASP	2.9
2	B	135	ARG	2.8
2	B	1179	GLN	2.8
2	B	436	VAL	2.8
1	A	1092	LYS	2.8
2	B	136	THR	2.7
10	L	26	THR	2.7
2	B	1108	ARG	2.7
1	A	1222	ASN	2.7
2	B	1221	SER	2.6
2	B	1101	ASP	2.6
1	A	1448	GLU	2.6
4	E	50	MET	2.6
2	B	1102	LYS	2.6
2	B	887	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLY	2.5
1	A	833	GLU	2.5
2	B	871	THR	2.5
7	I	79	HIS	2.4
1	A	157	ASP	2.4
2	B	866	TYR	2.4
1	A	1080	THR	2.4
2	B	1224	PHE	2.4
1	A	193	ASP	2.3
2	B	432	MET	2.3
2	B	90	ILE	2.3
2	B	1155	SER	2.3
1	A	37	PHE	2.2
2	B	1189	ILE	2.1
1	A	1173	HIS	2.1
4	E	3	GLN	2.1
4	E	52	ARG	2.1
10	L	45	ALA	2.1
2	B	131	ASP	2.1
1	A	8	SER	2.1
6	H	35	GLN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

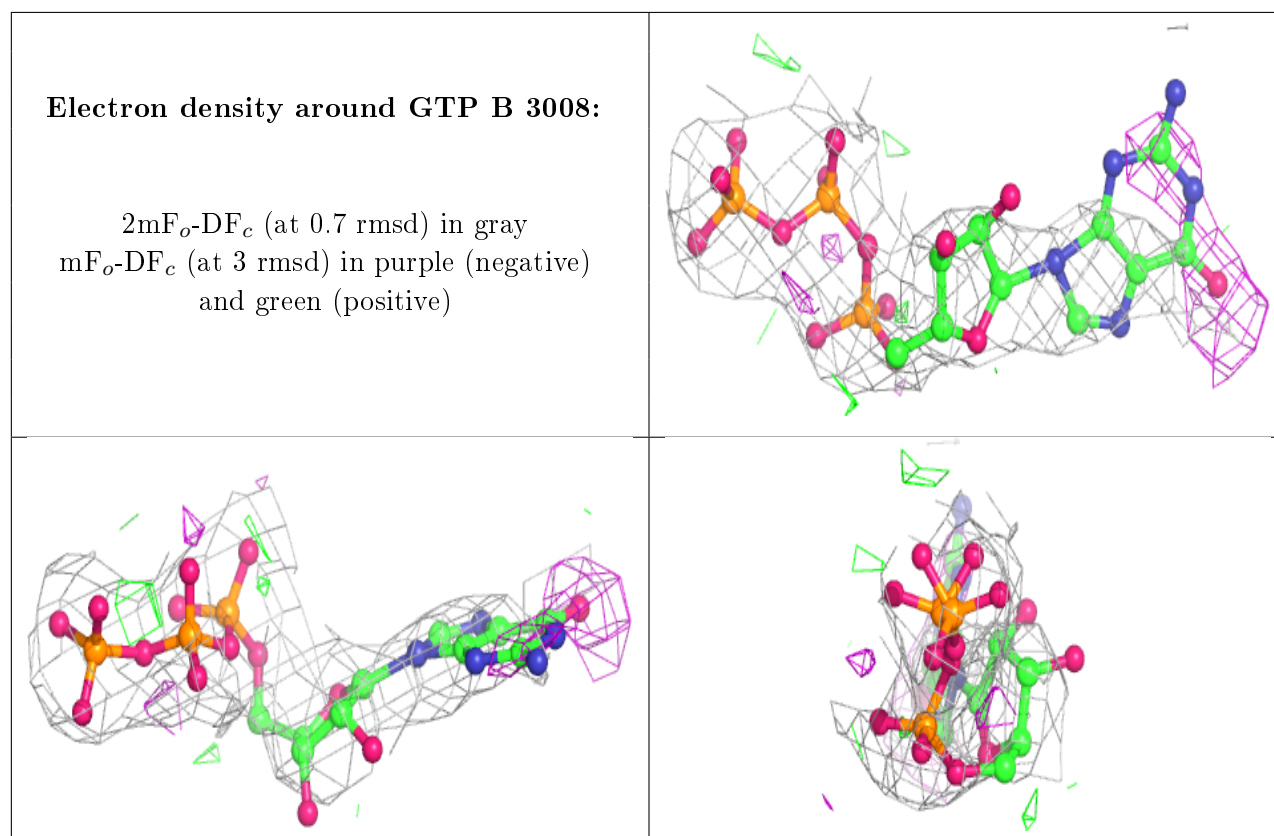
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	MN	A	3010	1/1	0.85	0.13	48,48,48,48	0
13	GTP	B	3008	32/32	0.90	0.23	96,112,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	ZN	A	3006	1/1	0.93	0.12	67,67,67,67	0
11	ZN	L	3005	1/1	0.93	0.09	96,96,96,96	0
11	ZN	B	3007	1/1	0.96	0.11	64,64,64,64	0
12	MN	A	3009	1/1	0.97	0.13	36,36,36,36	0
11	ZN	A	3008	1/1	0.98	0.12	91,91,91,91	0
11	ZN	I	3004	1/1	0.99	0.05	80,80,80,80	0
11	ZN	J	3001	1/1	0.99	0.16	47,47,47,47	0
11	ZN	C	3002	1/1	0.99	0.09	53,53,53,53	0
11	ZN	I	3003	1/1	0.99	0.12	59,59,59,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.