



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 01:49 AM EDT

PDB ID : 6DHK
Title : Bovine glutamate dehydrogenase complexed with ADP
Authors : Smith, T.J.
Deposited on : 2018-05-20
Resolution : 3.50 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

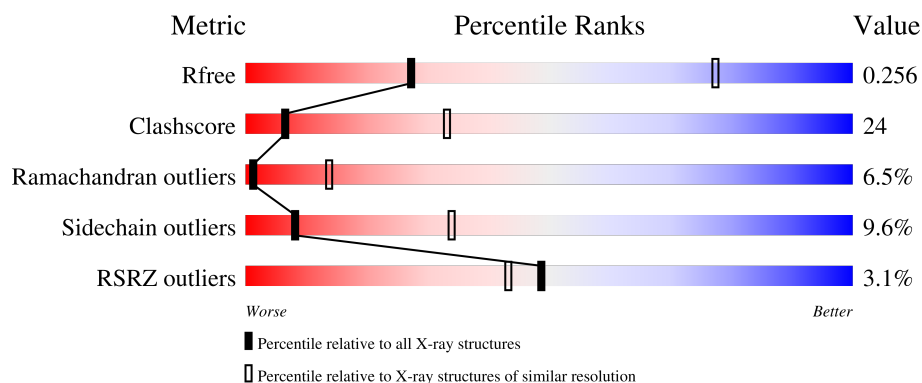
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	496	<div> <div>4%</div> <div>56% 32% 7% 5%</div> </div>
1	B	496	<div> <div>3%</div> <div>55% 32% 8% 5%</div> </div>
1	C	496	<div> <div>4%</div> <div>54% 33% 8% 5%</div> </div>
1	D	496	<div> <div>3%</div> <div>55% 31% 9% 5%</div> </div>
1	E	496	<div> <div>%</div> <div>57% 30% 7% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	496	<div><div></div><div>3%</div><div>56%</div><div>33%</div><div>7%</div><div></div></div>
1	G	496	<div><div></div><div>2%</div><div>58%</div><div>32%</div><div>5%</div><div>5%</div></div>
1	H	496	<div><div></div><div>3%</div><div>57%</div><div>31%</div><div>8%</div><div></div></div>
1	I	496	<div><div></div><div>6%</div><div>51%</div><div>34%</div><div>9%</div><div>5%</div></div>
1	J	496	<div><div></div><div>%</div><div>56%</div><div>31%</div><div>8%</div><div></div></div>
1	K	496	<div><div></div><div>3%</div><div>53%</div><div>34%</div><div>9%</div><div></div></div>
1	L	496	<div><div></div><div>4%</div><div>54%</div><div>32%</div><div>8%</div><div>5%</div></div>

2 Entry composition

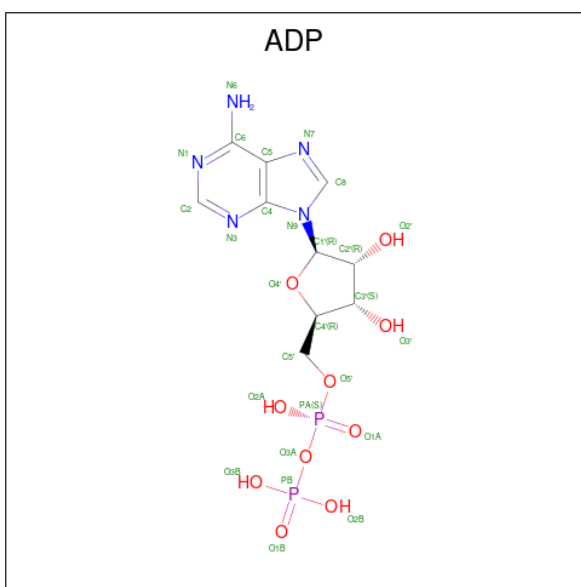
There are 2 unique types of molecules in this entry. The entry contains 46824 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate dehydrogenase 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3875	2451	679	726	19			
1	B	496	Total	C	N	O	S	0	0	0
			3875	2451	679	726	19			
1	C	496	Total	C	N	O	S	0	0	0
			3875	2451	679	726	19			
1	D	496	Total	C	N	O	S	0	0	0
			3875	2451	679	726	19			
1	E	496	Total	C	N	O	S	0	0	0
			3875	2451	679	726	19			
1	F	496	Total	C	N	O	S	0	0	0
			3875	2451	679	726	19			
1	G	496	Total	C	N	O	S	0	0	0
			3875	2451	679	726	19			
1	H	496	Total	C	N	O	S	0	0	0
			3875	2451	679	726	19			
1	I	496	Total	C	N	O	S	0	0	0
			3875	2451	679	726	19			
1	J	496	Total	C	N	O	S	0	0	0
			3875	2451	679	726	19			
1	K	496	Total	C	N	O	S	0	0	0
			3875	2451	679	726	19			
1	L	496	Total	C	N	O	S	0	0	0
			3875	2451	679	726	19			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

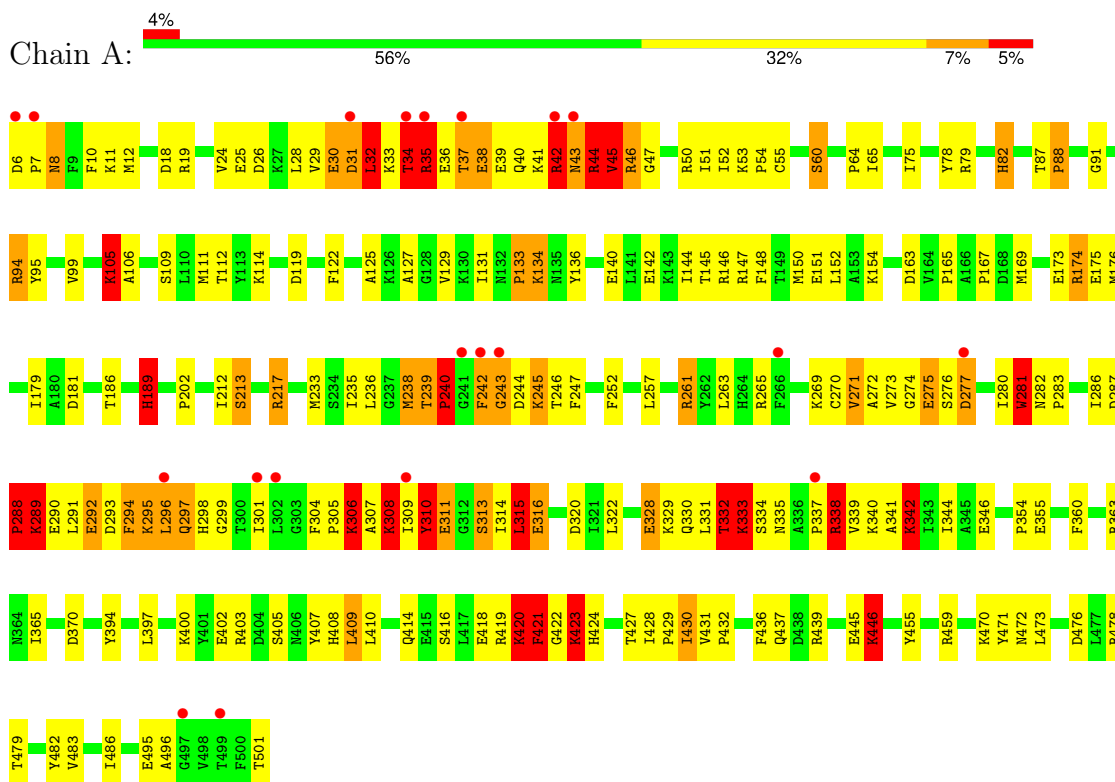


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	L	1	Total 27	C 10	N 5	O 10	P 2	0	0

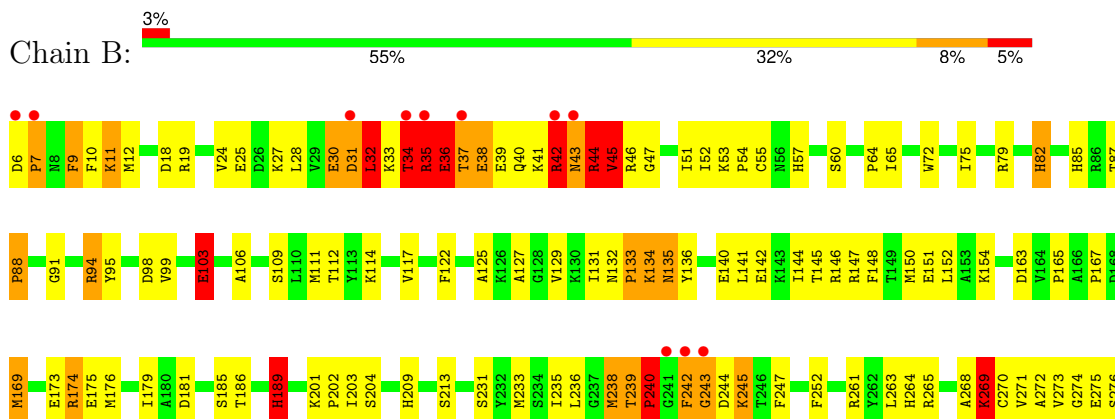
3 Residue-property plots

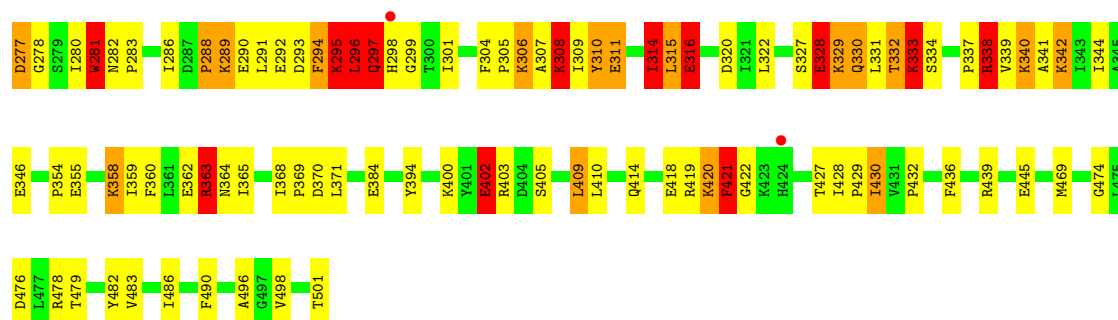
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutamate dehydrogenase 1, mitochondrial

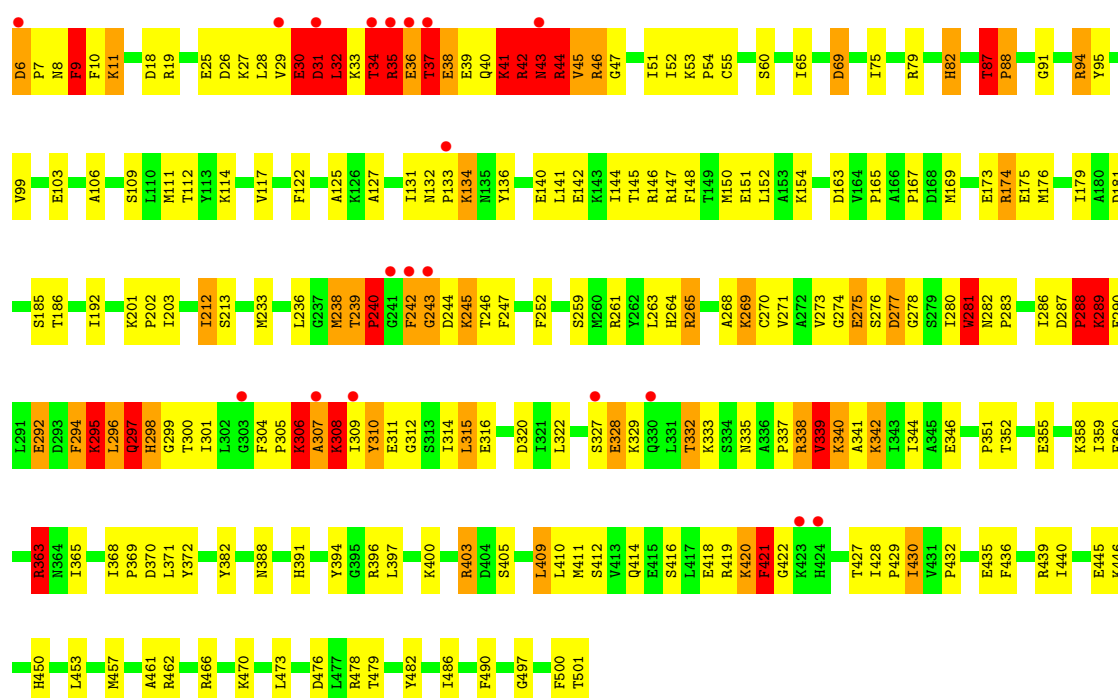


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

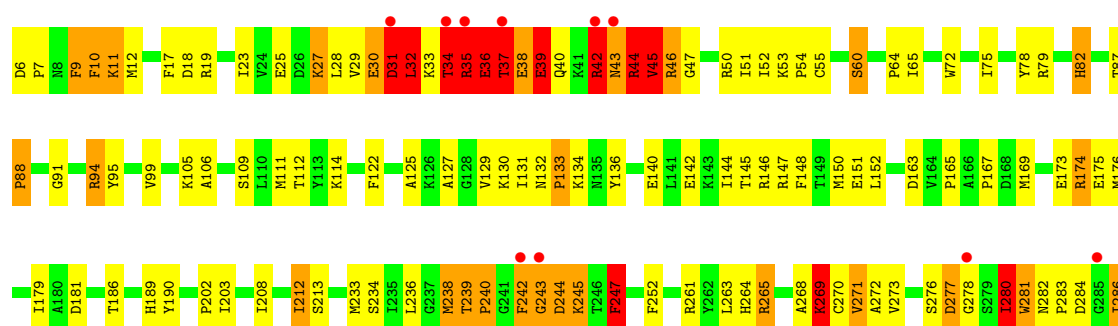


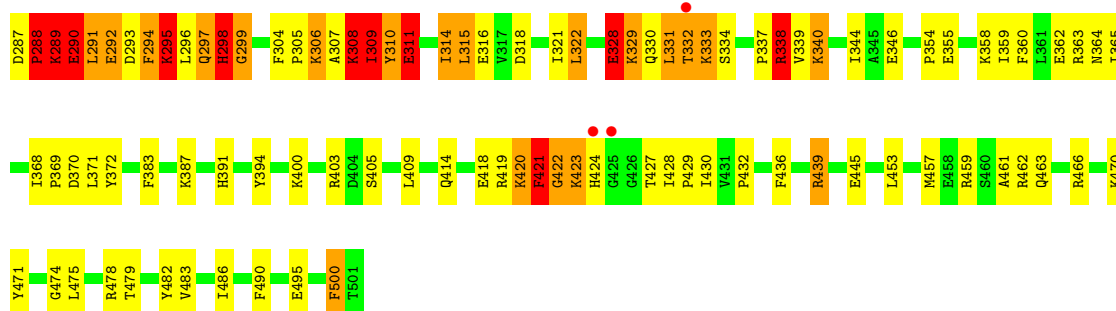


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

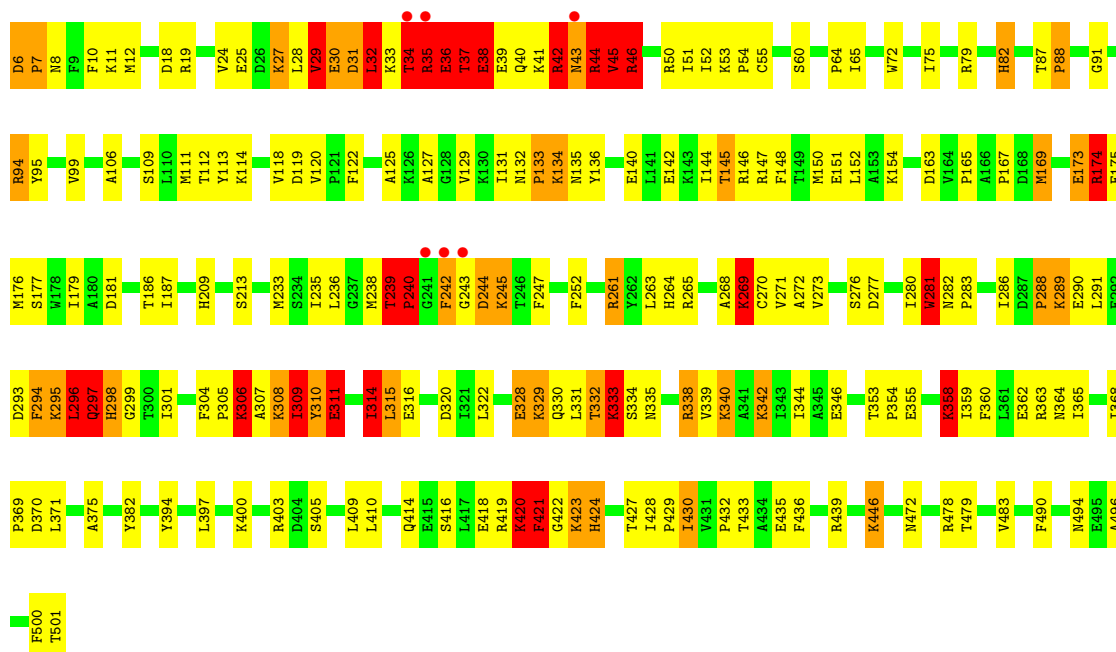


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

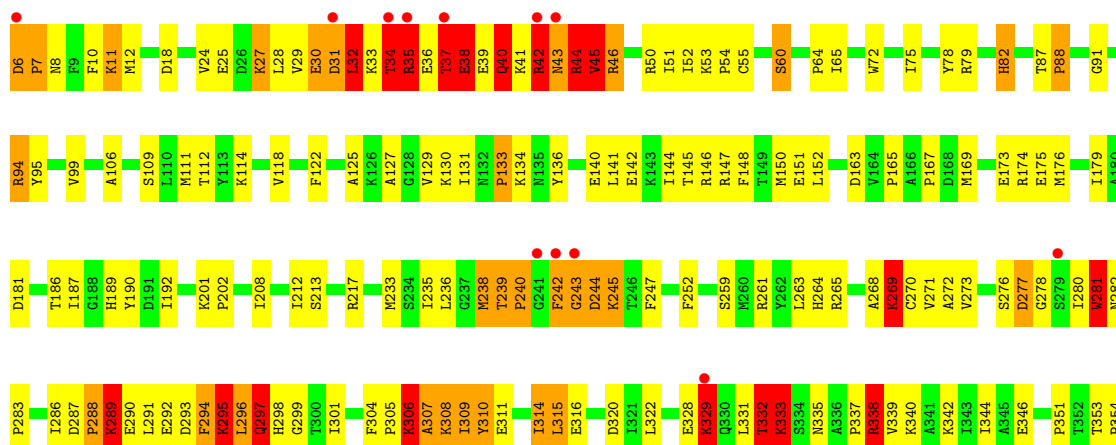


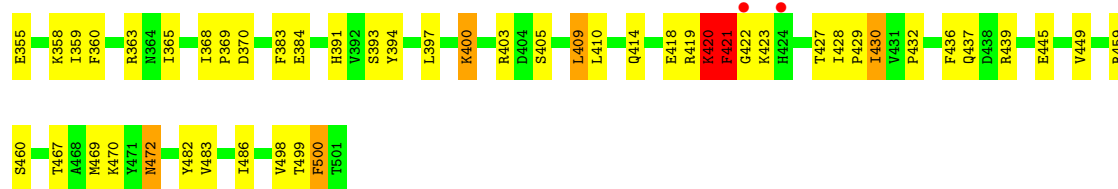


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

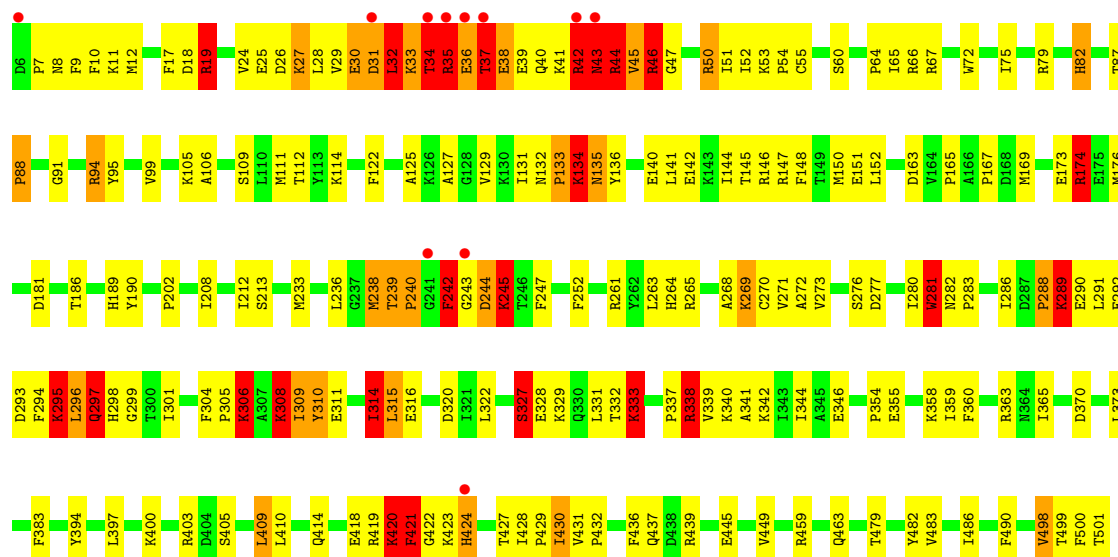


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

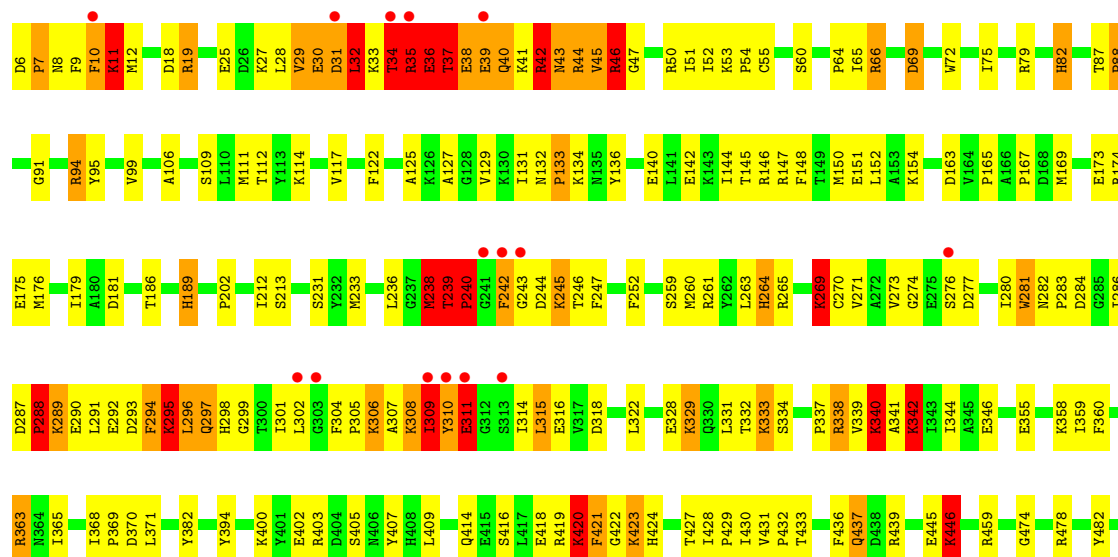




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

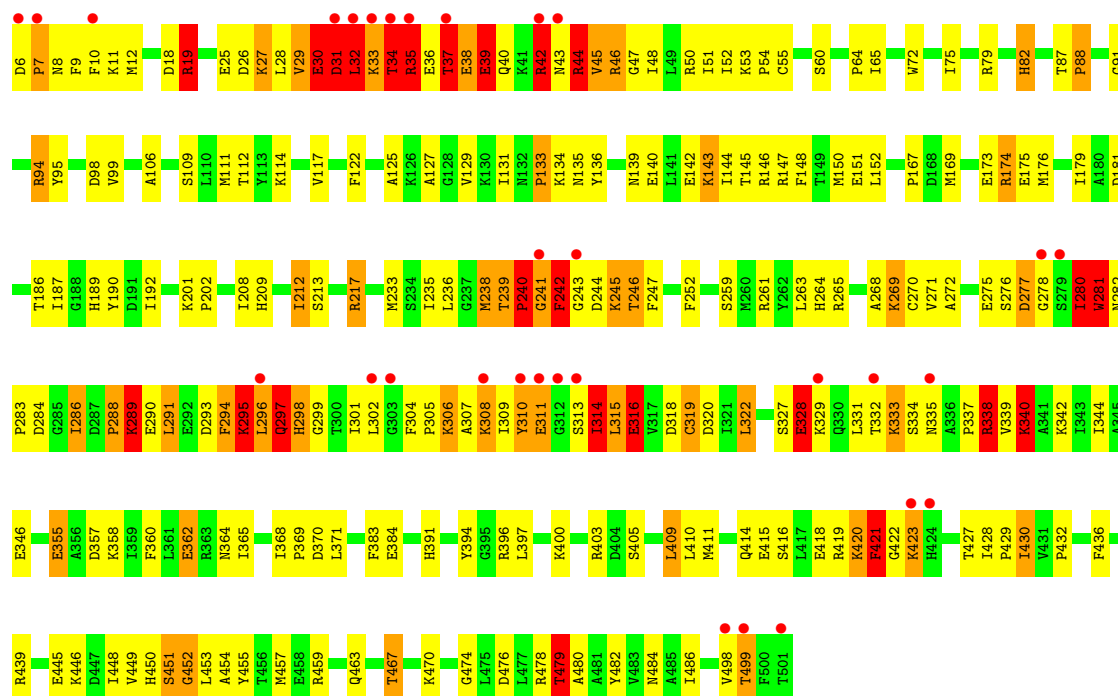


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

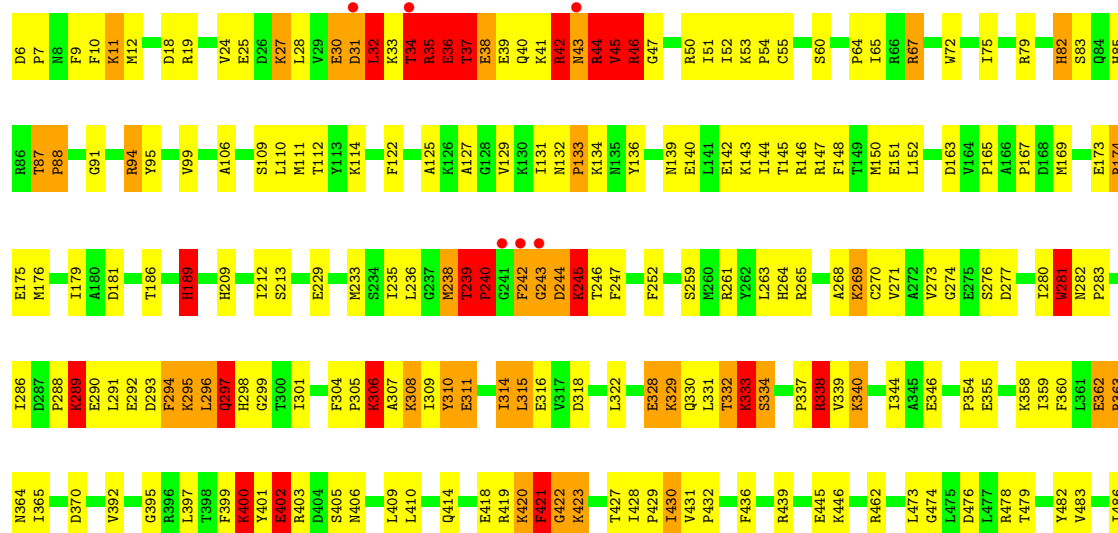




• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

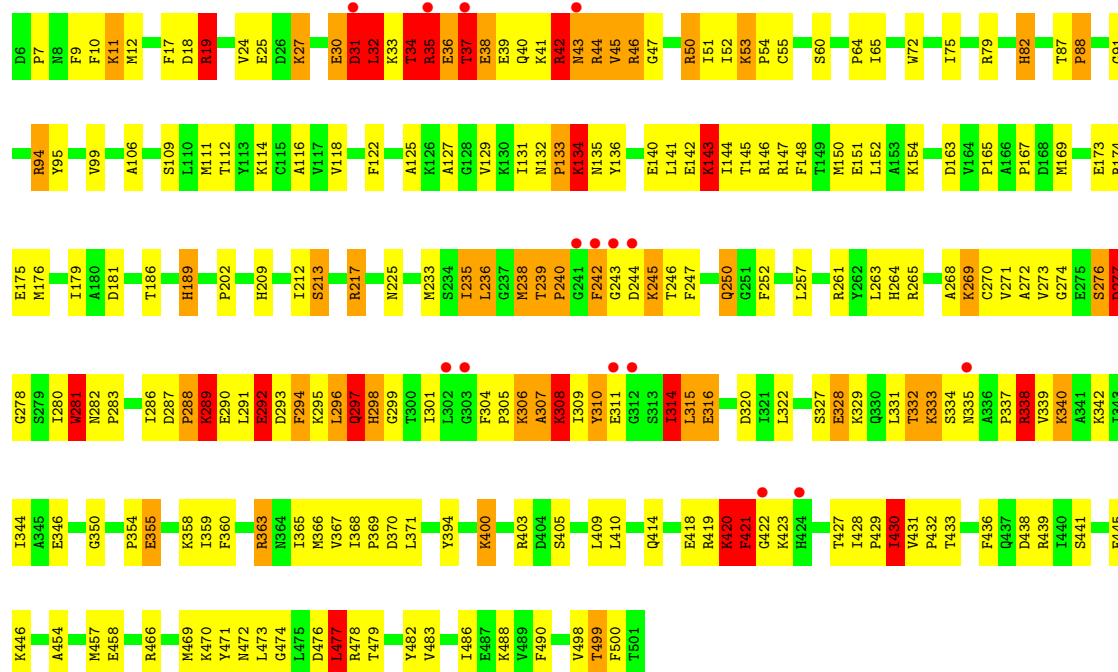


• Molecule 1: Glutamate dehydrogenase 1, mitochondrial

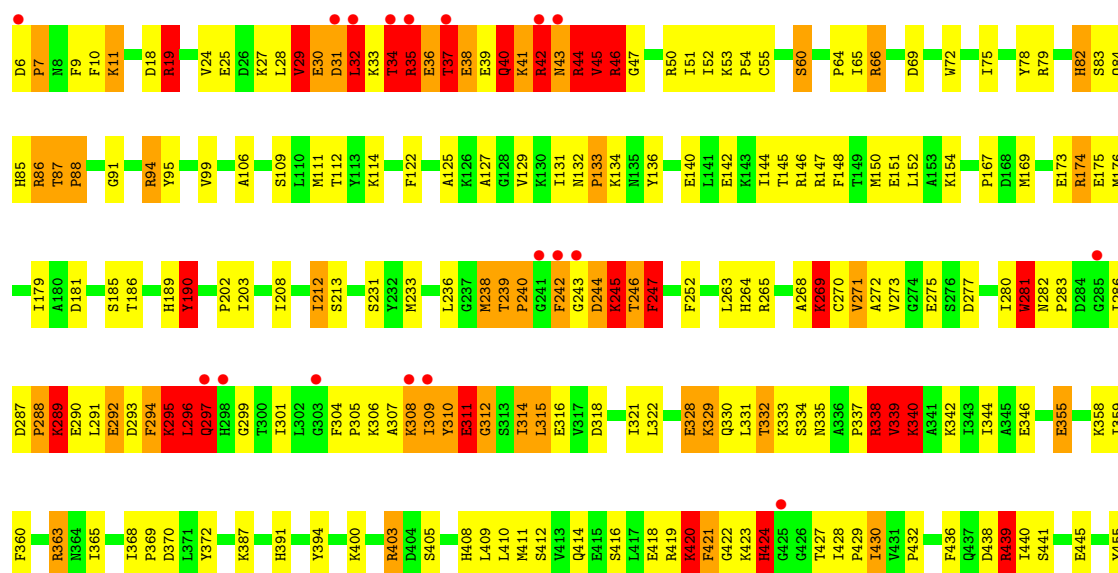




- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



- Molecule 1: Glutamate dehydrogenase 1, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.38Å 172.16Å 439.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 3.50 29.94 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.93-3.50) 94.0 (29.94-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 3.47Å)	Xtriage
Refinement program	PHENIX dev_1633	Depositor
R, R_{free}	0.216 , 0.254 0.221 , 0.256	Depositor DCC
R_{free} test set	2000 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å ²)	81.6	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	46824	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.16	40/3958 (1.0%)	1.62	75/5341 (1.4%)
1	B	1.16	41/3958 (1.0%)	1.43	77/5341 (1.4%)
1	C	1.08	31/3958 (0.8%)	1.34	60/5341 (1.1%)
1	D	1.23	45/3958 (1.1%)	1.56	70/5341 (1.3%)
1	E	1.11	41/3958 (1.0%)	1.49	71/5341 (1.3%)
1	F	1.02	23/3958 (0.6%)	1.35	68/5341 (1.3%)
1	G	1.12	40/3958 (1.0%)	1.53	91/5341 (1.7%)
1	H	1.06	38/3958 (1.0%)	1.37	76/5341 (1.4%)
1	I	1.19	39/3958 (1.0%)	1.63	81/5341 (1.5%)
1	J	1.05	41/3958 (1.0%)	1.51	63/5341 (1.2%)
1	K	1.10	34/3958 (0.9%)	1.50	81/5341 (1.5%)
1	L	1.13	35/3958 (0.9%)	1.66	87/5341 (1.6%)
All	All	1.12	448/47496 (0.9%)	1.50	900/64092 (1.4%)

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	14
1	B	0	16
1	C	0	15
1	D	0	16
1	E	0	16
1	F	1	17
1	G	0	14
1	H	0	11
1	I	0	19
1	J	0	13
1	K	0	15

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	18
All	All	1	184

All (448) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	GLU	CD-OE1	-22.14	1.01	1.25
1	B	30	GLU	CD-OE1	-19.86	1.03	1.25
1	I	328	GLU	CD-OE1	-19.63	1.04	1.25
1	E	261	ARG	CZ-NH1	-19.31	1.07	1.33
1	B	316	GLU	CD-OE1	-18.58	1.05	1.25
1	D	280	ILE	CB-CG2	-17.81	0.97	1.52
1	F	35	ARG	CD-NE	-17.48	1.16	1.46
1	A	35	ARG	CZ-NH2	-17.48	1.10	1.33
1	D	439	ARG	CZ-NH1	-17.39	1.10	1.33
1	I	35	ARG	CZ-NH2	-17.21	1.10	1.33
1	K	35	ARG	CZ-NH2	-17.08	1.10	1.33
1	F	35	ARG	CZ-NH2	-16.36	1.11	1.33
1	L	363	ARG	CZ-NH1	-16.04	1.12	1.33
1	L	265	ARG	CZ-NH1	-16.01	1.12	1.33
1	C	35	ARG	CD-NE	-15.98	1.19	1.46
1	B	35	ARG	CZ-NH2	-15.86	1.12	1.33
1	J	421	PHE	CD1-CE1	-14.80	1.09	1.39
1	K	35	ARG	CD-NE	-14.72	1.21	1.46
1	C	338	ARG	CG-CD	-14.62	1.15	1.51
1	G	42	ARG	CG-CD	-14.38	1.16	1.51
1	E	265	ARG	CZ-NH1	-14.36	1.14	1.33
1	G	35	ARG	CD-NE	-14.26	1.22	1.46
1	H	35	ARG	CZ-NH2	-14.23	1.14	1.33
1	D	35	ARG	CZ-NH2	-13.90	1.15	1.33
1	K	34	THR	CB-CG2	-13.79	1.06	1.52
1	B	35	ARG	CD-NE	-13.76	1.23	1.46
1	L	35	ARG	CD-NE	-13.46	1.23	1.46
1	D	35	ARG	CB-CG	-13.46	1.16	1.52
1	J	37	THR	CB-CG2	-13.05	1.09	1.52
1	E	37	THR	CB-CG2	-13.01	1.09	1.52
1	A	34	THR	CB-CG2	-12.98	1.09	1.52
1	F	35	ARG	CB-CG	-12.94	1.17	1.52
1	G	42	ARG	CB-CG	-12.94	1.17	1.52
1	B	103	GLU	CB-CG	-12.90	1.27	1.52
1	B	316	GLU	CD-OE2	-12.69	1.11	1.25
1	A	35	ARG	CD-NE	-12.64	1.25	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	245	LYS	CB-CG	-12.60	1.18	1.52
1	H	37	THR	CB-CG2	-12.57	1.10	1.52
1	H	35	ARG	CD-NE	-12.44	1.25	1.46
1	D	35	ARG	CD-NE	-12.32	1.25	1.46
1	J	35	ARG	CZ-NH2	-12.18	1.17	1.33
1	C	35	ARG	NE-CZ	-12.10	1.17	1.33
1	I	35	ARG	CZ-NH1	-12.09	1.17	1.33
1	D	314	ILE	CB-CG2	-11.82	1.16	1.52
1	I	34	THR	CB-CG2	-11.72	1.13	1.52
1	E	35	ARG	CD-NE	-11.72	1.26	1.46
1	G	35	ARG	CZ-NH2	-11.70	1.17	1.33
1	I	35	ARG	CD-NE	-11.67	1.26	1.46
1	I	35	ARG	CB-CG	-11.66	1.21	1.52
1	A	35	ARG	CB-CG	-11.53	1.21	1.52
1	C	41	LYS	CB-CG	-11.45	1.21	1.52
1	A	35	ARG	NE-CZ	-11.37	1.18	1.33
1	L	36	GLU	CB-CG	-11.34	1.30	1.52
1	L	44	ARG	CG-CD	-11.34	1.23	1.51
1	J	35	ARG	CD-NE	-11.29	1.27	1.46
1	I	35	ARG	NE-CZ	-11.27	1.18	1.33
1	B	42	ARG	CG-CD	-11.23	1.23	1.51
1	F	35	ARG	NE-CZ	-11.17	1.18	1.33
1	C	338	ARG	CB-CG	-11.00	1.22	1.52
1	H	35	ARG	NE-CZ	-11.00	1.18	1.33
1	L	37	THR	CB-CG2	-10.95	1.16	1.52
1	F	281	TRP	CZ3-CH2	10.82	1.57	1.40
1	K	44	ARG	CG-CD	-10.77	1.25	1.51
1	K	42	ARG	CG-CD	-10.69	1.25	1.51
1	G	328	GLU	CD-OE1	-10.61	1.14	1.25
1	L	338	ARG	CB-CG	-10.60	1.24	1.52
1	D	421	PHE	CB-CG	-10.59	1.33	1.51
1	B	35	ARG	NE-CZ	-10.46	1.19	1.33
1	L	424	HIS	CB-CG	-10.38	1.31	1.50
1	C	35	ARG	CZ-NH2	-10.38	1.19	1.33
1	D	296	LEU	CG-CD1	-10.35	1.13	1.51
1	K	35	ARG	NE-CZ	-10.22	1.19	1.33
1	B	296	LEU	CG-CD2	-10.16	1.14	1.51
1	J	36	GLU	CB-CG	-10.07	1.33	1.52
1	G	306	LYS	CB-CG	-9.98	1.25	1.52
1	A	35	ARG	CZ-NH1	-9.95	1.20	1.33
1	D	265	ARG	CZ-NH1	-9.85	1.20	1.33
1	I	44	ARG	CG-CD	-9.80	1.27	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	297	GLN	CD-OE1	-9.79	1.02	1.24
1	C	35	ARG	CZ-NH1	-9.79	1.20	1.33
1	K	297	GLN	CD-OE1	-9.72	1.02	1.24
1	A	295	LYS	CB-CG	-9.71	1.26	1.52
1	D	42	ARG	CB-CG	-9.65	1.26	1.52
1	I	245	LYS	CD-CE	-9.61	1.27	1.51
1	L	35	ARG	NE-CZ	-9.60	1.20	1.33
1	I	42	ARG	CB-CG	-9.57	1.26	1.52
1	D	37	THR	CB-CG2	-9.55	1.20	1.52
1	F	245	LYS	CG-CD	-9.51	1.20	1.52
1	E	338	ARG	CB-CG	-9.49	1.26	1.52
1	A	316	GLU	CB-CG	-9.45	1.34	1.52
1	G	37	THR	CB-CG2	-9.43	1.21	1.52
1	J	44	ARG	CB-CG	-9.43	1.27	1.52
1	D	36	GLU	CB-CG	-9.37	1.34	1.52
1	L	35	ARG	CB-CG	-9.35	1.27	1.52
1	G	35	ARG	NE-CZ	-9.32	1.21	1.33
1	D	245	LYS	CB-CG	-9.32	1.27	1.52
1	G	295	LYS	CB-CG	-9.30	1.27	1.52
1	H	245	LYS	CD-CE	-9.29	1.28	1.51
1	L	42	ARG	CG-CD	-9.24	1.28	1.51
1	D	35	ARG	NE-CZ	-9.22	1.21	1.33
1	B	103	GLU	CD-OE2	-9.22	1.15	1.25
1	D	291	LEU	CB-CG	-9.17	1.25	1.52
1	L	289	LYS	CB-CG	-9.06	1.28	1.52
1	E	36	GLU	CD-OE1	-9.05	1.15	1.25
1	K	37	THR	CB-CG2	-9.04	1.22	1.52
1	D	9	PHE	CB-CG	-8.92	1.36	1.51
1	J	400	LYS	CB-CG	-8.92	1.28	1.52
1	D	328	GLU	CD-OE1	-8.82	1.16	1.25
1	F	37	THR	CB-CG2	-8.79	1.23	1.52
1	K	328	GLU	CD-OE1	-8.77	1.16	1.25
1	H	44	ARG	CG-CD	-8.76	1.30	1.51
1	H	338	ARG	CB-CG	-8.74	1.28	1.52
1	H	298	HIS	CG-ND1	8.72	1.57	1.38
1	B	37	THR	CB-CG2	-8.66	1.23	1.52
1	C	340	LYS	CB-CG	-8.66	1.29	1.52
1	G	327	SER	CB-OG	-8.66	1.30	1.42
1	B	338	ARG	CB-CG	-8.64	1.29	1.52
1	E	42	ARG	CG-CD	-8.64	1.30	1.51
1	G	134	LYS	CB-CG	-8.64	1.29	1.52
1	I	42	ARG	CG-CD	-8.61	1.30	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	245	LYS	CB-CG	-8.60	1.29	1.52
1	E	35	ARG	NE-CZ	-8.54	1.22	1.33
1	C	245	LYS	CB-CG	-8.51	1.29	1.52
1	D	306	LYS	CB-CG	-8.49	1.29	1.52
1	L	340	LYS	CB-CG	-8.49	1.29	1.52
1	I	11	LYS	CB-CG	-8.44	1.29	1.52
1	C	342	LYS	CB-CG	-8.43	1.29	1.52
1	J	265	ARG	CZ-NH1	-8.41	1.22	1.33
1	I	338	ARG	CG-CD	-8.39	1.30	1.51
1	D	308	LYS	CB-CG	-8.38	1.29	1.52
1	F	34	THR	CB-CG2	-8.37	1.24	1.52
1	D	296	LEU	CG-CD2	-8.36	1.21	1.51
1	J	35	ARG	NE-CZ	-8.33	1.22	1.33
1	A	37	THR	CB-CG2	-8.30	1.25	1.52
1	A	316	GLU	CD-OE1	-8.28	1.16	1.25
1	F	338	ARG	CG-CD	-8.26	1.31	1.51
1	C	37	THR	CB-CG2	-8.25	1.25	1.52
1	E	42	ARG	CB-CG	-8.23	1.30	1.52
1	G	245	LYS	CD-CE	-8.17	1.30	1.51
1	I	33	LYS	CE-NZ	8.16	1.69	1.49
1	E	11	LYS	CB-CG	-8.11	1.30	1.52
1	K	245	LYS	CB-CG	-8.10	1.30	1.52
1	E	36	GLU	CB-CG	-8.09	1.36	1.52
1	D	291	LEU	CG-CD2	8.04	1.81	1.51
1	J	330	GLN	CB-CG	-8.02	1.30	1.52
1	K	245	LYS	CD-CE	-8.00	1.31	1.51
1	A	245	LYS	CD-CE	-7.99	1.31	1.51
1	D	338	ARG	CG-CD	-7.99	1.31	1.51
1	L	36	GLU	CG-CD	7.97	1.64	1.51
1	B	340	LYS	CE-NZ	-7.96	1.29	1.49
1	H	306	LYS	CB-CG	-7.94	1.31	1.52
1	J	421	PHE	CG-CD1	-7.90	1.26	1.38
1	J	174	ARG	CG-CD	-7.89	1.32	1.51
1	K	308	LYS	CB-CG	-7.83	1.31	1.52
1	K	35	ARG	CZ-NH1	-7.82	1.22	1.33
1	I	30	GLU	CD-OE1	-7.76	1.17	1.25
1	C	297	GLN	CD-OE1	-7.73	1.06	1.24
1	K	292	GLU	CD-OE1	-7.73	1.17	1.25
1	A	265	ARG	CZ-NH1	-7.70	1.23	1.33
1	H	298	HIS	ND1-CE1	-7.70	1.15	1.34
1	C	9	PHE	CB-CG	-7.68	1.38	1.51
1	F	30	GLU	CD-OE1	-7.68	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	338	ARG	CG-CD	-7.67	1.32	1.51
1	A	338	ARG	CB-CG	-7.67	1.31	1.52
1	J	338	ARG	CB-CG	-7.66	1.31	1.52
1	G	338	ARG	CB-CG	-7.62	1.31	1.52
1	H	308	LYS	CB-CG	-7.54	1.32	1.52
1	D	35	ARG	CZ-NH1	-7.53	1.23	1.33
1	D	291	LEU	CA-CB	7.52	1.71	1.53
1	E	245	LYS	CD-CE	-7.49	1.32	1.51
1	K	306	LYS	CB-CG	-7.47	1.32	1.52
1	J	245	LYS	CD-CE	-7.43	1.32	1.51
1	D	338	ARG	CB-CG	-7.42	1.32	1.52
1	L	36	GLU	CD-OE2	7.40	1.33	1.25
1	H	27	LYS	CB-CG	-7.38	1.32	1.52
1	J	297	GLN	CD-OE1	-7.38	1.07	1.24
1	H	265	ARG	CZ-NH1	-7.36	1.23	1.33
1	K	134	LYS	CB-CG	-7.35	1.32	1.52
1	C	11	LYS	CB-CG	-7.35	1.32	1.52
1	B	330	GLN	CB-CG	-7.34	1.32	1.52
1	D	340	LYS	CB-CG	-7.31	1.32	1.52
1	F	308	LYS	CB-CG	-7.28	1.32	1.52
1	L	295	LYS	CG-CD	-7.27	1.27	1.52
1	B	36	GLU	CB-CG	-7.26	1.38	1.52
1	C	42	ARG	CG-CD	-7.24	1.33	1.51
1	D	9	PHE	CD1-CE1	-7.23	1.24	1.39
1	E	174	ARG	CG-CD	-7.21	1.33	1.51
1	A	308	LYS	CB-CG	-7.21	1.33	1.52
1	G	36	GLU	CB-CG	-7.20	1.38	1.52
1	H	265	ARG	CB-CG	-7.20	1.33	1.52
1	H	245	LYS	CG-CD	-7.19	1.28	1.52
1	L	311	GLU	CD-OE1	-7.18	1.17	1.25
1	K	338	ARG	CG-CD	-7.16	1.34	1.51
1	C	328	GLU	CD-OE1	-7.14	1.17	1.25
1	I	39	GLU	CB-CG	-7.09	1.38	1.52
1	G	174	ARG	CZ-NH1	-6.97	1.24	1.33
1	H	340	LYS	CD-CE	-6.96	1.33	1.51
1	H	340	LYS	CB-CG	-6.92	1.33	1.52
1	J	289	LYS	CB-CG	-6.91	1.33	1.52
1	G	338	ARG	CG-CD	-6.89	1.34	1.51
1	C	269	LYS	CB-CG	-6.88	1.33	1.52
1	H	245	LYS	CB-CG	-6.88	1.33	1.52
1	G	50	ARG	CB-CG	-6.87	1.33	1.52
1	B	35	ARG	CZ-NH1	-6.86	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	46	ARG	CB-CG	-6.84	1.34	1.52
1	G	306	LYS	CG-CD	-6.83	1.29	1.52
1	D	295	LYS	CB-CG	-6.83	1.34	1.52
1	E	35	ARG	CZ-NH1	-6.79	1.24	1.33
1	A	42	ARG	CB-CG	-6.79	1.34	1.52
1	A	310	TYR	CD2-CE2	-6.78	1.29	1.39
1	B	245	LYS	CB-CG	-6.78	1.34	1.52
1	J	297	GLN	CB-CG	-6.75	1.34	1.52
1	B	245	LYS	CG-CD	-6.74	1.29	1.52
1	A	292	GLU	CB-CG	-6.73	1.39	1.52
1	B	308	LYS	CB-CG	-6.72	1.34	1.52
1	K	245	LYS	CE-NZ	-6.72	1.32	1.49
1	C	308	LYS	CB-CG	-6.72	1.34	1.52
1	G	297	GLN	CD-OE1	-6.72	1.09	1.24
1	B	41	LYS	CG-CD	-6.70	1.29	1.52
1	I	265	ARG	CZ-NH1	-6.70	1.24	1.33
1	A	46	ARG	CB-CG	-6.69	1.34	1.52
1	I	37	THR	CB-CG2	-6.69	1.30	1.52
1	A	340	LYS	CB-CG	-6.68	1.34	1.52
1	F	269	LYS	CB-CG	-6.67	1.34	1.52
1	I	316	GLU	CB-CG	-6.67	1.39	1.52
1	F	340	LYS	CB-CG	-6.66	1.34	1.52
1	L	275	GLU	CB-CG	-6.64	1.39	1.52
1	A	363	ARG	CG-CD	-6.62	1.35	1.51
1	D	292	GLU	CB-CG	-6.61	1.39	1.52
1	H	42	ARG	CG-CD	-6.53	1.35	1.51
1	A	245	LYS	CG-CD	-6.52	1.30	1.52
1	L	245	LYS	CD-CE	-6.49	1.35	1.51
1	B	306	LYS	CG-CD	-6.47	1.30	1.52
1	L	30	GLU	CD-OE1	-6.46	1.18	1.25
1	E	297	GLN	CB-CG	-6.44	1.35	1.52
1	E	269	LYS	CB-CG	-6.43	1.35	1.52
1	K	44	ARG	CB-CG	-6.39	1.35	1.52
1	H	30	GLU	CD-OE1	-6.39	1.18	1.25
1	H	11	LYS	CB-CG	-6.39	1.35	1.52
1	I	340	LYS	CD-CE	-6.39	1.35	1.51
1	I	242	PHE	CD1-CE1	-6.35	1.26	1.39
1	K	340	LYS	CB-CG	-6.34	1.35	1.52
1	F	308	LYS	CD-CE	-6.34	1.35	1.51
1	K	53	LYS	CB-CG	-6.34	1.35	1.52
1	B	30	GLU	CG-CD	-6.33	1.42	1.51
1	G	269	LYS	CB-CG	-6.32	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	328	GLU	CG-CD	-6.31	1.42	1.51
1	G	308	LYS	CB-CG	-6.30	1.35	1.52
1	E	245	LYS	CG-CD	-6.29	1.31	1.52
1	G	42	ARG	CD-NE	6.29	1.57	1.46
1	K	338	ARG	CB-CG	-6.27	1.35	1.52
1	B	240	PRO	CG-CD	-6.25	1.30	1.50
1	G	44	ARG	CB-CG	-6.25	1.35	1.52
1	K	50	ARG	CB-CG	-6.24	1.35	1.52
1	L	338	ARG	CG-CD	-6.23	1.36	1.51
1	A	44	ARG	CB-CG	-6.22	1.35	1.52
1	G	340	LYS	CB-CG	-6.21	1.35	1.52
1	J	340	LYS	CB-CG	-6.21	1.35	1.52
1	E	174	ARG	CB-CG	-6.20	1.35	1.52
1	I	11	LYS	CG-CD	-6.20	1.31	1.52
1	E	295	LYS	CB-CG	-6.20	1.35	1.52
1	J	340	LYS	CE-NZ	-6.19	1.33	1.49
1	E	306	LYS	CB-CG	-6.19	1.35	1.52
1	H	265	ARG	CZ-NH2	-6.18	1.25	1.33
1	H	340	LYS	CG-CD	-6.18	1.31	1.52
1	A	316	GLU	CD-OE2	-6.18	1.18	1.25
1	A	306	LYS	CD-CE	-6.17	1.35	1.51
1	E	308	LYS	CB-CG	-6.17	1.35	1.52
1	B	269	LYS	CB-CG	-6.16	1.35	1.52
1	E	340	LYS	CB-CG	-6.16	1.35	1.52
1	J	333	LYS	CB-CG	-6.16	1.35	1.52
1	D	289	LYS	CB-CG	-6.16	1.35	1.52
1	D	27	LYS	CB-CG	-6.15	1.35	1.52
1	G	269	LYS	CG-CD	-6.14	1.31	1.52
1	B	281	TRP	CG-CD1	-6.13	1.28	1.36
1	G	27	LYS	CB-CG	-6.12	1.36	1.52
1	C	42	ARG	CB-CG	-6.12	1.36	1.52
1	H	298	HIS	CB-CG	-6.10	1.39	1.50
1	F	265	ARG	CZ-NH1	-6.09	1.25	1.33
1	L	308	LYS	CB-CG	-6.08	1.36	1.52
1	K	35	ARG	CB-CG	-6.07	1.36	1.52
1	L	34	THR	CB-CG2	-6.07	1.32	1.52
1	F	338	ARG	CB-CG	-6.06	1.36	1.52
1	B	265	ARG	CZ-NH1	-6.06	1.25	1.33
1	I	30	GLU	CB-CG	-6.05	1.40	1.52
1	L	27	LYS	CB-CG	-6.04	1.36	1.52
1	E	30	GLU	CD-OE1	-6.03	1.19	1.25
1	J	34	THR	CB-CG2	-6.03	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	30	GLU	CG-CD	-6.02	1.43	1.51
1	D	290	GLU	C-O	6.01	1.34	1.23
1	H	19	ARG	CZ-NH2	6.00	1.40	1.33
1	B	316	GLU	CB-CG	-6.00	1.40	1.52
1	J	362	GLU	CG-CD	-6.00	1.43	1.51
1	L	44	ARG	CB-CG	-5.99	1.36	1.52
1	J	338	ARG	CG-CD	-5.98	1.36	1.51
1	I	44	ARG	CB-CG	-5.98	1.36	1.52
1	B	306	LYS	CB-CG	-5.97	1.36	1.52
1	E	35	ARG	CB-CG	-5.97	1.36	1.52
1	I	275	GLU	CB-CG	-5.95	1.40	1.52
1	C	46	ARG	CB-CG	-5.95	1.36	1.52
1	F	329	LYS	CB-CG	-5.93	1.36	1.52
1	J	340	LYS	CD-CE	-5.93	1.36	1.51
1	L	289	LYS	CG-CD	-5.92	1.32	1.52
1	B	330	GLN	CD-OE1	-5.92	1.10	1.24
1	H	269	LYS	CG-CD	-5.92	1.32	1.52
1	A	245	LYS	CB-CG	-5.88	1.36	1.52
1	A	338	ARG	CD-NE	-5.88	1.36	1.46
1	G	265	ARG	CZ-NH1	-5.88	1.25	1.33
1	C	30	GLU	CD-OE1	-5.86	1.19	1.25
1	E	297	GLN	CD-OE1	-5.86	1.11	1.24
1	J	30	GLU	CB-CG	-5.86	1.41	1.52
1	D	265	ARG	CB-CG	-5.85	1.36	1.52
1	E	340	LYS	CD-CE	-5.85	1.36	1.51
1	D	297	GLN	CB-CG	-5.84	1.36	1.52
1	F	35	ARG	CZ-NH1	-5.83	1.25	1.33
1	D	245	LYS	CD-CE	-5.83	1.36	1.51
1	L	311	GLU	CG-CD	-5.82	1.43	1.51
1	B	44	ARG	CZ-NH1	-5.81	1.25	1.33
1	I	240	PRO	CG-CD	-5.81	1.31	1.50
1	A	308	LYS	CD-CE	-5.81	1.36	1.51
1	C	269	LYS	CG-CD	-5.81	1.32	1.52
1	G	333	LYS	CG-CD	-5.80	1.32	1.52
1	A	275	GLU	CB-CG	-5.79	1.41	1.52
1	A	34	THR	CB-OG1	-5.78	1.31	1.43
1	D	35	ARG	CG-CD	-5.76	1.37	1.51
1	A	333	LYS	CB-CG	-5.75	1.37	1.52
1	I	242	PHE	CB-CG	-5.75	1.41	1.51
1	A	240	PRO	CG-CD	-5.74	1.31	1.50
1	K	265	ARG	CZ-NH1	-5.73	1.25	1.33
1	E	245	LYS	CB-CG	-5.72	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	LYS	CD-CE	-5.70	1.36	1.51
1	D	308	LYS	CD-CE	-5.70	1.37	1.51
1	K	250	GLN	CD-OE1	-5.69	1.11	1.24
1	B	245	LYS	CD-CE	-5.68	1.37	1.51
1	J	35	ARG	CB-CG	-5.67	1.37	1.52
1	L	269	LYS	CB-CG	-5.64	1.37	1.52
1	L	245	LYS	CB-CG	-5.64	1.37	1.52
1	I	289	LYS	CG-CD	-5.64	1.33	1.52
1	J	11	LYS	CG-CD	-5.64	1.33	1.52
1	B	44	ARG	CB-CG	-5.63	1.37	1.52
1	H	298	HIS	CE1-NE2	5.63	1.45	1.32
1	B	296	LEU	CG-CD1	-5.63	1.31	1.51
1	E	269	LYS	CG-CD	-5.63	1.33	1.52
1	G	30	GLU	CB-CG	-5.62	1.41	1.52
1	L	11	LYS	CB-CG	-5.62	1.37	1.52
1	E	421	PHE	CD1-CE1	-5.61	1.28	1.39
1	E	333	LYS	CB-CG	-5.61	1.37	1.52
1	J	340	LYS	CG-CD	-5.61	1.33	1.52
1	E	342	LYS	CG-CD	-5.60	1.33	1.52
1	J	240	PRO	CG-CD	-5.60	1.32	1.50
1	J	245	LYS	CE-NZ	-5.59	1.35	1.49
1	L	424	HIS	CG-ND1	5.59	1.51	1.38
1	C	306	LYS	CB-CG	-5.59	1.37	1.52
1	C	245	LYS	CD-CE	-5.59	1.37	1.51
1	H	36	GLU	CB-CG	-5.58	1.41	1.52
1	H	44	ARG	CB-CG	-5.58	1.37	1.52
1	H	240	PRO	CG-CD	-5.57	1.32	1.50
1	A	423	LYS	CB-CG	-5.56	1.37	1.52
1	J	11	LYS	CB-CG	-5.55	1.37	1.52
1	E	240	PRO	CG-CD	-5.54	1.32	1.50
1	B	340	LYS	CD-CE	-5.54	1.37	1.51
1	C	240	PRO	CG-CD	-5.54	1.32	1.50
1	B	289	LYS	CG-CD	-5.53	1.33	1.52
1	G	289	LYS	CB-CG	-5.53	1.37	1.52
1	E	134	LYS	CG-CD	-5.52	1.33	1.52
1	F	44	ARG	CZ-NH1	-5.52	1.25	1.33
1	G	308	LYS	CD-CE	-5.52	1.37	1.51
1	G	245	LYS	CE-NZ	-5.50	1.35	1.49
1	E	295	LYS	CD-CE	-5.50	1.37	1.51
1	I	245	LYS	CG-CD	-5.50	1.33	1.52
1	L	328	GLU	CD-OE1	-5.49	1.19	1.25
1	E	328	GLU	CD-OE1	-5.47	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	275	GLU	CB-CG	-5.47	1.41	1.52
1	I	19	ARG	CG-CD	-5.46	1.38	1.51
1	J	308	LYS	CB-CG	-5.46	1.37	1.52
1	F	245	LYS	CD-CE	-5.46	1.37	1.51
1	H	42	ARG	CB-CG	-5.45	1.37	1.52
1	E	281	TRP	CG-CD1	-5.45	1.29	1.36
1	K	42	ARG	CD-NE	-5.45	1.37	1.46
1	A	292	GLU	CG-CD	-5.43	1.43	1.51
1	B	289	LYS	CB-CG	-5.43	1.37	1.52
1	K	340	LYS	CD-CE	-5.43	1.37	1.51
1	J	308	LYS	CD-CE	-5.43	1.37	1.51
1	D	30	GLU	CD-OE1	-5.42	1.19	1.25
1	A	328	GLU	CD-OE1	-5.41	1.19	1.25
1	K	420	LYS	CG-CD	-5.39	1.34	1.52
1	D	306	LYS	CD-CE	-5.38	1.37	1.51
1	H	328	GLU	CD-OE1	-5.38	1.19	1.25
1	C	421	PHE	CB-CG	-5.37	1.42	1.51
1	D	9	PHE	CE2-CZ	-5.36	1.27	1.37
1	H	289	LYS	CB-CG	-5.33	1.38	1.52
1	I	27	LYS	CG-CD	-5.33	1.34	1.52
1	J	421	PHE	CA-CB	-5.33	1.42	1.53
1	F	35	ARG	CA-CB	-5.32	1.42	1.53
1	H	30	GLU	CG-CD	-5.32	1.44	1.51
1	I	35	ARG	CA-CB	-5.32	1.42	1.53
1	A	281	TRP	CE2-CZ2	-5.31	1.30	1.39
1	C	295	LYS	CG-CD	-5.31	1.34	1.52
1	H	264	HIS	CG-ND1	-5.31	1.27	1.38
1	K	329	LYS	CB-CG	-5.30	1.38	1.52
1	B	328	GLU	CB-CG	-5.28	1.42	1.52
1	C	292	GLU	CD-OE1	-5.28	1.19	1.25
1	D	247	PHE	CE2-CZ	5.26	1.47	1.37
1	B	329	LYS	CB-CG	-5.26	1.38	1.52
1	D	245	LYS	CG-CD	-5.24	1.34	1.52
1	I	340	LYS	CB-CG	-5.24	1.38	1.52
1	F	306	LYS	CG-CD	-5.23	1.34	1.52
1	G	27	LYS	CD-CE	-5.23	1.38	1.51
1	D	340	LYS	CG-CD	-5.21	1.34	1.52
1	B	342	LYS	CB-CG	-5.20	1.38	1.52
1	J	27	LYS	CB-CG	-5.19	1.38	1.52
1	A	42	ARG	CG-CD	-5.18	1.39	1.51
1	E	45	VAL	CB-CG2	-5.18	1.42	1.52
1	H	342	LYS	CB-CG	-5.17	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	27	LYS	CB-CG	-5.17	1.38	1.52
1	F	295	LYS	CB-CG	-5.16	1.38	1.52
1	B	297	GLN	CG-CD	-5.16	1.39	1.51
1	D	247	PHE	CG-CD2	5.14	1.46	1.38
1	D	269	LYS	CB-CG	-5.14	1.38	1.52
1	G	308	LYS	CG-CD	-5.14	1.34	1.52
1	G	333	LYS	CD-CE	-5.14	1.38	1.51
1	L	42	ARG	CB-CG	-5.13	1.38	1.52
1	K	269	LYS	CB-CG	-5.12	1.38	1.52
1	E	45	VAL	CB-CG1	-5.11	1.42	1.52
1	K	446	LYS	CD-CE	-5.10	1.38	1.51
1	J	421	PHE	CB-CG	-5.10	1.42	1.51
1	J	35	ARG	CZ-NH1	-5.10	1.26	1.33
1	K	308	LYS	CG-CD	-5.10	1.35	1.52
1	G	30	GLU	CD-OE1	-5.09	1.20	1.25
1	E	134	LYS	CB-CG	-5.08	1.38	1.52
1	A	261	ARG	CB-CG	-5.08	1.38	1.52
1	H	295	LYS	CB-CG	-5.07	1.38	1.52
1	J	328	GLU	CD-OE1	-5.07	1.20	1.25
1	G	329	LYS	CB-CG	-5.07	1.38	1.52
1	I	421	PHE	CD1-CE1	-5.07	1.29	1.39
1	C	358	LYS	CB-CG	-5.06	1.38	1.52
1	G	35	ARG	CB-CG	-5.06	1.38	1.52
1	C	363	ARG	CG-CD	-5.05	1.39	1.51
1	J	421	PHE	CE1-CZ	-5.05	1.27	1.37
1	H	306	LYS	CG-CD	-5.05	1.35	1.52
1	A	329	LYS	CB-CG	-5.05	1.39	1.52
1	B	27	LYS	CB-CG	-5.05	1.39	1.52
1	I	308	LYS	CB-CG	-5.04	1.39	1.52
1	J	42	ARG	CG-CD	-5.02	1.39	1.51
1	L	265	ARG	CZ-NH2	-5.02	1.26	1.33
1	E	421	PHE	CB-CG	-5.01	1.42	1.51
1	G	340	LYS	CD-CE	-5.01	1.38	1.51
1	I	297	GLN	CD-OE1	-5.00	1.12	1.24

All (900) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	421	PHE	CB-CG-CD1	-41.88	91.48	120.80
1	I	242	PHE	CB-CG-CD1	-39.63	93.06	120.80
1	L	35	ARG	NE-CZ-NH2	-38.88	100.86	120.30
1	L	363	ARG	NE-CZ-NH2	38.76	139.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	261	ARG	NE-CZ-NH2	37.43	139.01	120.30
1	J	421	PHE	CB-CG-CD2	36.58	146.41	120.80
1	A	338	ARG	NE-CZ-NH2	35.80	138.20	120.30
1	A	338	ARG	NE-CZ-NH1	-33.53	103.53	120.30
1	L	265	ARG	NE-CZ-NH2	32.88	136.74	120.30
1	D	439	ARG	NE-CZ-NH2	32.13	136.37	120.30
1	E	265	ARG	NE-CZ-NH2	29.92	135.26	120.30
1	D	280	ILE	CG1-CB-CG2	-29.56	46.36	111.40
1	I	242	PHE	CB-CG-CD2	28.75	140.92	120.80
1	B	35	ARG	NE-CZ-NH2	-28.06	106.27	120.30
1	D	314	ILE	CG1-CB-CG2	-28.03	49.73	111.40
1	C	35	ARG	NE-CZ-NH2	-27.33	106.63	120.30
1	F	35	ARG	NE-CZ-NH2	-26.87	106.86	120.30
1	L	363	ARG	NE-CZ-NH1	-25.71	107.44	120.30
1	A	35	ARG	CG-CD-NE	-25.68	57.87	111.80
1	L	35	ARG	CG-CD-NE	-25.33	58.60	111.80
1	G	314	ILE	CG1-CB-CG2	-23.40	59.92	111.40
1	K	217	ARG	NE-CZ-NH1	-22.54	109.03	120.30
1	H	35	ARG	NE-CZ-NH2	-22.37	109.11	120.30
1	D	439	ARG	NE-CZ-NH1	-22.02	109.29	120.30
1	E	261	ARG	NE-CZ-NH1	-21.48	109.56	120.30
1	K	217	ARG	NE-CZ-NH2	21.27	130.94	120.30
1	D	35	ARG	CG-CD-NE	-21.07	67.55	111.80
1	G	174	ARG	NE-CZ-NH2	20.67	130.63	120.30
1	F	50	ARG	NE-CZ-NH1	-20.19	110.20	120.30
1	I	50	ARG	NE-CZ-NH1	-20.10	110.25	120.30
1	G	66	ARG	NE-CZ-NH1	-19.66	110.47	120.30
1	A	217	ARG	NE-CZ-NH1	-19.41	110.60	120.30
1	G	35	ARG	CA-CB-CG	19.37	156.01	113.40
1	I	32	LEU	CA-CB-CG	19.27	159.61	115.30
1	B	316	GLU	OE1-CD-OE2	-19.24	100.21	123.30
1	H	296	LEU	CA-CB-CG	19.19	159.44	115.30
1	C	35	ARG	CG-CD-NE	-19.10	71.69	111.80
1	D	265	ARG	NE-CZ-NH2	19.04	129.82	120.30
1	F	35	ARG	CG-CD-NE	-18.77	72.38	111.80
1	K	296	LEU	CA-CB-CG	18.76	158.46	115.30
1	J	265	ARG	NE-CZ-NH2	18.54	129.57	120.30
1	I	322	LEU	CB-CG-CD2	-18.29	79.90	111.00
1	F	50	ARG	NE-CZ-NH2	17.54	129.07	120.30
1	I	50	ARG	NE-CZ-NH2	17.52	129.06	120.30
1	E	32	LEU	CA-CB-CG	17.28	155.05	115.30
1	G	66	ARG	NE-CZ-NH2	16.95	128.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	LYS	CD-CE-NZ	16.88	150.51	111.70
1	G	358	LYS	CD-CE-NZ	16.78	150.29	111.70
1	A	420	LYS	CD-CE-NZ	16.76	150.25	111.70
1	J	94	ARG	NE-CZ-NH1	-16.49	112.06	120.30
1	K	94	ARG	NE-CZ-NH1	-16.48	112.06	120.30
1	A	94	ARG	NE-CZ-NH1	-16.42	112.09	120.30
1	I	94	ARG	NE-CZ-NH1	-16.40	112.10	120.30
1	I	94	ARG	NE-CZ-NH2	16.30	128.45	120.30
1	J	94	ARG	NE-CZ-NH2	16.25	128.42	120.30
1	K	94	ARG	NE-CZ-NH2	16.23	128.42	120.30
1	A	94	ARG	NE-CZ-NH2	16.16	128.38	120.30
1	A	265	ARG	NE-CZ-NH2	16.09	128.35	120.30
1	A	217	ARG	NE-CZ-NH2	16.00	128.30	120.30
1	G	35	ARG	NE-CZ-NH2	-15.90	112.35	120.30
1	I	34	THR	OG1-CB-CG2	-15.63	74.05	110.00
1	F	239	THR	C-N-CD	-15.59	86.30	120.60
1	K	239	THR	C-N-CD	-15.45	86.62	120.60
1	K	245	LYS	CD-CE-NZ	15.23	146.74	111.70
1	K	35	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	I	239	THR	C-N-CD	-14.81	88.02	120.60
1	I	322	LEU	CA-CB-CG	14.79	149.32	115.30
1	A	338	ARG	CD-NE-CZ	14.56	143.98	123.60
1	B	239	THR	C-N-CD	-14.47	88.78	120.60
1	E	46	ARG	CG-CD-NE	14.44	142.12	111.80
1	A	292	GLU	CA-CB-CG	14.41	145.10	113.40
1	B	296	LEU	CA-CB-CG	14.41	148.44	115.30
1	C	239	THR	C-N-CD	-14.34	89.05	120.60
1	G	174	ARG	NE-CZ-NH1	-14.16	113.22	120.30
1	A	34	THR	OG1-CB-CG2	-14.11	77.54	110.00
1	L	265	ARG	NE-CZ-NH1	-13.94	113.33	120.30
1	B	169	MET	CG-SD-CE	13.94	122.50	100.20
1	G	239	THR	C-N-CD	-13.85	90.12	120.60
1	D	296	LEU	CD1-CG-CD2	-13.76	69.21	110.50
1	H	239	THR	C-N-CD	-13.75	90.35	120.60
1	F	32	LEU	CA-CB-CG	13.65	146.70	115.30
1	L	363	ARG	CG-CD-NE	13.59	140.34	111.80
1	D	130	LYS	CD-CE-NZ	13.58	142.94	111.70
1	A	239	THR	C-N-CD	-13.52	90.86	120.60
1	G	42	ARG	NH1-CZ-NH2	-13.45	104.61	119.40
1	G	42	ARG	NE-CZ-NH1	13.38	126.99	120.30
1	A	30	GLU	CA-CB-CG	13.35	142.77	113.40
1	C	41	LYS	CA-CB-CG	13.30	142.66	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	ARG	NE-CZ-NH2	13.16	126.88	120.30
1	H	46	ARG	CG-CD-NE	13.09	139.28	111.80
1	E	169	MET	CG-SD-CE	13.06	121.10	100.20
1	F	265	ARG	NE-CZ-NH2	13.06	126.83	120.30
1	K	308	LYS	CA-CB-CG	13.00	142.00	113.40
1	G	42	ARG	NE-CZ-NH2	12.99	126.79	120.30
1	G	35	ARG	CD-NE-CZ	-12.98	105.42	123.60
1	J	35	ARG	CG-CD-NE	-12.97	84.56	111.80
1	B	32	LEU	CA-CB-CG	12.89	144.95	115.30
1	J	35	ARG	NE-CZ-NH2	-12.86	113.87	120.30
1	D	311	GLU	CA-CB-CG	12.82	141.61	113.40
1	C	44	ARG	NE-CZ-NH2	12.76	126.68	120.30
1	E	311	GLU	CA-CB-CG	12.72	141.39	113.40
1	H	44	ARG	CA-CB-CG	-12.71	85.44	113.40
1	A	42	ARG	NE-CZ-NH1	-12.71	113.95	120.30
1	G	245	LYS	CD-CE-NZ	12.64	140.78	111.70
1	I	35	ARG	CG-CD-NE	-12.61	85.32	111.80
1	E	358	LYS	CD-CE-NZ	12.50	140.44	111.70
1	K	308	LYS	CD-CE-NZ	12.47	140.39	111.70
1	G	35	ARG	CG-CD-NE	-12.46	85.63	111.80
1	H	35	ARG	CG-CD-NE	-12.41	85.73	111.80
1	D	421	PHE	CB-CG-CD2	-12.39	112.13	120.80
1	H	46	ARG	NE-CZ-NH2	-12.35	114.12	120.30
1	E	265	ARG	NE-CZ-NH1	-12.33	114.14	120.30
1	C	30	GLU	CA-CB-CG	12.28	140.42	113.40
1	H	35	ARG	CD-NE-CZ	-12.28	106.41	123.60
1	G	314	ILE	CA-CB-CG1	12.22	134.22	111.00
1	L	169	MET	CG-SD-CE	12.16	119.66	100.20
1	L	239	THR	C-N-CD	-12.13	93.92	120.60
1	D	296	LEU	CA-CB-CG	12.12	143.17	115.30
1	I	33	LYS	CD-CE-NZ	12.10	139.53	111.70
1	K	32	LEU	CA-CB-CG	12.10	143.13	115.30
1	B	306	LYS	CA-CB-CG	12.06	139.94	113.40
1	L	424	HIS	N-CA-CB	12.04	132.28	110.60
1	J	32	LEU	CA-CB-CG	12.03	142.96	115.30
1	H	32	LEU	CA-CB-CG	11.99	142.88	115.30
1	E	239	THR	C-N-CD	-11.98	94.23	120.60
1	E	32	LEU	CB-CG-CD2	-11.96	90.67	111.00
1	B	296	LEU	CD1-CG-CD2	-11.94	74.67	110.50
1	K	328	GLU	CA-CB-CG	11.93	139.64	113.40
1	H	169	MET	CG-SD-CE	11.89	119.22	100.20
1	A	292	GLU	CG-CD-OE2	11.87	142.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	MET	CG-SD-CE	11.85	119.16	100.20
1	J	239	THR	C-N-CD	-11.79	94.67	120.60
1	C	35	ARG	NE-CZ-NH1	11.75	126.17	120.30
1	D	239	THR	C-N-CD	-11.75	94.76	120.60
1	A	42	ARG	NE-CZ-NH2	11.70	126.15	120.30
1	L	32	LEU	CA-CB-CG	11.69	142.18	115.30
1	L	35	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	B	342	LYS	CD-CE-NZ	11.68	138.55	111.70
1	G	35	ARG	N-CA-CB	-11.67	89.59	110.60
1	A	333	LYS	CA-CB-CG	11.58	138.87	113.40
1	B	340	LYS	CB-CG-CD	-11.51	81.67	111.60
1	K	53	LYS	CA-CB-CG	11.50	138.70	113.40
1	D	169	MET	CG-SD-CE	11.44	118.51	100.20
1	J	333	LYS	CA-CB-CG	11.43	138.56	113.40
1	K	169	MET	CG-SD-CE	11.43	118.48	100.20
1	K	217	ARG	CD-NE-CZ	11.37	139.51	123.60
1	K	269	LYS	CB-CG-CD	-11.30	82.21	111.60
1	C	269	LYS	CD-CE-NZ	-11.27	85.79	111.70
1	K	53	LYS	CB-CG-CD	11.23	140.81	111.60
1	J	362	GLU	CA-CB-CG	11.20	138.03	113.40
1	I	296	LEU	CA-CB-CG	11.19	141.03	115.30
1	D	174	ARG	NE-CZ-NH1	-11.16	114.72	120.30
1	K	50	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	F	269	LYS	CD-CE-NZ	-11.11	86.14	111.70
1	H	35	ARG	N-CA-CB	-11.09	90.64	110.60
1	D	30	GLU	CA-CB-CG	11.07	137.76	113.40
1	G	105	LYS	CG-CD-CE	11.04	145.02	111.90
1	K	245	LYS	CG-CD-CE	-10.97	78.98	111.90
1	I	44	ARG	CA-CB-CG	-10.96	89.30	113.40
1	B	35	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	E	174	ARG	CA-CB-CG	10.94	137.46	113.40
1	G	105	LYS	CD-CE-NZ	10.93	136.84	111.70
1	C	295	LYS	CD-CE-NZ	10.92	136.81	111.70
1	F	329	LYS	CA-CB-CG	10.90	137.37	113.40
1	H	338	ARG	NE-CZ-NH1	-10.88	114.86	120.30
1	C	169	MET	CG-SD-CE	10.81	117.49	100.20
1	B	44	ARG	NE-CZ-NH2	10.79	125.69	120.30
1	J	329	LYS	CD-CE-NZ	10.74	136.40	111.70
1	G	30	GLU	CA-CB-CG	10.67	136.88	113.40
1	C	296	LEU	CA-CB-CG	10.61	139.71	115.30
1	A	35	ARG	CA-CB-CG	10.55	136.61	113.40
1	A	35	ARG	N-CA-CB	-10.52	91.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	LYS	CD-CE-NZ	10.50	135.85	111.70
1	L	35	ARG	NH1-CZ-NH2	10.50	130.95	119.40
1	F	35	ARG	N-CA-C	10.45	139.22	111.00
1	K	265	ARG	NE-CZ-NH2	10.45	125.53	120.30
1	F	169	MET	CG-SD-CE	10.43	116.89	100.20
1	J	306	LYS	CD-CE-NZ	10.42	135.67	111.70
1	J	30	GLU	CA-CB-CG	10.38	136.23	113.40
1	L	363	ARG	CB-CG-CD	-10.38	84.62	111.60
1	A	35	ARG	CD-NE-CZ	-10.36	109.10	123.60
1	C	32	LEU	CB-CG-CD1	10.35	128.59	111.00
1	L	308	LYS	CB-CG-CD	-10.34	84.72	111.60
1	H	306	LYS	CA-CB-CG	10.33	136.13	113.40
1	D	265	ARG	NE-CZ-NH1	-10.33	115.14	120.30
1	K	329	LYS	CD-CE-NZ	10.30	135.38	111.70
1	K	333	LYS	CA-CB-CG	10.30	136.05	113.40
1	H	298	HIS	ND1-CG-CD2	-10.28	91.61	106.00
1	D	245	LYS	CG-CD-CE	-10.21	81.26	111.90
1	K	35	ARG	CG-CD-NE	-10.18	90.42	111.80
1	B	330	GLN	CA-CB-CG	10.17	135.78	113.40
1	I	19	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	G	296	LEU	CA-CB-CG	10.08	138.48	115.30
1	A	310	TYR	CB-CG-CD2	-10.08	114.95	121.00
1	H	44	ARG	NE-CZ-NH1	-10.07	115.26	120.30
1	F	296	LEU	CA-CB-CG	10.05	138.43	115.30
1	E	42	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	G	265	ARG	NE-CZ-NH2	10.03	125.31	120.30
1	B	35	ARG	CG-CD-NE	-10.02	90.75	111.80
1	B	30	GLU	CG-CD-OE2	10.01	138.31	118.30
1	J	46	ARG	CG-CD-NE	10.00	132.79	111.80
1	G	27	LYS	CB-CG-CD	-9.92	85.81	111.60
1	G	42	ARG	CA-CB-CG	-9.91	91.61	113.40
1	G	27	LYS	CA-CB-CG	9.90	135.18	113.40
1	B	35	ARG	N-CA-CB	-9.89	92.80	110.60
1	G	35	ARG	CB-CG-CD	9.82	137.12	111.60
1	A	296	LEU	CA-CB-CG	9.81	137.86	115.30
1	A	329	LYS	CD-CE-NZ	9.81	134.25	111.70
1	I	35	ARG	N-CA-C	9.80	137.45	111.00
1	J	265	ARG	NE-CZ-NH1	-9.79	115.41	120.30
1	B	35	ARG	CA-CB-CG	9.77	134.90	113.40
1	I	44	ARG	NE-CZ-NH1	-9.72	115.44	120.30
1	B	103	GLU	CB-CA-C	-9.71	90.98	110.40
1	K	27	LYS	CB-CG-CD	-9.70	86.38	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	105	LYS	CB-CG-CD	-9.70	86.39	111.60
1	E	37	THR	OG1-CB-CG2	-9.69	87.71	110.00
1	C	308	LYS	CA-CB-CG	9.69	134.71	113.40
1	I	328	GLU	OE1-CD-OE2	-9.66	111.71	123.30
1	B	338	ARG	CG-CD-NE	9.66	132.08	111.80
1	C	27	LYS	CB-CG-CD	-9.63	86.55	111.60
1	D	35	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	I	169	MET	CG-SD-CE	9.62	115.59	100.20
1	G	169	MET	CG-SD-CE	9.61	115.58	100.20
1	J	296	LEU	CA-CB-CG	9.60	137.37	115.30
1	L	27	LYS	CA-CB-CG	9.57	134.45	113.40
1	L	37	THR	OG1-CB-CG2	-9.52	88.11	110.00
1	F	245	LYS	CD-CE-NZ	-9.51	89.82	111.70
1	D	247	PHE	CB-CG-CD2	-9.51	114.14	120.80
1	G	358	LYS	CB-CG-CD	-9.51	86.89	111.60
1	B	41	LYS	CD-CE-NZ	9.48	133.50	111.70
1	F	35	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	B	36	GLU	CA-CB-CG	9.45	134.19	113.40
1	E	296	LEU	CA-CB-CG	9.45	137.02	115.30
1	K	420	LYS	CD-CE-NZ	9.43	133.39	111.70
1	J	169	MET	CG-SD-CE	9.40	115.24	100.20
1	L	40	GLN	CA-CB-CG	9.38	134.04	113.40
1	B	42	ARG	CG-CD-NE	9.36	131.46	111.80
1	I	289	LYS	CB-CG-CD	9.32	135.84	111.60
1	D	314	ILE	CA-CB-CG1	9.32	128.70	111.00
1	H	35	ARG	CA-CB-CG	9.30	133.87	113.40
1	E	42	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	K	37	THR	OG1-CB-CG2	-9.29	88.64	110.00
1	A	265	ARG	NE-CZ-NH1	-9.25	115.68	120.30
1	C	69	ASP	CB-CG-OD1	9.25	126.62	118.30
1	J	338	ARG	CG-CD-NE	9.24	131.21	111.80
1	F	40	GLN	CA-CB-CG	9.23	133.72	113.40
1	K	44	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	C	46	ARG	CG-CD-NE	9.20	131.12	111.80
1	A	37	THR	OG1-CB-CG2	-9.20	88.85	110.00
1	K	44	ARG	CA-CB-CG	-9.19	93.17	113.40
1	E	245	LYS	CD-CE-NZ	-9.19	90.56	111.70
1	G	295	LYS	CD-CE-NZ	9.19	132.82	111.70
1	H	30	GLU	CA-CB-CG	9.19	133.61	113.40
1	L	363	ARG	NH1-CZ-NH2	-9.17	109.31	119.40
1	B	329	LYS	CD-CE-NZ	9.16	132.78	111.70
1	A	292	GLU	CG-CD-OE1	-9.16	99.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	42	ARG	CB-CG-CD	9.14	135.37	111.60
1	K	42	ARG	CG-CD-NE	9.13	130.98	111.80
1	K	35	ARG	CD-NE-CZ	-9.12	110.83	123.60
1	L	174	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	F	35	ARG	CD-NE-CZ	-9.12	110.84	123.60
1	I	19	ARG	CD-NE-CZ	9.10	136.33	123.60
1	I	19	ARG	CG-CD-NE	9.09	130.90	111.80
1	K	174	ARG	NE-CZ-NH1	-9.08	115.76	120.30
1	D	439	ARG	CG-CD-NE	9.07	130.84	111.80
1	J	333	LYS	CB-CA-C	-9.05	92.30	110.40
1	D	174	ARG	CG-CD-NE	9.04	130.79	111.80
1	E	30	GLU	CA-CB-CG	9.04	133.29	113.40
1	F	174	ARG	NE-CZ-NH1	-9.03	115.78	120.30
1	A	235	ILE	CG1-CB-CG2	-9.01	91.58	111.40
1	K	333	LYS	N-CA-CB	-8.99	94.42	110.60
1	H	338	ARG	CG-CD-NE	8.96	130.62	111.80
1	B	306	LYS	CD-CE-NZ	8.93	132.24	111.70
1	A	217	ARG	CD-NE-CZ	8.90	136.06	123.60
1	E	35	ARG	CD-NE-CZ	-8.90	111.14	123.60
1	C	421	PHE	CB-CG-CD2	-8.89	114.58	120.80
1	K	35	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	L	289	LYS	CA-CB-CG	8.89	132.97	113.40
1	F	37	THR	OG1-CB-CG2	-8.89	89.56	110.00
1	H	35	ARG	NH1-CZ-NH2	8.89	129.18	119.40
1	B	338	ARG	NE-CZ-NH1	-8.85	115.87	120.30
1	A	35	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	H	69	ASP	CB-CG-OD1	8.85	126.26	118.30
1	G	245	LYS	CG-CD-CE	-8.84	85.39	111.90
1	A	32	LEU	CB-CG-CD2	8.84	126.02	111.00
1	I	242	PHE	CG-CD1-CE1	8.82	130.51	120.80
1	H	306	LYS	CB-CA-C	-8.80	92.81	110.40
1	K	50	ARG	CA-CB-CG	8.79	132.74	113.40
1	E	36	GLU	OE1-CD-OE2	8.76	133.81	123.30
1	L	19	ARG	CG-CD-NE	8.75	130.18	111.80
1	G	328	GLU	CA-CB-CG	8.74	132.63	113.40
1	F	42	ARG	NE-CZ-NH2	8.73	124.67	120.30
1	I	44	ARG	CG-CD-NE	8.72	130.12	111.80
1	E	265	ARG	CG-CD-NE	8.71	130.09	111.80
1	L	329	LYS	CD-CE-NZ	8.70	131.72	111.70
1	H	37	THR	OG1-CB-CG2	-8.69	90.01	110.00
1	K	420	LYS	CB-CG-CD	8.64	134.06	111.60
1	H	44	ARG	NE-CZ-NH2	8.63	124.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	46	ARG	CG-CD-NE	8.62	129.90	111.80
1	L	265	ARG	NH1-CZ-NH2	-8.61	109.92	119.40
1	H	19	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	B	35	ARG	N-CA-C	8.57	134.15	111.00
1	J	400	LYS	CA-CB-CG	8.56	132.24	113.40
1	D	174	ARG	NE-CZ-NH2	8.55	124.57	120.30
1	F	421	PHE	CB-CG-CD2	-8.52	114.84	120.80
1	I	306	LYS	CD-CE-NZ	8.52	131.29	111.70
1	H	296	LEU	CB-CG-CD1	8.52	125.48	111.00
1	I	328	GLU	CG-CD-OE2	8.51	135.33	118.30
1	L	19	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	B	35	ARG	CB-CG-CD	8.51	133.73	111.60
1	G	421	PHE	CB-CG-CD2	-8.51	114.85	120.80
1	L	296	LEU	CA-CB-CG	8.47	134.79	115.30
1	B	44	ARG	NE-CZ-NH1	-8.47	116.07	120.30
1	D	329	LYS	CD-CE-NZ	8.45	131.14	111.70
1	J	289	LYS	CA-CB-CG	8.45	132.00	113.40
1	F	295	LYS	CD-CE-NZ	8.42	131.07	111.70
1	B	409	LEU	CA-CB-CG	8.41	134.66	115.30
1	H	311	GLU	CA-CB-CG	8.39	131.85	113.40
1	L	424	HIS	CG-ND1-CE1	8.38	119.93	108.20
1	H	338	ARG	CD-NE-CZ	-8.38	111.87	123.60
1	G	50	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	J	400	LYS	CD-CE-NZ	8.35	130.91	111.70
1	A	363	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	K	42	ARG	CB-CG-CD	-8.32	89.96	111.60
1	I	333	LYS	CD-CE-NZ	8.31	130.82	111.70
1	I	338	ARG	CB-CG-CD	-8.30	90.02	111.60
1	H	36	GLU	CA-CB-CG	8.29	131.64	113.40
1	I	280	ILE	CG1-CB-CG2	-8.26	93.24	111.40
1	L	296	LEU	CB-CG-CD2	-8.25	96.98	111.00
1	C	35	ARG	N-CA-C	8.24	133.26	111.00
1	L	27	LYS	CD-CE-NZ	8.24	130.66	111.70
1	E	35	ARG	CB-CG-CD	8.24	133.02	111.60
1	L	289	LYS	CB-CA-C	-8.24	93.92	110.40
1	C	295	LYS	CA-CB-CG	8.23	131.51	113.40
1	G	338	ARG	NE-CZ-NH1	-8.22	116.19	120.30
1	J	37	THR	OG1-CB-CG2	-8.22	91.09	110.00
1	I	235	ILE	CG1-CB-CG2	-8.21	93.33	111.40
1	G	174	ARG	CG-CD-NE	8.19	128.99	111.80
1	F	35	ARG	CB-CA-C	-8.18	94.04	110.40
1	L	247	PHE	CB-CG-CD2	-8.16	115.08	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	94	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	G	420	LYS	CB-CG-CD	8.15	132.78	111.60
1	B	42	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	B	94	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	E	29	VAL	CG1-CB-CG2	8.11	123.87	110.90
1	F	94	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	D	94	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	I	479	THR	CA-CB-CG2	-8.09	101.08	112.40
1	I	242	PHE	N-CA-CB	-8.07	96.07	110.60
1	I	94	ARG	CD-NE-CZ	8.05	134.88	123.60
1	C	94	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	E	94	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	E	265	ARG	NH1-CZ-NH2	-8.05	110.55	119.40
1	A	94	ARG	CD-NE-CZ	8.04	134.86	123.60
1	G	94	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	J	27	LYS	CA-CB-CG	8.04	131.09	113.40
1	J	94	ARG	CD-NE-CZ	8.01	134.81	123.60
1	H	94	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	I	50	ARG	CD-NE-CZ	7.99	134.79	123.60
1	K	94	ARG	CD-NE-CZ	7.99	134.79	123.60
1	C	27	LYS	CA-CB-CG	7.99	130.98	113.40
1	F	44	ARG	NE-CZ-NH1	-7.97	116.32	120.30
1	D	174	ARG	CB-CG-CD	-7.95	90.92	111.60
1	F	50	ARG	CD-NE-CZ	7.93	134.71	123.60
1	I	242	PHE	CA-CB-CG	7.93	132.94	113.90
1	C	340	LYS	CA-CB-CG	7.93	130.84	113.40
1	C	306	LYS	CD-CE-NZ	7.90	129.87	111.70
1	K	306	LYS	CB-CA-C	-7.90	94.61	110.40
1	G	306	LYS	CA-CB-CG	7.88	130.74	113.40
1	D	35	ARG	CD-NE-CZ	-7.87	112.58	123.60
1	L	308	LYS	CA-CB-CG	7.86	130.70	113.40
1	E	306	LYS	CA-CB-CG	7.85	130.67	113.40
1	C	297	GLN	CA-CB-CG	7.84	130.64	113.40
1	G	314	ILE	CA-CB-CG2	-7.83	95.23	110.90
1	K	35	ARG	CB-CG-CD	7.83	131.94	111.60
1	F	287	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	A	174	ARG	NE-CZ-NH1	-7.82	116.39	120.30
1	G	424	HIS	N-CA-CB	-7.82	96.53	110.60
1	E	35	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	I	291	LEU	CB-CG-CD2	7.81	124.27	111.00
1	H	35	ARG	N-CA-C	7.78	132.02	111.00
1	E	35	ARG	N-CA-C	7.78	131.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	362	GLU	CB-CG-CD	7.75	135.14	114.20
1	L	190	TYR	CB-CG-CD2	-7.74	116.35	121.00
1	K	174	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	K	477	LEU	CB-CG-CD2	-7.74	97.84	111.00
1	D	35	ARG	N-CA-CB	-7.74	96.67	110.60
1	E	423	LYS	CA-CB-CG	7.70	130.34	113.40
1	K	446	LYS	CD-CE-NZ	7.70	129.41	111.70
1	H	338	ARG	NE-CZ-NH2	7.69	124.15	120.30
1	E	333	LYS	N-CA-CB	-7.67	96.79	110.60
1	I	314	ILE	CG1-CB-CG2	-7.67	94.53	111.40
1	I	32	LEU	CB-CG-CD2	-7.67	97.97	111.00
1	E	446	LYS	CB-CG-CD	-7.64	91.75	111.60
1	G	333	LYS	N-CA-CB	-7.64	96.85	110.60
1	D	94	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	D	291	LEU	CB-CG-CD1	-7.63	98.03	111.00
1	A	245	LYS	CD-CE-NZ	7.61	129.21	111.70
1	I	265	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	E	94	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	H	46	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	J	400	LYS	N-CA-CB	7.61	124.29	110.60
1	C	94	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	H	295	LYS	CD-CE-NZ	7.59	129.17	111.70
1	L	439	ARG	NE-CZ-NH1	-7.59	116.50	120.30
1	F	308	LYS	CA-CB-CG	7.59	130.09	113.40
1	I	35	ARG	CD-NE-CZ	-7.57	113.00	123.60
1	G	94	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	B	94	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	H	340	LYS	CA-CB-CG	7.56	130.03	113.40
1	F	11	LYS	CD-CE-NZ	7.56	129.08	111.70
1	I	322	LEU	CB-CG-CD1	7.56	123.85	111.00
1	L	94	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	G	358	LYS	CG-CD-CE	7.55	134.55	111.90
1	I	295	LYS	CD-CE-NZ	7.55	129.06	111.70
1	I	338	ARG	CG-CD-NE	7.53	127.61	111.80
1	F	94	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	C	338	ARG	CG-CD-NE	-7.52	96.00	111.80
1	C	41	LYS	CB-CA-C	7.52	125.44	110.40
1	D	35	ARG	N-CA-C	7.51	131.28	111.00
1	A	363	ARG	CB-CG-CD	-7.51	92.08	111.60
1	I	242	PHE	N-CA-C	7.51	131.28	111.00
1	I	306	LYS	CB-CG-CD	-7.51	92.08	111.60
1	J	174	ARG	CG-CD-NE	7.49	127.52	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	261	ARG	CG-CD-NE	7.47	127.49	111.80
1	H	94	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	J	362	GLU	CB-CA-C	-7.45	95.50	110.40
1	J	338	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	D	50	ARG	CD-NE-CZ	7.42	134.00	123.60
1	A	292	GLU	CB-CA-C	-7.42	95.56	110.40
1	L	340	LYS	CA-CB-CG	7.42	129.71	113.40
1	A	446	LYS	CD-CE-NZ	7.41	128.73	111.70
1	D	50	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	C	32	LEU	CA-CB-CG	7.39	132.30	115.30
1	K	44	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	B	333	LYS	N-CA-CB	-7.37	97.33	110.60
1	B	314	ILE	CG1-CB-CG2	-7.37	95.19	111.40
1	H	44	ARG	CG-CD-NE	7.36	127.26	111.80
1	H	446	LYS	CD-CE-NZ	7.36	128.63	111.70
1	H	306	LYS	CD-CE-NZ	7.36	128.63	111.70
1	G	239	THR	C-N-CA	7.36	152.90	122.00
1	H	46	ARG	CA-CB-CG	7.35	129.56	113.40
1	D	286	ILE	CG1-CB-CG2	-7.34	95.24	111.40
1	E	239	THR	C-N-CA	7.34	152.82	122.00
1	J	338	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	B	42	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	D	174	ARG	CD-NE-CZ	-7.33	113.34	123.60
1	K	314	ILE	CG1-CB-CG2	-7.32	95.29	111.40
1	E	306	LYS	CB-CG-CD	-7.32	92.57	111.60
1	L	311	GLU	OE1-CD-OE2	7.32	132.08	123.30
1	L	42	ARG	NE-CZ-NH1	-7.29	116.65	120.30
1	H	342	LYS	CD-CE-NZ	7.28	128.45	111.70
1	K	296	LEU	CB-CG-CD1	7.28	123.38	111.00
1	A	35	ARG	N-CA-C	7.28	130.65	111.00
1	H	46	ARG	CB-CG-CD	-7.27	92.69	111.60
1	D	306	LYS	CA-CB-CG	7.27	129.39	113.40
1	E	261	ARG	NH1-CZ-NH2	-7.26	111.41	119.40
1	E	11	LYS	CB-CA-C	-7.25	95.90	110.40
1	D	36	GLU	CA-CB-CG	7.24	129.33	113.40
1	F	239	THR	C-N-CA	7.24	152.41	122.00
1	G	245	LYS	CB-CA-C	-7.23	95.94	110.40
1	B	30	GLU	CG-CD-OE1	-7.22	103.86	118.30
1	D	245	LYS	CB-CA-C	-7.22	95.96	110.40
1	E	342	LYS	CB-CG-CD	7.19	130.29	111.60
1	A	340	LYS	CB-CG-CD	-7.18	92.92	111.60
1	D	306	LYS	CB-CA-C	-7.17	96.05	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	34	THR	CA-CB-OG1	7.17	124.05	109.00
1	J	306	LYS	CB-CG-CD	-7.17	92.97	111.60
1	E	329	LYS	CD-CE-NZ	7.15	128.15	111.70
1	I	32	LEU	CB-CA-C	-7.15	96.62	110.20
1	C	174	ARG	NE-CZ-NH1	-7.15	116.73	120.30
1	I	245	LYS	CB-CA-C	-7.14	96.11	110.40
1	A	423	LYS	CG-CD-CE	7.14	133.32	111.90
1	L	269	LYS	CB-CA-C	-7.14	96.13	110.40
1	L	41	LYS	CD-CE-NZ	7.13	128.11	111.70
1	L	66	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	F	32	LEU	CB-CG-CD2	7.11	123.09	111.00
1	B	338	ARG	CD-NE-CZ	-7.10	113.66	123.60
1	A	281	TRP	CB-CG-CD2	7.09	135.81	126.60
1	F	42	ARG	CB-CG-CD	-7.09	93.18	111.60
1	F	306	LYS	CA-CB-CG	7.07	128.96	113.40
1	I	340	LYS	CB-CG-CD	-7.06	93.24	111.60
1	K	245	LYS	CB-CA-C	-7.05	96.30	110.40
1	L	44	ARG	CA-CB-CG	-7.05	97.89	113.40
1	K	143	LYS	CB-CG-CD	7.05	129.92	111.60
1	A	281	TRP	CG-CD1-NE1	7.04	117.14	110.10
1	B	330	GLN	CB-CA-C	7.03	124.46	110.40
1	A	289	LYS	N-CA-C	7.02	129.95	111.00
1	E	134	LYS	CB-CG-CD	7.02	129.85	111.60
1	B	306	LYS	CB-CA-C	-7.02	96.37	110.40
1	E	42	ARG	CB-CG-CD	7.00	129.80	111.60
1	L	35	ARG	N-CA-C	7.00	129.90	111.00
1	I	32	LEU	CB-CG-CD1	-7.00	99.11	111.00
1	G	306	LYS	CB-CA-C	-7.00	96.41	110.40
1	J	340	LYS	CA-CB-CG	6.99	128.77	113.40
1	J	245	LYS	CD-CE-NZ	6.97	127.74	111.70
1	C	35	ARG	NH1-CZ-NH2	6.97	127.07	119.40
1	B	37	THR	OG1-CB-CG2	-6.97	93.98	110.00
1	B	239	THR	C-N-CA	6.96	151.22	122.00
1	I	423	LYS	CD-CE-NZ	6.96	127.70	111.70
1	B	103	GLU	CA-CB-CG	6.94	128.68	113.40
1	H	66	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	C	69	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	E	329	LYS	CB-CG-CD	-6.92	93.61	111.60
1	I	239	THR	C-N-CA	6.92	151.05	122.00
1	L	314	ILE	CG1-CB-CG2	-6.92	96.18	111.40
1	E	134	LYS	CA-CB-CG	-6.92	98.19	113.40
1	A	363	ARG	CA-CB-CG	6.90	128.59	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	32	LEU	CB-CG-CD1	6.89	122.72	111.00
1	J	42	ARG	NE-CZ-NH1	-6.89	116.85	120.30
1	D	44	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	H	36	GLU	N-CA-CB	-6.88	98.22	110.60
1	K	34	THR	CA-CB-CG2	6.86	122.01	112.40
1	J	27	LYS	CB-CG-CD	-6.86	93.76	111.60
1	F	314	ILE	CG1-CB-CG2	-6.85	96.32	111.40
1	H	239	THR	C-N-CA	6.85	150.76	122.00
1	F	30	GLU	CA-CB-CG	6.84	128.44	113.40
1	I	35	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	L	36	GLU	CB-CA-C	-6.83	96.73	110.40
1	I	35	ARG	CB-CA-C	-6.82	96.76	110.40
1	I	308	LYS	CA-CB-CG	6.82	128.39	113.40
1	E	27	LYS	CA-CB-CG	6.81	128.38	113.40
1	A	174	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	L	40	GLN	CB-CA-C	6.80	124.01	110.40
1	E	446	LYS	CD-CE-NZ	6.80	127.34	111.70
1	L	174	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	J	34	THR	OG1-CB-CG2	-6.80	94.37	110.00
1	D	265	ARG	NH1-CZ-NH2	-6.79	111.93	119.40
1	A	281	TRP	CD1-NE1-CE2	-6.78	102.90	109.00
1	K	50	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	H	69	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	E	269	LYS	CD-CE-NZ	-6.78	96.11	111.70
1	D	423	LYS	CA-CB-CG	6.77	128.30	113.40
1	C	239	THR	C-N-CA	6.77	150.42	122.00
1	E	174	ARG	CB-CG-CD	6.76	129.19	111.60
1	B	103	GLU	N-CA-CB	6.76	122.77	110.60
1	K	239	THR	C-N-CA	6.76	150.39	122.00
1	J	421	PHE	N-CA-C	6.75	129.23	111.00
1	D	36	GLU	CB-CA-C	-6.75	96.90	110.40
1	D	297	GLN	CA-CB-CG	-6.75	98.55	113.40
1	F	44	ARG	CD-NE-CZ	6.74	133.04	123.60
1	E	306	LYS	CB-CA-C	-6.73	96.93	110.40
1	G	338	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	C	342	LYS	CB-CA-C	6.71	123.83	110.40
1	K	35	ARG	N-CA-C	6.70	129.10	111.00
1	A	239	THR	C-N-CA	6.70	150.12	122.00
1	A	289	LYS	CB-CA-C	-6.68	97.03	110.40
1	B	36	GLU	N-CA-CB	-6.68	98.57	110.60
1	E	174	ARG	N-CA-CB	-6.68	98.57	110.60
1	G	30	GLU	CB-CA-C	-6.68	97.05	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	35	ARG	CD-NE-CZ	-6.67	114.25	123.60
1	K	134	LYS	CG-CD-CE	6.67	131.90	111.90
1	J	35	ARG	N-CA-C	6.66	128.99	111.00
1	J	421	PHE	CA-CB-CG	6.66	129.89	113.90
1	D	314	ILE	CA-CB-CG2	-6.65	97.60	110.90
1	G	35	ARG	N-CA-C	6.64	128.92	111.00
1	H	245	LYS	CD-CE-NZ	6.63	126.95	111.70
1	H	420	LYS	CD-CE-NZ	6.63	126.95	111.70
1	B	35	ARG	NH1-CZ-NH2	6.62	126.68	119.40
1	A	235	ILE	CB-CG1-CD1	6.60	132.39	113.90
1	B	289	LYS	CB-CA-C	-6.60	97.19	110.40
1	D	309	ILE	CG1-CB-CG2	6.60	125.92	111.40
1	H	46	ARG	CD-NE-CZ	6.59	132.83	123.60
1	C	306	LYS	CA-CB-CG	6.57	127.86	113.40
1	B	265	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	F	338	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	G	333	LYS	CA-CB-CG	6.54	127.78	113.40
1	K	53	LYS	CB-CA-C	-6.53	97.33	110.40
1	F	281	TRP	CB-CG-CD2	6.52	135.08	126.60
1	B	42	ARG	CB-CG-CD	-6.52	94.65	111.60
1	F	174	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	H	287	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	E	36	GLU	CG-CD-OE1	-6.48	105.34	118.30
1	D	130	LYS	CG-CD-CE	6.48	131.33	111.90
1	L	239	THR	C-N-CA	6.48	149.20	122.00
1	I	284	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	B	296	LEU	CB-CG-CD1	6.47	121.99	111.00
1	G	34	THR	OG1-CB-CG2	-6.46	95.13	110.00
1	E	11	LYS	CA-CB-CG	6.46	127.61	113.40
1	K	296	LEU	CB-CG-CD2	-6.45	100.04	111.00
1	L	424	HIS	ND1-CE1-NE2	-6.44	95.73	109.90
1	B	296	LEU	CB-CG-CD2	-6.44	100.06	111.00
1	L	311	GLU	CG-CD-OE1	-6.43	105.44	118.30
1	D	329	LYS	CB-CG-CD	-6.43	94.89	111.60
1	G	66	ARG	CD-NE-CZ	6.42	132.59	123.60
1	L	44	ARG	NE-CZ-NH1	-6.41	117.09	120.30
1	L	19	ARG	CD-NE-CZ	6.40	132.57	123.60
1	H	311	GLU	N-CA-CB	-6.40	99.08	110.60
1	L	275	GLU	CB-CA-C	-6.39	97.61	110.40
1	L	269	LYS	CB-CG-CD	6.39	128.20	111.60
1	B	402	GLU	CA-CB-CG	6.38	127.43	113.40
1	F	27	LYS	CA-CB-CG	6.38	127.43	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	239	THR	C-N-CA	6.38	148.78	122.00
1	K	306	LYS	CA-CB-CG	6.35	127.38	113.40
1	K	363	ARG	NE-CZ-NH1	-6.35	117.13	120.30
1	F	338	ARG	CG-CD-NE	6.35	125.13	111.80
1	J	400	LYS	CG-CD-CE	6.34	130.93	111.90
1	G	50	ARG	CG-CD-NE	-6.34	98.49	111.80
1	L	30	GLU	CA-CB-CG	6.33	127.34	113.40
1	F	265	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	F	245	LYS	CB-CA-C	-6.33	97.74	110.40
1	G	174	ARG	CB-CG-CD	-6.33	95.15	111.60
1	K	27	LYS	CA-CB-CG	6.32	127.31	113.40
1	A	308	LYS	CD-CE-NZ	6.29	126.18	111.70
1	B	174	ARG	CG-CD-NE	6.29	125.00	111.80
1	I	30	GLU	CG-CD-OE2	6.28	130.86	118.30
1	K	34	THR	OG1-CB-CG2	-6.27	95.57	110.00
1	L	363	ARG	CD-NE-CZ	-6.27	114.82	123.60
1	I	30	GLU	CG-CD-OE1	-6.26	105.77	118.30
1	L	439	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	J	30	GLU	CB-CA-C	-6.25	97.90	110.40
1	J	239	THR	C-N-CA	6.24	148.22	122.00
1	J	289	LYS	CD-CE-NZ	6.24	126.05	111.70
1	A	46	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	C	245	LYS	CB-CA-C	-6.17	98.06	110.40
1	G	295	LYS	CA-CB-CG	6.17	126.98	113.40
1	B	27	LYS	CA-CB-CG	6.17	126.97	113.40
1	L	27	LYS	CB-CG-CD	-6.17	95.57	111.60
1	G	420	LYS	CD-CE-NZ	6.16	125.87	111.70
1	D	296	LEU	CB-CG-CD2	6.16	121.47	111.00
1	H	245	LYS	N-CA-C	6.14	127.59	111.00
1	G	338	ARG	CD-NE-CZ	-6.14	115.01	123.60
1	H	44	ARG	CD-NE-CZ	-6.13	115.01	123.60
1	E	423	LYS	CB-CA-C	-6.13	98.15	110.40
1	K	11	LYS	CD-CE-NZ	6.13	125.79	111.70
1	H	363	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	I	143	LYS	CB-CG-CD	6.12	127.50	111.60
1	E	35	ARG	CG-CD-NE	-6.11	98.96	111.80
1	H	329	LYS	CB-CG-CD	-6.11	95.71	111.60
1	A	42	ARG	CD-NE-CZ	-6.11	115.05	123.60
1	J	400	LYS	CB-CA-C	-6.10	98.20	110.40
1	G	308	LYS	CA-CB-CG	6.10	126.82	113.40
1	F	42	ARG	CA-CB-CG	6.10	126.82	113.40
1	K	34	THR	N-CA-CB	-6.10	98.72	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	34	THR	OG1-CB-CG2	-6.09	95.99	110.00
1	C	174	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	H	44	ARG	CB-CG-CD	6.08	127.41	111.60
1	E	363	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	B	363	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	E	30	GLU	CB-CA-C	-6.06	98.29	110.40
1	E	333	LYS	CA-CB-CG	6.06	126.73	113.40
1	A	340	LYS	CD-CE-NZ	-6.05	97.78	111.70
1	D	328	GLU	CA-CB-CG	6.04	126.70	113.40
1	E	295	LYS	CD-CE-NZ	6.04	125.60	111.70
1	H	245	LYS	CB-CA-C	-6.04	98.33	110.40
1	F	363	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	G	32	LEU	CB-CG-CD2	6.03	121.25	111.00
1	B	296	LEU	CB-CA-C	-6.02	98.76	110.20
1	J	308	LYS	CB-CA-C	-6.01	98.38	110.40
1	C	44	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	I	242	PHE	CG-CD2-CE2	-6.00	114.20	120.80
1	B	333	LYS	CA-CB-CG	5.99	126.57	113.40
1	A	420	LYS	CG-CD-CE	5.98	129.85	111.90
1	F	340	LYS	CA-CB-CG	5.98	126.55	113.40
1	G	363	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	C	41	LYS	CB-CG-CD	-5.97	96.07	111.60
1	H	423	LYS	CA-CB-CG	5.97	126.53	113.40
1	I	308	LYS	CB-CA-C	-5.97	98.46	110.40
1	I	235	ILE	CB-CG1-CD1	5.96	130.60	113.90
1	D	46	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	L	275	GLU	CG-CD-OE1	-5.96	106.37	118.30
1	K	308	LYS	N-CA-CB	-5.96	99.88	110.60
1	G	329	LYS	CA-CB-CG	5.95	126.49	113.40
1	K	143	LYS	CG-CD-CE	5.95	129.75	111.90
1	L	424	HIS	CB-CA-C	-5.95	98.51	110.40
1	G	295	LYS	CB-CA-C	-5.94	98.51	110.40
1	L	312	GLY	N-CA-C	-5.93	98.26	113.10
1	C	275	GLU	CA-CB-CG	5.93	126.44	113.40
1	C	42	ARG	CA-CB-CG	5.92	126.43	113.40
1	H	423	LYS	CB-CA-C	-5.91	98.57	110.40
1	L	269	LYS	CD-CE-NZ	-5.91	98.11	111.70
1	E	311	GLU	N-CA-CB	-5.90	99.99	110.60
1	L	424	HIS	ND1-CG-CD2	-5.89	97.75	106.00
1	D	245	LYS	CD-CE-NZ	5.89	125.25	111.70
1	A	292	GLU	N-CA-CB	5.89	121.20	110.60
1	I	174	ARG	NE-CZ-NH1	-5.89	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	42	ARG	CD-NE-CZ	-5.88	115.36	123.60
1	G	245	LYS	N-CA-C	5.88	126.88	111.00
1	K	308	LYS	CB-CA-C	5.88	122.16	110.40
1	C	421	PHE	N-CA-CB	-5.88	100.02	110.60
1	G	67	ARG	CD-NE-CZ	-5.87	115.38	123.60
1	G	327	SER	CA-CB-OG	5.87	127.05	111.20
1	I	35	ARG	CA-CB-CG	5.85	126.27	113.40
1	I	289	LYS	CB-CA-C	-5.83	98.73	110.40
1	G	269	LYS	CA-CB-CG	-5.83	100.58	113.40
1	F	340	LYS	CB-CA-C	-5.82	98.77	110.40
1	D	363	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	A	46	ARG	NE-CZ-NH2	5.81	123.20	120.30
1	L	46	ARG	CG-CD-NE	5.80	123.98	111.80
1	K	35	ARG	CA-CB-CG	-5.80	100.64	113.40
1	J	174	ARG	CA-CB-CG	5.79	126.14	113.40
1	L	174	ARG	CG-CD-NE	5.79	123.95	111.80
1	G	269	LYS	CD-CE-NZ	-5.79	98.39	111.70
1	K	363	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	I	328	GLU	CG-CD-OE1	-5.78	106.74	118.30
1	G	333	LYS	N-CA-C	5.78	126.60	111.00
1	L	423	LYS	CB-CA-C	-5.77	98.86	110.40
1	I	11	LYS	CB-CG-CD	5.76	126.58	111.60
1	E	38	GLU	CA-CB-CG	5.76	126.06	113.40
1	A	338	ARG	CG-CD-NE	-5.75	99.72	111.80
1	L	46	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	B	316	GLU	CG-CD-OE2	5.75	129.79	118.30
1	D	328	GLU	CG-CD-OE2	5.75	129.79	118.30
1	F	329	LYS	N-CA-CB	-5.74	100.26	110.60
1	K	27	LYS	CG-CD-CE	5.73	129.10	111.90
1	E	169	MET	CA-CB-CG	-5.72	103.58	113.30
1	D	9	PHE	CB-CA-C	-5.71	98.99	110.40
1	G	174	ARG	CD-NE-CZ	-5.70	115.62	123.60
1	L	338	ARG	CA-CB-CG	-5.70	100.87	113.40
1	L	338	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	44	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	L	329	LYS	CB-CG-CD	-5.68	96.82	111.60
1	J	35	ARG	CB-CG-CD	-5.68	96.82	111.60
1	H	265	ARG	CB-CA-C	-5.68	99.04	110.40
1	G	308	LYS	CB-CA-C	-5.68	99.05	110.40
1	J	363	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	L	190	TYR	CB-CG-CD1	5.67	124.40	121.00
1	J	289	LYS	N-CA-C	5.67	126.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	LYS	N-CA-C	5.63	126.22	111.00
1	A	261	ARG	N-CA-CB	5.63	120.74	110.60
1	B	289	LYS	N-CA-C	5.63	126.21	111.00
1	I	35	ARG	N-CA-CB	-5.63	100.46	110.60
1	K	174	ARG	CB-CG-CD	-5.63	96.96	111.60
1	D	31	ASP	CB-CG-OD1	5.63	123.37	118.30
1	E	32	LEU	CB-CA-C	-5.63	99.51	110.20
1	I	11	LYS	CA-CB-CG	-5.62	101.05	113.40
1	I	33	LYS	N-CA-C	-5.61	95.86	111.00
1	J	306	LYS	CA-CB-CG	5.61	125.74	113.40
1	K	134	LYS	CD-CE-NZ	5.61	124.59	111.70
1	D	295	LYS	CD-CE-NZ	5.59	124.57	111.70
1	H	174	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	K	446	LYS	CB-CG-CD	-5.59	97.06	111.60
1	G	44	ARG	CB-CG-CD	5.59	126.13	111.60
1	J	421	PHE	CG-CD2-CE2	-5.59	114.66	120.80
1	A	44	ARG	CB-CG-CD	5.58	126.11	111.60
1	F	34	THR	N-CA-CB	-5.58	99.70	110.30
1	A	174	ARG	CG-CD-NE	5.58	123.51	111.80
1	K	289	LYS	CB-CA-C	-5.57	99.26	110.40
1	D	421	PHE	N-CA-CB	-5.56	100.58	110.60
1	F	281	TRP	CD1-NE1-CE2	-5.56	103.99	109.00
1	F	358	LYS	CB-CG-CD	-5.56	97.14	111.60
1	B	169	MET	CB-CG-SD	5.56	129.07	112.40
1	C	339	VAL	N-CA-C	-5.55	96.01	111.00
1	G	265	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	L	289	LYS	N-CA-C	5.55	125.98	111.00
1	H	333	LYS	CB-CG-CD	-5.54	97.20	111.60
1	A	316	GLU	CG-CD-OE2	5.53	129.37	118.30
1	L	29	VAL	CG1-CB-CG2	5.53	119.75	110.90
1	H	308	LYS	CD-CE-NZ	5.53	124.42	111.70
1	A	105	LYS	CG-CD-CE	-5.53	95.31	111.90
1	F	297	GLN	CA-CB-CG	5.53	125.56	113.40
1	C	37	THR	OG1-CB-CG2	-5.52	97.29	110.00
1	D	338	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	B	311	GLU	CA-CB-CG	5.52	125.54	113.40
1	B	245	LYS	N-CA-C	5.49	125.83	111.00
1	H	298	HIS	CA-CB-CG	5.49	122.93	113.60
1	C	27	LYS	CG-CD-CE	5.47	128.32	111.90
1	A	363	ARG	CG-CD-NE	5.46	123.25	111.80
1	C	338	ARG	CB-CA-C	-5.45	99.50	110.40
1	I	42	ARG	CG-CD-NE	-5.45	100.36	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	32	LEU	CB-CG-CD1	5.45	120.26	111.00
1	H	298	HIS	CG-CD2-NE2	5.45	119.55	109.20
1	A	245	LYS	CA-CB-CG	-5.44	101.43	113.40
1	B	269	LYS	CB-CA-C	-5.44	99.52	110.40
1	K	269	LYS	N-CA-C	5.44	125.68	111.00
1	G	50	ARG	CA-CB-CG	5.43	125.35	113.40
1	L	295	LYS	CA-CB-CG	5.43	125.35	113.40
1	C	265	ARG	CB-CA-C	-5.43	99.55	110.40
1	L	265	ARG	CG-CD-NE	5.43	123.20	111.80
1	D	50	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	F	329	LYS	CD-CE-NZ	5.42	124.18	111.70
1	G	338	ARG	CA-CB-CG	-5.42	101.47	113.40
1	F	306	LYS	N-CA-CB	-5.41	100.87	110.60
1	I	286	ILE	CG1-CB-CG2	-5.40	99.51	111.40
1	J	265	ARG	CB-CG-CD	-5.40	97.57	111.60
1	H	340	LYS	CB-CA-C	-5.39	99.61	110.40
1	F	38	GLU	N-CA-C	-5.39	96.45	111.00
1	D	311	GLU	N-CA-CB	-5.38	100.91	110.60
1	H	306	LYS	CG-CD-CE	-5.38	95.75	111.90
1	I	44	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	292	GLU	OE1-CD-OE2	-5.38	116.85	123.30
1	F	243	GLY	N-CA-C	-5.37	99.67	113.10
1	K	19	ARG	CD-NE-CZ	-5.37	116.08	123.60
1	H	238	MET	CA-CB-CG	5.37	122.43	113.30
1	G	327	SER	CB-CA-C	-5.37	99.90	110.10
1	B	169	MET	CA-CB-CG	-5.36	104.18	113.30
1	C	295	LYS	N-CA-CB	5.36	120.25	110.60
1	L	86	ARG	N-CA-CB	5.36	120.24	110.60
1	L	424	HIS	CB-CG-ND1	5.36	136.59	123.20
1	J	329	LYS	CB-CG-CD	-5.35	97.68	111.60
1	H	265	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	G	328	GLU	CG-CD-OE2	5.35	129.00	118.30
1	I	340	LYS	CA-CB-CG	5.34	125.16	113.40
1	B	245	LYS	CB-CA-C	-5.34	99.71	110.40
1	A	261	ARG	CA-CB-CG	5.34	125.15	113.40
1	D	290	GLU	CG-CD-OE1	-5.34	107.63	118.30
1	F	46	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	G	340	LYS	CA-CB-CG	5.33	125.13	113.40
1	F	329	LYS	CB-CA-C	5.33	121.06	110.40
1	A	261	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	H	437	GLN	CA-CB-CG	-5.32	101.69	113.40
1	L	295	LYS	N-CA-CB	-5.32	101.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	GLY	N-CA-C	-5.31	99.82	113.10
1	L	84	GLN	CB-CA-C	-5.31	99.78	110.40
1	B	308	LYS	CB-CA-C	-5.31	99.79	110.40
1	D	243	GLY	N-CA-C	-5.30	99.85	113.10
1	L	296	LEU	CD1-CG-CD2	-5.30	94.60	110.50
1	G	27	LYS	CB-CA-C	5.29	120.99	110.40
1	E	358	LYS	CG-CD-CE	5.29	127.77	111.90
1	G	421	PHE	N-CA-CB	-5.29	101.08	110.60
1	I	333	LYS	CB-CG-CD	-5.28	97.86	111.60
1	K	340	LYS	CA-CB-CG	5.28	125.02	113.40
1	K	423	LYS	CD-CE-NZ	-5.28	99.55	111.70
1	G	19	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	316	GLU	OE1-CD-OE2	-5.27	116.97	123.30
1	F	281	TRP	CB-CG-CD1	-5.27	120.15	127.00
1	F	333	LYS	N-CA-C	5.27	125.23	111.00
1	C	332	THR	N-CA-C	-5.26	96.79	111.00
1	C	338	ARG	CA-CB-CG	5.26	124.98	113.40
1	I	297	GLN	CA-CB-CG	5.26	124.98	113.40
1	C	246	THR	OG1-CB-CG2	5.25	122.08	110.00
1	I	37	THR	OG1-CB-CG2	-5.25	97.94	110.00
1	G	32	LEU	CA-CB-CG	5.24	127.36	115.30
1	L	245	LYS	CB-CA-C	-5.24	99.92	110.40
1	A	311	GLU	CA-CB-CG	5.24	124.92	113.40
1	G	340	LYS	CB-CG-CD	-5.23	98.00	111.60
1	B	409	LEU	CB-CG-CD2	5.23	119.89	111.00
1	L	423	LYS	N-CA-C	5.22	125.09	111.00
1	C	44	ARG	CG-CD-NE	-5.21	100.85	111.80
1	C	339	VAL	CG1-CB-CG2	5.21	119.24	110.90
1	I	11	LYS	CB-CA-C	-5.21	99.98	110.40
1	I	11	LYS	N-CA-C	5.21	125.06	111.00
1	F	338	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	J	265	ARG	CG-CD-NE	5.20	122.72	111.80
1	F	44	ARG	CB-CG-CD	5.19	125.10	111.60
1	K	265	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	F	38	GLU	CA-CB-CG	5.19	124.82	113.40
1	D	333	LYS	N-CA-C	5.18	125.00	111.00
1	G	36	GLU	CA-C-N	-5.18	105.80	117.20
1	B	38	GLU	CA-CB-CG	5.18	124.80	113.40
1	H	174	ARG	CG-CD-NE	5.18	122.67	111.80
1	E	420	LYS	CD-CE-NZ	5.18	123.61	111.70
1	G	340	LYS	CB-CA-C	-5.18	100.05	110.40
1	B	134	LYS	CG-CD-CE	5.17	127.41	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	LYS	N-CA-CB	-5.17	101.30	110.60
1	F	281	TRP	CZ3-CH2-CZ2	-5.17	115.40	121.60
1	I	415	GLU	CA-CB-CG	5.17	124.76	113.40
1	E	342	LYS	CG-CD-CE	-5.16	96.41	111.90
1	K	38	GLU	CA-CB-CG	5.16	124.75	113.40
1	B	340	LYS	CA-CB-CG	5.16	124.74	113.40
1	L	338	ARG	CB-CG-CD	5.16	125.00	111.60
1	J	36	GLU	CA-C-N	-5.15	105.86	117.20
1	H	311	GLU	CB-CA-C	5.15	120.70	110.40
1	C	295	LYS	CB-CA-C	-5.15	100.11	110.40
1	H	340	LYS	CG-CD-CE	-5.14	96.47	111.90
1	L	36	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	F	306	LYS	CD-CE-NZ	5.14	123.52	111.70
1	D	322	LEU	CB-CG-CD2	5.13	119.73	111.00
1	E	297	GLN	CA-CB-CG	-5.13	102.11	113.40
1	J	243	GLY	N-CA-C	-5.13	100.28	113.10
1	J	423	LYS	CB-CA-C	-5.12	100.16	110.40
1	D	37	THR	OG1-CB-CG2	-5.12	98.22	110.00
1	B	41	LYS	CG-CD-CE	5.12	127.25	111.90
1	C	87	THR	C-N-CD	5.11	139.14	128.40
1	C	11	LYS	CB-CG-CD	5.11	124.89	111.60
1	E	44	ARG	CG-CD-NE	5.11	122.53	111.80
1	C	243	GLY	N-CA-C	-5.11	100.33	113.10
1	K	174	ARG	CD-NE-CZ	-5.11	116.45	123.60
1	L	420	LYS	CD-CE-NZ	5.11	123.44	111.70
1	J	42	ARG	CA-CB-CG	5.10	124.62	113.40
1	K	41	LYS	CA-CB-CG	5.10	124.62	113.40
1	B	11	LYS	CB-CG-CD	-5.10	98.35	111.60
1	K	38	GLU	N-CA-C	-5.10	97.24	111.00
1	F	174	ARG	CB-CG-CD	-5.08	98.40	111.60
1	B	243	GLY	N-CA-C	-5.08	100.41	113.10
1	H	42	ARG	CB-CA-C	-5.07	100.25	110.40
1	C	9	PHE	N-CA-C	5.07	124.68	111.00
1	C	11	LYS	CB-CA-C	-5.07	100.26	110.40
1	H	269	LYS	N-CA-C	5.06	124.65	111.00
1	D	32	LEU	CA-CB-CG	5.05	126.92	115.30
1	E	314	ILE	CG1-CB-CG2	-5.04	100.31	111.40
1	G	297	GLN	CA-CB-CG	5.04	124.50	113.40
1	H	309	ILE	CG1-CB-CG2	5.04	122.50	111.40
1	E	35	ARG	CA-CB-CG	-5.04	102.31	113.40
1	B	338	ARG	CA-CB-CG	-5.04	102.32	113.40
1	E	35	ARG	N-CA-CB	-5.04	101.53	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	402	GLU	CA-CB-CG	5.04	124.48	113.40
1	K	174	ARG	CG-CD-NE	5.04	122.38	111.80
1	A	342	LYS	CD-CE-NZ	5.03	123.28	111.70
1	G	340	LYS	CD-CE-NZ	-5.03	100.12	111.70
1	E	296	LEU	CD1-CG-CD2	-5.03	95.40	110.50
1	D	31	ASP	CB-CA-C	5.03	120.46	110.40
1	H	245	LYS	CA-CB-CG	-5.03	102.35	113.40
1	J	245	LYS	CA-CB-CG	-5.02	102.36	113.40
1	K	287	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	E	46	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	I	286	ILE	N-CA-C	-5.01	97.47	111.00
1	G	134	LYS	CG-CD-CE	5.01	126.93	111.90
1	B	358	LYS	CB-CG-CD	-5.01	98.58	111.60
1	C	265	ARG	CB-CG-CD	-5.00	98.59	111.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	34	THR	CB

All (184) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	HIS	Sidechain
1	A	238	MET	Peptide
1	A	281	TRP	Peptide
1	A	288	PRO	Peptide
1	A	296	LEU	Peptide
1	A	31	ASP	Peptide
1	A	310	TYR	Peptide
1	A	332	THR	Peptide
1	A	337	PRO	Peptide
1	A	34	THR	Peptide
1	A	35	ARG	Sidechain
1	A	42	ARG	Peptide
1	A	420	LYS	Peptide
1	A	43	ASN	Peptide
1	B	189	HIS	Sidechain
1	B	238	MET	Peptide
1	B	281	TRP	Peptide
1	B	288	PRO	Peptide
1	B	296	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	B	31	ASP	Peptide
1	B	310	TYR	Peptide
1	B	316	GLU	Sidechain
1	B	328	GLU	Peptide
1	B	332	THR	Peptide
1	B	337	PRO	Peptide
1	B	34	THR	Peptide
1	B	36	GLU	Peptide
1	B	42	ARG	Peptide
1	B	420	LYS	Peptide
1	B	43	ASN	Peptide
1	C	238	MET	Peptide
1	C	281	TRP	Peptide
1	C	288	PRO	Peptide
1	C	296	LEU	Peptide
1	C	307	ALA	Peptide
1	C	31	ASP	Peptide
1	C	310	TYR	Peptide
1	C	332	THR	Peptide
1	C	337	PRO	Peptide
1	C	339	VAL	Peptide
1	C	34	THR	Peptide
1	C	42	ARG	Peptide
1	C	420	LYS	Peptide
1	C	421	PHE	Sidechain
1	C	43	ASN	Peptide
1	D	238	MET	Peptide
1	D	288	PRO	Peptide
1	D	29	VAL	Peptide
1	D	298	HIS	Sidechain
1	D	31	ASP	Peptide
1	D	310	TYR	Peptide
1	D	328	GLU	Peptide
1	D	332	THR	Peptide
1	D	337	PRO	Peptide
1	D	34	THR	Peptide
1	D	36	GLU	Peptide
1	D	38	GLU	Peptide
1	D	42	ARG	Peptide
1	D	420	LYS	Peptide
1	D	421	PHE	Sidechain
1	D	43	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	E	173	GLU	Peptide
1	E	174	ARG	Sidechain
1	E	239	THR	Peptide
1	E	281	TRP	Peptide
1	E	288	PRO	Peptide
1	E	296	LEU	Peptide
1	E	31	ASP	Peptide
1	E	310	TYR	Peptide
1	E	32	LEU	Mainchain
1	E	332	THR	Peptide
1	E	34	THR	Peptide
1	E	36	GLU	Peptide
1	E	37	THR	Peptide
1	E	42	ARG	Peptide
1	E	420	LYS	Peptide
1	E	424	HIS	Mainchain
1	F	238	MET	Peptide
1	F	281	TRP	Peptide
1	F	288	PRO	Peptide
1	F	29	VAL	Peptide
1	F	296	LEU	Peptide
1	F	307	ALA	Peptide
1	F	31	ASP	Peptide
1	F	310	TYR	Peptide
1	F	328	GLU	Peptide
1	F	332	THR	Peptide
1	F	337	PRO	Peptide
1	F	34	THR	Peptide
1	F	37	THR	Peptide
1	F	42	ARG	Peptide
1	F	420	LYS	Peptide
1	F	43	ASN	Peptide
1	F	44	ARG	Sidechain
1	G	238	MET	Peptide
1	G	281	TRP	Peptide
1	G	288	PRO	Peptide
1	G	296	LEU	Peptide
1	G	308	LYS	Peptide
1	G	31	ASP	Peptide
1	G	310	TYR	Peptide
1	G	332	THR	Peptide
1	G	337	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	G	34	THR	Peptide
1	G	35	ARG	Sidechain
1	G	42	ARG	Peptide
1	G	420	LYS	Peptide
1	G	43	ASN	Peptide
1	H	238	MET	Peptide
1	H	288	PRO	Peptide
1	H	29	VAL	Peptide
1	H	296	LEU	Peptide
1	H	31	ASP	Peptide
1	H	310	TYR	Peptide
1	H	337	PRO	Peptide
1	H	34	THR	Peptide
1	H	42	ARG	Peptide
1	H	420	LYS	Peptide
1	H	43	ASN	Peptide
1	I	19	ARG	Sidechain
1	I	238	MET	Peptide
1	I	241	GLY	Peptide
1	I	242	PHE	Sidechain
1	I	281	TRP	Peptide
1	I	288	PRO	Peptide
1	I	29	VAL	Peptide
1	I	296	LEU	Peptide
1	I	30	GLU	Sidechain
1	I	31	ASP	Peptide
1	I	310	TYR	Peptide
1	I	328	GLU	Peptide,Sidechain
1	I	337	PRO	Peptide
1	I	34	THR	Peptide
1	I	38	GLU	Peptide
1	I	42	ARG	Peptide
1	I	420	LYS	Peptide
1	I	44	ARG	Sidechain
1	J	189	HIS	Sidechain
1	J	238	MET	Peptide
1	J	281	TRP	Peptide
1	J	296	LEU	Peptide
1	J	298	HIS	Sidechain
1	J	31	ASP	Peptide
1	J	310	TYR	Peptide
1	J	332	THR	Peptide

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Mol	Chain	Res	Type	Group
1	J	337	PRO	Peptide
1	J	34	THR	Peptide
1	J	42	ARG	Peptide
1	J	421	PHE	Sidechain
1	J	499	THR	Peptide
1	K	238	MET	Peptide
1	K	281	TRP	Peptide
1	K	288	PRO	Peptide
1	K	298	HIS	Sidechain
1	K	307	ALA	Peptide
1	K	31	ASP	Peptide
1	K	310	TYR	Peptide
1	K	332	THR	Peptide
1	K	337	PRO	Peptide
1	K	34	THR	Peptide
1	K	37	THR	Peptide
1	K	42	ARG	Peptide
1	K	420	LYS	Peptide
1	K	43	ASN	Peptide
1	K	476	ASP	Peptide
1	L	19	ARG	Sidechain
1	L	238	MET	Peptide
1	L	281	TRP	Peptide
1	L	29	VAL	Peptide
1	L	292	GLU	Sidechain
1	L	295	LYS	Peptide
1	L	296	LEU	Peptide
1	L	31	ASP	Peptide
1	L	310	TYR	Peptide
1	L	332	THR	Peptide
1	L	339	VAL	Peptide
1	L	34	THR	Peptide
1	L	35	ARG	Sidechain
1	L	37	THR	Peptide
1	L	42	ARG	Peptide
1	L	420	LYS	Peptide
1	L	424	HIS	Mainchain
1	L	43	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3875	0	3844	220	0
1	B	3875	0	3845	188	0
1	C	3875	0	3845	190	2
1	D	3875	0	3845	199	0
1	E	3875	0	3845	199	2
1	F	3875	0	3845	194	0
1	G	3875	0	3845	188	0
1	H	3875	0	3845	184	0
1	I	3875	0	3844	202	0
1	J	3875	0	3845	185	0
1	K	3875	0	3845	194	0
1	L	3875	0	3845	210	0
2	A	27	0	12	0	0
2	B	27	0	12	2	0
2	C	54	0	24	2	0
2	D	27	0	12	1	0
2	F	27	0	12	1	0
2	G	27	0	12	0	0
2	H	27	0	12	2	0
2	I	27	0	12	0	0
2	J	27	0	12	0	0
2	K	27	0	12	0	0
2	L	27	0	12	1	0
All	All	46824	0	46282	2215	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (2215) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:LEU:CD2	1:D:291:LEU:CG	1.81	1.54
1:I:33:LYS:NZ	1:I:33:LYS:CE	1.69	1.52
1:A:423:LYS:NZ	1:H:437:GLN:HE21	1.42	1.16
1:I:241:GLY:O	1:I:242:PHE:HB3	1.39	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:239:THR:HG21	1:G:428:ILE:HD13	1.30	1.11
1:I:32:LEU:HD13	1:I:33:LYS:HD2	1.25	1.10
1:F:437:GLN:HG2	1:G:244:ASP:HB2	1.35	1.08
1:I:281:TRP:HE1	1:I:283:PRO:HD3	1.18	1.08
1:D:240:PRO:HG3	1:D:245:LYS:HZ3	1.14	1.08
1:D:240:PRO:HG3	1:D:245:LYS:NZ	1.71	1.04
1:D:18:ASP:OD1	1:D:53:LYS:NZ	1.90	1.03
1:G:240:PRO:HG2	1:G:245:LYS:NZ	1.73	1.03
1:G:18:ASP:OD1	1:G:53:LYS:NZ	1.92	1.01
1:I:18:ASP:OD1	1:I:53:LYS:NZ	1.95	1.00
1:C:240:PRO:HG2	1:C:245:LYS:NZ	1.78	0.99
1:J:419:ARG:C	1:J:421:PHE:H	1.61	0.98
1:C:35:ARG:HB3	1:C:35:ARG:HH21	1.25	0.98
1:J:18:ASP:OD1	1:J:53:LYS:NZ	1.97	0.97
1:B:44:ARG:HH11	1:B:44:ARG:HG2	1.27	0.97
1:C:18:ASP:OD1	1:C:53:LYS:NZ	1.98	0.97
1:B:18:ASP:OD1	1:B:53:LYS:NZ	1.97	0.96
1:E:18:ASP:OD1	1:E:53:LYS:NZ	1.97	0.96
1:A:423:LYS:HZ2	1:H:437:GLN:NE2	1.63	0.96
1:F:18:ASP:OD1	1:F:53:LYS:NZ	1.97	0.96
1:A:18:ASP:OD1	1:A:53:LYS:NZ	1.96	0.96
1:H:18:ASP:OD1	1:H:53:LYS:NZ	1.97	0.96
1:I:281:TRP:HE1	1:I:283:PRO:CD	1.78	0.96
1:A:281:TRP:HE1	1:A:283:PRO:HD3	1.26	0.96
1:K:18:ASP:OD1	1:K:53:LYS:NZ	1.98	0.96
1:E:335:ASN:HA	1:E:338:ARG:HD2	1.44	0.95
1:L:33:LYS:O	1:L:35:ARG:N	2.01	0.94
1:E:400:LYS:HD2	1:E:403:ARG:HH21	1.33	0.93
1:K:31:ASP:OD2	1:K:470:LYS:NZ	2.02	0.93
1:L:18:ASP:OD1	1:L:53:LYS:NZ	2.00	0.93
1:F:244:ASP:HB2	1:G:437:GLN:HG2	1.50	0.92
1:D:291:LEU:CD2	1:D:291:LEU:CB	2.46	0.92
1:A:240:PRO:HG2	1:A:245:LYS:NZ	1.86	0.91
1:J:400:LYS:HD2	1:J:403:ARG:HH21	1.33	0.91
1:J:33:LYS:O	1:J:35:ARG:N	2.04	0.91
1:L:240:PRO:HG3	1:L:245:LYS:NZ	1.85	0.91
1:B:240:PRO:HG2	1:B:245:LYS:NZ	1.85	0.91
1:F:400:LYS:HD2	1:F:403:ARG:HH21	1.35	0.90
1:D:33:LYS:O	1:D:35:ARG:N	2.05	0.90
1:L:33:LYS:HB3	1:L:36:GLU:HG3	1.52	0.90
1:B:305:PRO:O	1:B:306:LYS:HB2	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:240:PRO:HG3	1:J:245:LYS:HZ2	1.35	0.89
1:E:42:ARG:C	1:E:44:ARG:H	1.72	0.89
1:E:240:PRO:HG3	1:E:245:LYS:NZ	1.88	0.89
1:C:33:LYS:O	1:C:35:ARG:N	2.06	0.88
1:D:9:PHE:CZ	1:D:328:GLU:OE2	2.26	0.88
1:F:394:TYR:HB2	1:F:445:GLU:HG3	1.54	0.88
1:K:240:PRO:HG2	1:K:245:LYS:HZ3	1.38	0.88
1:C:233:MET:HB3	1:C:239:THR:H	1.39	0.88
1:E:33:LYS:O	1:E:35:ARG:N	2.05	0.88
1:I:42:ARG:C	1:I:44:ARG:H	1.77	0.87
1:K:33:LYS:O	1:K:35:ARG:N	2.05	0.87
1:H:240:PRO:HG2	1:H:245:LYS:NZ	1.90	0.87
1:A:423:LYS:HZ2	1:H:437:GLN:HE21	0.90	0.87
1:G:30:GLU:O	1:G:32:LEU:N	2.08	0.87
1:I:240:PRO:HG2	1:I:245:LYS:NZ	1.90	0.87
1:I:499:THR:HA	1:L:66:ARG:HH11	1.41	0.86
1:G:394:TYR:HB2	1:G:445:GLU:HG3	1.57	0.86
1:G:240:PRO:HG2	1:G:245:LYS:HZ3	1.39	0.86
1:A:233:MET:HB3	1:A:239:THR:H	1.41	0.86
1:A:281:TRP:C	1:A:281:TRP:HD1	1.79	0.86
1:D:33:LYS:HB3	1:D:36:GLU:HG3	1.55	0.86
1:E:233:MET:HB3	1:E:239:THR:H	1.40	0.86
1:E:294:PHE:CE1	1:E:298:HIS:HE1	1.92	0.86
1:B:328:GLU:HB3	1:B:329:LYS:HG3	1.58	0.85
1:G:233:MET:HB3	1:G:239:THR:H	1.41	0.85
1:C:281:TRP:HE1	1:C:283:PRO:HD3	1.42	0.85
1:G:281:TRP:HE1	1:G:283:PRO:HD3	1.42	0.85
1:J:42:ARG:C	1:J:44:ARG:H	1.78	0.84
1:B:233:MET:HB3	1:B:239:THR:H	1.40	0.84
1:F:233:MET:HB3	1:F:239:THR:H	1.43	0.84
1:L:233:MET:HB3	1:L:239:THR:H	1.42	0.84
1:G:439:ARG:NH2	1:H:405:SER:OG	2.11	0.84
1:K:225:ASN:HD21	1:K:458:GLU:CD	1.81	0.84
1:I:233:MET:HB3	1:I:239:THR:H	1.40	0.84
1:K:240:PRO:HG2	1:K:245:LYS:NZ	1.92	0.84
1:F:240:PRO:HG2	1:F:245:LYS:NZ	1.92	0.84
1:J:233:MET:HB3	1:J:239:THR:H	1.43	0.83
1:H:233:MET:HB3	1:H:239:THR:H	1.42	0.83
1:C:33:LYS:HB3	1:C:36:GLU:HG2	1.60	0.83
1:C:240:PRO:HG2	1:C:245:LYS:HZ2	1.43	0.83
1:K:261:ARG:NH2	1:K:292:GLU:OE2	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:O	1:A:32:LEU:N	2.12	0.83
1:A:33:LYS:O	1:A:35:ARG:N	2.12	0.83
1:H:281:TRP:HE1	1:H:283:PRO:HD3	1.41	0.83
1:J:281:TRP:HE1	1:J:283:PRO:HD3	1.41	0.83
1:E:30:GLU:O	1:E:32:LEU:N	2.12	0.82
1:F:281:TRP:HE1	1:F:283:PRO:CD	1.92	0.82
1:H:281:TRP:C	1:H:281:TRP:HD1	1.82	0.82
1:L:34:THR:O	1:L:35:ARG:HB3	1.78	0.82
1:C:396:ARG:NH1	1:E:119:ASP:O	2.11	0.82
1:B:9:PHE:CE2	1:B:103:GLU:OE2	2.33	0.81
1:I:439:ARG:NH2	1:J:405:SER:OG	2.13	0.81
1:D:233:MET:HB3	1:D:239:THR:H	1.46	0.81
1:H:439:ARG:NH2	1:L:405:SER:OG	2.14	0.81
1:D:281:TRP:HE1	1:D:283:PRO:HD3	1.44	0.81
1:K:19:ARG:HE	1:K:479:THR:HG21	1.46	0.81
1:K:233:MET:HB3	1:K:239:THR:H	1.45	0.81
1:E:281:TRP:HE1	1:E:283:PRO:CD	1.94	0.81
1:B:189:HIS:HD2	1:E:154:LYS:HE2	1.45	0.81
1:A:41:LYS:HG3	1:A:44:ARG:NH1	1.95	0.81
1:L:281:TRP:HD1	1:L:281:TRP:C	1.83	0.80
1:A:281:TRP:HE1	1:A:283:PRO:CD	1.94	0.80
1:E:42:ARG:C	1:E:44:ARG:N	2.33	0.80
1:I:281:TRP:HD1	1:I:282:ASN:N	1.80	0.80
1:D:291:LEU:CD2	1:D:291:LEU:CD1	2.59	0.80
1:I:281:TRP:HD1	1:I:281:TRP:C	1.85	0.80
1:J:240:PRO:HG3	1:J:245:LYS:NZ	1.95	0.80
1:H:42:ARG:C	1:H:44:ARG:N	2.35	0.79
1:H:281:TRP:C	1:H:281:TRP:CD1	2.55	0.79
1:C:281:TRP:C	1:C:281:TRP:HD1	1.86	0.79
1:G:281:TRP:HD1	1:G:281:TRP:C	1.85	0.79
1:H:42:ARG:C	1:H:44:ARG:H	1.86	0.79
1:I:35:ARG:HG2	1:I:35:ARG:NH1	1.91	0.79
1:K:281:TRP:HE1	1:K:283:PRO:CD	1.94	0.79
1:I:42:ARG:C	1:I:44:ARG:N	2.34	0.79
1:L:42:ARG:O	1:L:44:ARG:N	2.15	0.79
1:J:35:ARG:C	1:J:37:THR:H	1.85	0.79
1:D:281:TRP:HD1	1:D:281:TRP:C	1.86	0.79
1:K:30:GLU:O	1:K:34:THR:N	2.15	0.79
1:D:19:ARG:HE	1:D:479:THR:HG21	1.48	0.79
1:I:32:LEU:CD1	1:I:33:LYS:HD2	2.12	0.78
1:B:281:TRP:HE1	1:B:283:PRO:CD	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:405:SER:OG	1:L:439:ARG:NH2	2.17	0.78
1:L:281:TRP:HE1	1:L:283:PRO:HD3	1.46	0.78
1:D:9:PHE:HZ	1:D:328:GLU:OE2	1.67	0.78
1:J:19:ARG:HE	1:J:479:THR:HG21	1.49	0.78
1:J:406:ASN:HD22	1:J:436:PHE:HZ	1.28	0.78
1:I:30:GLU:O	1:I:32:LEU:N	2.17	0.78
1:A:34:THR:HB	1:A:35:ARG:CB	2.14	0.78
1:K:281:TRP:C	1:K:281:TRP:HD1	1.87	0.77
1:D:419:ARG:O	1:D:421:PHE:N	2.18	0.77
1:F:281:TRP:CD1	1:F:281:TRP:C	2.57	0.77
1:A:42:ARG:C	1:A:44:ARG:N	2.37	0.77
1:J:419:ARG:C	1:J:421:PHE:N	2.38	0.77
1:A:281:TRP:C	1:A:281:TRP:CD1	2.57	0.76
1:J:189:HIS:HD2	1:L:154:LYS:HE2	1.49	0.76
1:K:42:ARG:C	1:K:44:ARG:H	1.88	0.76
1:D:44:ARG:C	1:D:46:ARG:H	1.89	0.76
1:G:42:ARG:C	1:G:44:ARG:H	1.89	0.76
1:L:42:ARG:C	1:L:44:ARG:N	2.39	0.76
1:J:281:TRP:HE1	1:J:283:PRO:CD	1.97	0.76
1:D:42:ARG:C	1:D:44:ARG:H	1.89	0.76
1:D:281:TRP:HE1	1:D:283:PRO:CD	1.99	0.76
1:F:239:THR:CG2	1:G:428:ILE:HD13	2.13	0.76
1:C:37:THR:OG1	1:C:40:GLN:HA	1.86	0.76
1:G:281:TRP:HE1	1:G:283:PRO:CD	1.98	0.76
1:I:35:ARG:C	1:I:37:THR:H	1.89	0.76
1:A:42:ARG:C	1:A:44:ARG:H	1.88	0.76
1:A:44:ARG:C	1:A:46:ARG:H	1.88	0.76
1:A:189:HIS:HD2	1:C:154:LYS:HE2	1.49	0.76
1:C:281:TRP:HE1	1:C:283:PRO:CD	1.99	0.76
1:C:281:TRP:C	1:C:281:TRP:CD1	2.59	0.76
1:E:44:ARG:C	1:E:46:ARG:H	1.88	0.76
1:L:281:TRP:HD1	1:L:282:ASN:N	1.84	0.76
1:A:41:LYS:HG3	1:A:44:ARG:HH12	1.50	0.75
1:H:30:GLU:O	1:H:32:LEU:N	2.19	0.75
1:E:243:GLY:O	1:E:245:LYS:N	2.20	0.75
1:K:44:ARG:C	1:K:46:ARG:H	1.89	0.75
1:L:42:ARG:C	1:L:44:ARG:H	1.89	0.75
1:B:44:ARG:C	1:B:46:ARG:H	1.90	0.75
1:J:281:TRP:HD1	1:J:281:TRP:C	1.89	0.75
1:D:281:TRP:C	1:D:281:TRP:CD1	2.59	0.75
1:D:42:ARG:C	1:D:44:ARG:N	2.39	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ARG:HE	1:B:479:THR:HG21	1.51	0.75
1:C:41:LYS:HG3	1:C:44:ARG:NH1	2.01	0.75
1:G:42:ARG:C	1:G:44:ARG:N	2.40	0.75
1:A:314:ILE:O	1:A:316:GLU:N	2.20	0.74
1:I:479:THR:OG1	1:I:480:ALA:N	2.18	0.74
1:K:281:TRP:HE1	1:K:283:PRO:HD3	1.52	0.74
1:B:42:ARG:C	1:B:44:ARG:N	2.40	0.74
1:D:30:GLU:O	1:D:32:LEU:N	2.20	0.74
1:J:281:TRP:C	1:J:281:TRP:CD1	2.60	0.74
1:H:281:TRP:HE1	1:H:283:PRO:CD	2.00	0.74
1:K:281:TRP:C	1:K:281:TRP:CD1	2.57	0.74
1:C:294:PHE:HA	1:C:297:GLN:HG3	1.69	0.74
1:E:281:TRP:CD1	1:E:281:TRP:C	2.61	0.74
1:J:42:ARG:C	1:J:44:ARG:N	2.39	0.74
1:B:186:THR:HG23	1:E:186:THR:HG23	1.67	0.74
1:E:281:TRP:C	1:E:281:TRP:HD1	1.91	0.74
1:G:33:LYS:O	1:G:35:ARG:N	2.21	0.74
1:K:42:ARG:C	1:K:44:ARG:N	2.39	0.74
1:B:42:ARG:C	1:B:44:ARG:H	1.90	0.74
1:E:419:ARG:O	1:E:421:PHE:N	2.21	0.73
1:J:44:ARG:C	1:J:46:ARG:H	1.89	0.73
1:A:30:GLU:O	1:A:34:THR:N	2.21	0.73
1:C:240:PRO:HG2	1:C:245:LYS:HZ1	1.53	0.73
1:G:44:ARG:C	1:G:46:ARG:H	1.91	0.73
1:B:30:GLU:O	1:B:34:THR:N	2.20	0.73
1:H:33:LYS:O	1:H:35:ARG:N	2.21	0.73
1:B:33:LYS:O	1:B:35:ARG:N	2.21	0.73
1:E:19:ARG:HE	1:E:479:THR:HG21	1.52	0.73
1:F:33:LYS:HB3	1:F:36:GLU:HG2	1.69	0.73
1:C:403:ARG:HG3	1:C:440:ILE:HG23	1.69	0.73
1:L:281:TRP:HE1	1:L:283:PRO:CD	2.00	0.73
1:A:290:GLU:O	1:A:294:PHE:N	2.14	0.73
1:A:305:PRO:O	1:A:306:LYS:HG3	1.89	0.73
1:I:281:TRP:NE1	1:I:283:PRO:HD3	1.99	0.73
1:A:186:THR:HG23	1:C:186:THR:HG23	1.71	0.73
1:D:245:LYS:O	1:D:269:LYS:HB2	1.88	0.73
1:L:394:TYR:HB2	1:L:445:GLU:HG3	1.71	0.73
1:G:44:ARG:HG2	1:G:44:ARG:HH11	1.54	0.73
1:C:42:ARG:O	1:C:44:ARG:N	2.22	0.73
1:K:30:GLU:O	1:K:32:LEU:N	2.22	0.73
1:L:243:GLY:O	1:L:245:LYS:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:ARG:C	1:E:37:THR:H	1.91	0.72
1:E:240:PRO:HG3	1:E:245:LYS:HZ1	1.50	0.72
1:J:186:THR:HG23	1:L:186:THR:HG23	1.69	0.72
1:F:243:GLY:O	1:F:245:LYS:N	2.22	0.72
1:H:428:ILE:O	1:L:416:SER:HB3	1.89	0.72
1:I:42:ARG:O	1:I:44:ARG:N	2.17	0.72
1:D:42:ARG:O	1:D:44:ARG:N	2.18	0.72
1:A:19:ARG:HH21	1:A:479:THR:HG21	1.53	0.72
1:A:281:TRP:HD1	1:A:282:ASN:N	1.87	0.72
1:H:240:PRO:HG2	1:H:245:LYS:CE	2.18	0.72
1:I:44:ARG:C	1:I:46:ARG:H	1.92	0.72
1:A:419:ARG:O	1:A:421:PHE:N	2.23	0.72
1:B:35:ARG:O	1:B:37:THR:HG22	1.88	0.72
1:C:42:ARG:C	1:C:44:ARG:N	2.41	0.72
1:D:328:GLU:HB3	1:D:329:LYS:HG3	1.70	0.72
1:E:236:LEU:HB3	1:E:342:LYS:HE3	1.71	0.72
1:K:53:LYS:HB2	1:K:54:PRO:HD3	1.71	0.72
1:K:42:ARG:O	1:K:44:ARG:N	2.17	0.72
1:L:44:ARG:C	1:L:46:ARG:H	1.93	0.72
1:C:335:ASN:HA	1:C:338:ARG:HG3	1.70	0.71
1:I:419:ARG:O	1:I:421:PHE:N	2.23	0.71
1:B:281:TRP:CD1	1:B:281:TRP:C	2.63	0.71
1:E:281:TRP:HE1	1:E:283:PRO:HD3	1.54	0.71
1:H:44:ARG:C	1:H:46:ARG:H	1.93	0.71
1:C:396:ARG:NH2	1:E:118:VAL:O	2.23	0.71
1:C:419:ARG:O	1:C:421:PHE:N	2.23	0.71
1:A:252:PHE:HD2	1:A:295:LYS:HZ2	1.36	0.71
1:C:44:ARG:C	1:C:46:ARG:H	1.93	0.71
1:H:39:GLU:HB3	1:H:41:LYS:HG2	1.73	0.71
1:F:44:ARG:C	1:F:46:ARG:H	1.94	0.71
1:J:243:GLY:O	1:J:245:LYS:N	2.24	0.71
1:L:281:TRP:C	1:L:281:TRP:CD1	2.59	0.71
1:E:286:ILE:HG21	1:E:291:LEU:HD22	1.73	0.71
1:K:346:GLU:OE2	1:K:478:ARG:NH2	2.24	0.71
1:B:37:THR:OG1	1:B:40:GLN:HA	1.90	0.71
1:F:42:ARG:C	1:F:44:ARG:N	2.44	0.71
1:G:37:THR:OG1	1:G:40:GLN:HA	1.91	0.71
1:E:33:LYS:HB3	1:E:36:GLU:HB2	1.73	0.71
1:F:33:LYS:O	1:F:35:ARG:N	2.23	0.71
1:A:41:LYS:HB3	1:A:44:ARG:HG2	1.72	0.70
1:F:286:ILE:HG21	1:F:291:LEU:HD22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:419:ARG:O	1:F:421:PHE:N	2.22	0.70
1:I:33:LYS:O	1:I:35:ARG:N	2.24	0.70
1:I:37:THR:OG1	1:I:40:GLN:HA	1.90	0.70
1:I:143:LYS:HG2	1:K:499:THR:HG21	1.73	0.70
1:I:240:PRO:HG2	1:I:245:LYS:HZ2	1.54	0.70
1:I:394:TYR:HB2	1:I:445:GLU:HG3	1.73	0.70
1:F:281:TRP:CD1	1:F:282:ASN:N	2.59	0.70
1:D:293:ASP:O	1:D:297:GLN:HB2	1.92	0.70
1:H:30:GLU:O	1:H:34:THR:N	2.24	0.70
1:B:290:GLU:O	1:B:294:PHE:N	2.22	0.70
1:H:419:ARG:O	1:H:421:PHE:N	2.23	0.70
1:L:236:LEU:HB3	1:L:342:LYS:HE3	1.72	0.70
1:G:36:GLU:HG2	1:G:42:ARG:HH21	1.55	0.70
1:C:315:LEU:HD23	1:C:322:LEU:HD11	1.74	0.70
1:L:30:GLU:O	1:L:32:LEU:N	2.23	0.70
1:L:286:ILE:HG21	1:L:291:LEU:HD22	1.73	0.70
1:C:117:VAL:HG21	1:C:371:LEU:HG	1.73	0.70
1:G:281:TRP:C	1:G:281:TRP:CD1	2.59	0.70
1:G:42:ARG:O	1:G:44:ARG:N	2.23	0.69
1:J:41:LYS:HD2	1:J:44:ARG:HH12	1.57	0.69
1:J:328:GLU:HB3	1:J:329:LYS:HG3	1.74	0.69
1:L:419:ARG:O	1:L:421:PHE:N	2.24	0.69
1:J:43:ASN:O	1:J:46:ARG:HD3	1.92	0.69
1:H:382:TYR:OH	1:L:391:HIS:O	2.09	0.69
1:A:405:SER:OG	1:F:439:ARG:NH2	2.25	0.69
1:F:281:TRP:HE1	1:F:283:PRO:N	1.91	0.69
1:F:281:TRP:C	1:F:281:TRP:HD1	1.95	0.69
1:D:37:THR:OG1	1:D:40:GLN:HA	1.91	0.69
1:L:33:LYS:C	1:L:35:ARG:H	1.94	0.69
1:C:405:SER:OG	1:E:439:ARG:NH2	2.22	0.69
1:E:37:THR:CG2	1:E:40:GLN:HA	2.23	0.69
1:J:30:GLU:O	1:J:32:LEU:N	2.25	0.69
1:L:83:SER:OG	1:L:85:HIS:ND1	2.23	0.69
1:A:33:LYS:HB3	1:A:36:GLU:HG2	1.75	0.69
1:F:308:LYS:HZ3	1:L:469:MET:HB3	1.58	0.69
1:H:286:ILE:HG21	1:H:291:LEU:HD22	1.73	0.69
1:C:30:GLU:O	1:C:34:THR:N	2.25	0.69
1:G:35:ARG:O	1:G:37:THR:HG22	1.93	0.69
1:J:286:ILE:HG21	1:J:291:LEU:HD22	1.74	0.69
1:B:30:GLU:O	1:B:32:LEU:N	2.26	0.68
1:F:30:GLU:H	1:F:32:LEU:HD12	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:PRO:HG2	1:F:245:LYS:HZ1	1.55	0.68
1:J:419:ARG:O	1:J:421:PHE:N	2.25	0.68
1:K:315:LEU:HD23	1:K:322:LEU:HD11	1.75	0.68
1:J:315:LEU:HD23	1:J:322:LEU:HD11	1.75	0.68
1:L:315:LEU:HD23	1:L:322:LEU:HD11	1.75	0.68
1:A:286:ILE:HG21	1:A:291:LEU:HD22	1.75	0.68
1:B:240:PRO:HG2	1:B:245:LYS:HZ1	1.58	0.68
1:B:281:TRP:C	1:B:281:TRP:HD1	1.95	0.68
1:G:12:MET:SD	1:G:354:PRO:HD3	2.34	0.68
1:G:240:PRO:HG2	1:G:245:LYS:HZ2	1.56	0.68
1:G:252:PHE:CD2	1:G:295:LYS:HE3	2.28	0.68
1:K:286:ILE:HG21	1:K:291:LEU:HD22	1.74	0.68
1:D:459:ARG:O	1:D:463:GLN:HG3	1.93	0.68
1:H:186:THR:HG23	1:K:186:THR:HG23	1.76	0.68
1:K:400:LYS:HD2	1:K:403:ARG:HH21	1.57	0.68
1:B:314:ILE:O	1:B:316:GLU:N	2.26	0.68
1:L:240:PRO:HG3	1:L:245:LYS:HZ1	1.56	0.68
1:F:281:TRP:HE1	1:F:283:PRO:HD3	1.58	0.68
1:H:315:LEU:HD23	1:H:322:LEU:HD11	1.75	0.68
1:H:439:ARG:HH21	1:L:405:SER:HG	1.41	0.68
1:K:419:ARG:O	1:K:421:PHE:N	2.26	0.68
1:F:30:GLU:O	1:F:34:THR:N	2.27	0.68
1:H:42:ARG:O	1:H:44:ARG:N	2.20	0.68
1:A:294:PHE:CE1	1:A:298:HIS:HE1	2.12	0.68
1:K:369:PRO:HD3	1:K:477:LEU:HG	1.75	0.68
1:B:439:ARG:NH2	1:F:405:SER:OG	2.27	0.68
1:F:35:ARG:C	1:F:37:THR:H	1.97	0.68
1:C:35:ARG:C	1:C:37:THR:H	1.94	0.67
1:A:428:ILE:HD13	1:H:428:ILE:HD13	1.76	0.67
1:G:281:TRP:HD1	1:G:282:ASN:N	1.93	0.67
1:G:315:LEU:HD23	1:G:322:LEU:HD11	1.76	0.67
1:F:42:ARG:O	1:F:44:ARG:N	2.24	0.67
1:E:315:LEU:HD23	1:E:322:LEU:HD11	1.75	0.67
1:G:19:ARG:HH21	1:G:479:THR:HG21	1.60	0.67
1:H:35:ARG:C	1:H:37:THR:H	1.96	0.67
1:A:257:LEU:HD11	1:A:292:GLU:OE1	1.95	0.67
1:B:281:TRP:HE1	1:B:283:PRO:HD3	1.59	0.67
1:B:315:LEU:HD23	1:B:322:LEU:HD11	1.75	0.67
1:G:286:ILE:HG21	1:G:291:LEU:HD22	1.76	0.67
1:A:42:ARG:O	1:A:44:ARG:N	2.22	0.67
1:D:30:GLU:O	1:D:34:THR:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:LEU:HD23	1:F:322:LEU:HD11	1.75	0.67
1:K:33:LYS:HB3	1:K:36:GLU:HG2	1.76	0.67
1:A:240:PRO:HG2	1:A:245:LYS:HZ1	1.59	0.67
1:G:419:ARG:O	1:G:421:PHE:N	2.27	0.66
1:H:240:PRO:CG	1:H:245:LYS:HE2	2.26	0.66
1:I:35:ARG:O	1:I:37:THR:HG22	1.94	0.66
1:H:146:ARG:NH2	1:H:181:ASP:OD2	2.29	0.66
1:H:355:GLU:O	1:H:358:LYS:HB3	1.94	0.66
1:K:243:GLY:O	1:K:245:LYS:N	2.27	0.66
1:D:35:ARG:C	1:D:37:THR:H	1.95	0.66
1:E:12:MET:SD	1:E:354:PRO:HD3	2.36	0.66
1:E:355:GLU:O	1:E:358:LYS:HB3	1.94	0.66
1:H:281:TRP:HD1	1:H:282:ASN:N	1.93	0.66
1:I:7:PRO:O	1:I:329:LYS:NZ	2.27	0.66
1:D:394:TYR:HB2	1:D:445:GLU:HG3	1.77	0.66
1:E:42:ARG:O	1:E:44:ARG:N	2.17	0.66
1:H:240:PRO:HG2	1:H:245:LYS:HZ3	1.56	0.66
1:F:290:GLU:O	1:F:294:PHE:N	2.15	0.66
1:A:34:THR:HB	1:A:35:ARG:HB3	1.77	0.66
1:E:236:LEU:HB2	1:E:238:MET:HG3	1.76	0.66
1:B:243:GLY:O	1:B:245:LYS:N	2.29	0.66
1:G:281:TRP:CD1	1:G:282:ASN:N	2.63	0.66
1:F:146:ARG:NH2	1:F:181:ASP:OD2	2.29	0.66
1:I:476:ASP:OD2	1:I:479:THR:HG21	1.96	0.66
1:L:52:ILE:O	1:L:82:HIS:NE2	2.29	0.66
1:B:64:PRO:HB3	1:D:51:ILE:HG12	1.77	0.65
1:B:72:TRP:HB2	1:D:47:GLY:HA3	1.77	0.65
1:E:293:ASP:O	1:E:297:GLN:HB2	1.96	0.65
1:B:346:GLU:OE1	1:B:370:ASP:N	2.30	0.65
1:I:281:TRP:C	1:I:281:TRP:CD1	2.63	0.65
1:B:419:ARG:O	1:B:421:PHE:N	2.29	0.65
1:E:52:ILE:O	1:E:82:HIS:NE2	2.29	0.65
1:K:281:TRP:CD1	1:K:282:ASN:N	2.63	0.65
1:C:52:ILE:O	1:C:82:HIS:NE2	2.29	0.65
1:E:346:GLU:OE1	1:E:370:ASP:N	2.30	0.65
1:F:467:THR:HA	1:F:470:LYS:HE3	1.77	0.65
1:I:30:GLU:O	1:I:34:THR:N	2.29	0.65
1:A:44:ARG:HG2	1:A:44:ARG:HH11	1.61	0.65
1:D:53:LYS:HB3	1:D:54:PRO:HD3	1.79	0.65
1:F:346:GLU:OE1	1:F:370:ASP:N	2.30	0.65
1:K:17:PHE:CD2	1:K:53:LYS:HD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:281:TRP:CD1	1:L:282:ASN:N	2.64	0.65
1:C:281:TRP:CD1	1:C:282:ASN:N	2.64	0.65
1:D:10:PHE:HA	1:D:106:ALA:HB2	1.78	0.65
1:E:290:GLU:O	1:E:294:PHE:N	2.16	0.65
1:G:290:GLU:O	1:G:294:PHE:N	2.15	0.65
1:H:281:TRP:CD1	1:H:282:ASN:N	2.64	0.65
1:I:476:ASP:CG	1:I:479:THR:HG21	2.17	0.65
1:B:52:ILE:O	1:B:82:HIS:NE2	2.29	0.65
1:D:272:ALA:HB1	1:D:314:ILE:HD12	1.78	0.65
1:G:245:LYS:O	1:G:269:LYS:HB2	1.97	0.65
1:H:240:PRO:HG2	1:H:245:LYS:HE2	1.79	0.65
1:K:146:ARG:NH2	1:K:181:ASP:OD2	2.30	0.65
1:K:290:GLU:O	1:K:294:PHE:N	2.15	0.65
1:E:7:PRO:O	1:E:329:LYS:NZ	2.30	0.65
1:J:293:ASP:O	1:J:297:GLN:HB2	1.96	0.65
1:G:439:ARG:HH21	1:H:405:SER:HG	1.41	0.65
1:J:406:ASN:ND2	1:J:436:PHE:HZ	1.94	0.65
1:A:423:LYS:NZ	1:H:437:GLN:NE2	2.28	0.64
1:D:281:TRP:CD1	1:D:282:ASN:N	2.65	0.64
1:H:433:THR:HG21	1:L:411:MET:HB3	1.77	0.64
1:B:51:ILE:HG12	1:D:64:PRO:HB3	1.79	0.64
1:D:281:TRP:HD1	1:D:282:ASN:N	1.95	0.64
1:D:346:GLU:OE1	1:D:370:ASP:N	2.30	0.64
1:A:315:LEU:HD23	1:A:322:LEU:HD11	1.77	0.64
1:D:36:GLU:HB2	1:D:42:ARG:HH21	1.61	0.64
1:G:346:GLU:OE1	1:G:370:ASP:N	2.30	0.64
1:A:240:PRO:HG2	1:A:245:LYS:CE	2.27	0.64
1:C:146:ARG:NH2	1:C:181:ASP:OD2	2.31	0.64
1:E:245:LYS:O	1:E:269:LYS:HB2	1.97	0.64
1:F:142:GLU:OE2	1:F:146:ARG:NH1	2.31	0.64
1:K:346:GLU:OE1	1:K:370:ASP:N	2.30	0.64
1:C:281:TRP:HD1	1:C:282:ASN:N	1.95	0.64
1:H:346:GLU:OE1	1:H:370:ASP:N	2.30	0.64
1:I:346:GLU:OE2	1:I:478:ARG:NH2	2.28	0.64
1:I:346:GLU:OE1	1:I:370:ASP:N	2.30	0.64
1:J:346:GLU:OE1	1:J:370:ASP:N	2.30	0.64
1:F:42:ARG:C	1:F:44:ARG:H	2.01	0.64
1:G:305:PRO:O	1:G:306:LYS:HB2	1.97	0.64
1:A:142:GLU:OE2	1:A:146:ARG:NH1	2.31	0.64
1:B:346:GLU:OE2	1:B:478:ARG:NH2	2.29	0.64
1:C:243:GLY:O	1:C:245:LYS:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:TRP:CD1	1:F:282:ASN:CA	2.81	0.64
1:A:146:ARG:NH2	1:A:181:ASP:OD2	2.31	0.64
1:D:186:THR:HG23	1:F:186:THR:HG23	1.79	0.64
1:D:315:LEU:HD23	1:D:322:LEU:HD21	1.79	0.64
1:E:42:ARG:HA	1:E:45:VAL:HG22	1.80	0.64
1:I:281:TRP:HD1	1:I:282:ASN:CA	2.11	0.64
1:B:286:ILE:HG21	1:B:291:LEU:HD22	1.78	0.63
1:J:146:ARG:NH2	1:J:181:ASP:OD2	2.31	0.63
1:L:41:LYS:HB3	1:L:44:ARG:HH11	1.63	0.63
1:L:240:PRO:HG3	1:L:245:LYS:HZ2	1.61	0.63
1:L:346:GLU:OE1	1:L:370:ASP:N	2.30	0.63
1:C:476:ASP:OD2	1:C:479:THR:OG1	2.12	0.63
1:F:60:SER:HB3	1:F:78:TYR:HD1	1.62	0.63
1:G:52:ILE:O	1:G:82:HIS:NE2	2.30	0.63
1:L:146:ARG:NH2	1:L:181:ASP:OD2	2.31	0.63
1:A:294:PHE:CZ	1:A:304:PHE:HA	2.32	0.63
1:J:281:TRP:CD1	1:J:282:ASN:N	2.66	0.63
1:A:272:ALA:HB1	1:A:314:ILE:HD13	1.79	0.63
1:B:42:ARG:O	1:B:44:ARG:N	2.20	0.63
1:C:142:GLU:OE2	1:C:146:ARG:NH1	2.32	0.63
1:C:201:LYS:NZ	1:C:388:ASN:OD1	2.21	0.63
1:C:290:GLU:O	1:C:294:PHE:N	2.19	0.63
1:I:146:ARG:NH2	1:I:181:ASP:OD2	2.31	0.63
1:A:240:PRO:HG2	1:A:245:LYS:HE2	1.80	0.63
1:A:346:GLU:OE1	1:A:370:ASP:N	2.30	0.63
1:A:394:TYR:HB2	1:A:445:GLU:HG3	1.81	0.63
1:D:142:GLU:OE2	1:D:146:ARG:NH1	2.32	0.63
1:G:17:PHE:CE2	1:G:53:LYS:HD2	2.33	0.63
1:A:424:HIS:ND1	1:H:407:TYR:CE2	2.66	0.63
1:J:360:PHE:CD1	1:J:365:ILE:HD11	2.34	0.63
1:K:142:GLU:OE2	1:K:146:ARG:NH1	2.32	0.63
1:D:243:GLY:O	1:D:245:LYS:N	2.31	0.63
1:E:146:ARG:NH2	1:E:181:ASP:OD2	2.31	0.63
1:H:247:PHE:CD2	1:H:263:LEU:HD23	2.34	0.63
1:B:9:PHE:CE2	1:B:328:GLU:OE2	2.52	0.63
1:D:146:ARG:NH2	1:D:181:ASP:OD2	2.31	0.63
1:C:42:ARG:C	1:C:44:ARG:H	2.01	0.62
1:D:360:PHE:CD1	1:D:365:ILE:HD11	2.34	0.62
1:E:281:TRP:CD1	1:E:282:ASN:N	2.67	0.62
1:G:360:PHE:CD1	1:G:365:ILE:HD11	2.34	0.62
1:J:236:LEU:HB2	1:J:238:MET:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:366:MET:HG2	1:K:477:LEU:HD21	1.80	0.62
1:E:33:LYS:HE3	1:E:494:ASN:HD21	1.64	0.62
1:G:146:ARG:NH2	1:G:181:ASP:OD2	2.32	0.62
1:H:142:GLU:OE2	1:H:146:ARG:NH1	2.32	0.62
1:I:34:THR:HB	1:I:35:ARG:HG2	1.82	0.62
1:I:142:GLU:OE2	1:I:146:ARG:NH1	2.32	0.62
1:I:360:PHE:CD1	1:I:365:ILE:HD11	2.34	0.62
1:I:498:VAL:O	1:I:499:THR:OG1	2.13	0.62
1:B:146:ARG:NH2	1:B:181:ASP:OD2	2.31	0.62
1:E:142:GLU:OE2	1:E:146:ARG:NH1	2.32	0.62
1:H:360:PHE:CD1	1:H:365:ILE:HD11	2.34	0.62
1:C:9:PHE:CZ	1:C:103:GLU:OE2	2.52	0.62
1:C:252:PHE:HD2	1:C:295:LYS:HZ1	1.47	0.62
1:E:247:PHE:CD2	1:E:263:LEU:HD23	2.35	0.62
1:G:142:GLU:OE2	1:G:146:ARG:NH1	2.32	0.62
1:K:35:ARG:C	1:K:37:THR:H	2.00	0.62
1:B:142:GLU:OE2	1:B:146:ARG:NH1	2.32	0.62
1:C:247:PHE:CD2	1:C:263:LEU:HD23	2.34	0.62
1:G:186:THR:HG23	1:I:186:THR:HG23	1.79	0.62
1:G:247:PHE:CD2	1:G:263:LEU:HD23	2.35	0.62
1:K:360:PHE:CD1	1:K:365:ILE:HD11	2.35	0.62
1:A:243:GLY:O	1:A:245:LYS:N	2.32	0.62
1:F:52:ILE:O	1:F:82:HIS:NE2	2.29	0.62
1:K:247:PHE:CD2	1:K:263:LEU:HD23	2.35	0.62
1:B:272:ALA:HB1	1:B:314:ILE:HD11	1.80	0.62
1:C:346:GLU:OE1	1:C:370:ASP:N	2.33	0.62
1:F:41:LYS:HD2	1:F:44:ARG:HH12	1.65	0.62
1:I:27:LYS:HE3	1:I:470:LYS:HE2	1.82	0.62
1:J:52:ILE:O	1:J:82:HIS:NE2	2.29	0.62
1:J:247:PHE:CD2	1:J:263:LEU:HD23	2.35	0.62
1:K:471:TYR:O	1:K:473:LEU:HG	2.00	0.62
1:K:34:THR:HG22	1:K:35:ARG:HB2	1.82	0.62
1:K:272:ALA:HB1	1:K:314:ILE:HD11	1.80	0.62
1:A:52:ILE:O	1:A:82:HIS:NE2	2.31	0.62
1:B:247:PHE:CD2	1:B:263:LEU:HD23	2.35	0.61
1:C:314:ILE:O	1:C:316:GLU:N	2.33	0.61
1:E:12:MET:SD	1:E:353:THR:HA	2.40	0.61
1:I:28:LEU:O	1:I:32:LEU:HD11	2.00	0.61
1:J:142:GLU:OE2	1:J:146:ARG:NH1	2.32	0.61
1:E:360:PHE:CD1	1:E:365:ILE:HD11	2.35	0.61
1:G:236:LEU:HB2	1:G:238:MET:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:52:ILE:O	1:H:82:HIS:NE2	2.30	0.61
1:B:360:PHE:CD1	1:B:365:ILE:HD11	2.35	0.61
1:F:335:ASN:HA	1:F:338:ARG:HD2	1.81	0.61
1:G:51:ILE:HG12	1:K:64:PRO:HB3	1.82	0.61
1:J:12:MET:SD	1:J:354:PRO:HD3	2.40	0.61
1:L:35:ARG:C	1:L:37:THR:H	2.02	0.61
1:A:294:PHE:CE1	1:A:298:HIS:CE1	2.89	0.61
1:A:360:PHE:CD1	1:A:365:ILE:HD11	2.35	0.61
1:D:9:PHE:HE1	1:D:328:GLU:HG2	1.65	0.61
1:D:52:ILE:O	1:D:82:HIS:NE2	2.32	0.61
1:F:360:PHE:CD1	1:F:365:ILE:HD11	2.35	0.61
1:K:53:LYS:HB2	1:K:54:PRO:CD	2.30	0.61
1:A:236:LEU:HB3	1:A:342:LYS:HE3	1.82	0.61
1:D:236:LEU:HB2	1:D:238:MET:HG3	1.83	0.61
1:I:52:ILE:O	1:I:82:HIS:NE2	2.29	0.61
1:J:38:GLU:O	1:J:39:GLU:HB2	2.00	0.61
1:A:439:ARG:NH2	1:B:405:SER:OG	2.29	0.61
1:D:6:ASP:OD2	1:D:329:LYS:HE3	2.01	0.61
1:G:47:GLY:HA3	1:K:72:TRP:HB2	1.83	0.61
1:A:247:PHE:CD2	1:A:263:LEU:HD23	2.35	0.61
1:G:297:GLN:HG3	1:G:298:HIS:ND1	2.16	0.61
1:H:51:ILE:HG12	1:J:64:PRO:HB3	1.82	0.61
1:E:30:GLU:O	1:E:34:THR:N	2.34	0.61
1:F:247:PHE:CD2	1:F:263:LEU:HD23	2.35	0.61
1:I:10:PHE:HA	1:I:106:ALA:HB2	1.82	0.61
1:A:272:ALA:HB1	1:A:314:ILE:CD1	2.31	0.60
1:D:418:GLU:HB3	1:D:423:LYS:HB2	1.84	0.60
1:F:428:ILE:HD13	1:G:239:THR:HG21	1.83	0.60
1:I:383:PHE:CD1	1:J:397:LEU:HD21	2.35	0.60
1:J:9:PHE:HZ	1:J:110:LEU:HD22	1.64	0.60
1:J:314:ILE:O	1:J:316:GLU:N	2.34	0.60
1:D:9:PHE:O	1:D:11:LYS:N	2.34	0.60
1:A:53:LYS:HB3	1:A:54:PRO:HD3	1.83	0.60
1:E:240:PRO:HG3	1:E:245:LYS:CE	2.32	0.60
1:I:243:GLY:O	1:I:245:LYS:N	2.34	0.60
1:L:314:ILE:O	1:L:316:GLU:N	2.35	0.60
1:B:281:TRP:CD1	1:B:282:ASN:N	2.69	0.60
1:H:34:THR:CA	1:H:35:ARG:HB3	2.16	0.60
1:L:142:GLU:OE2	1:L:146:ARG:NH1	2.33	0.60
1:A:281:TRP:CD1	1:A:282:ASN:N	2.69	0.60
1:F:30:GLU:O	1:F:32:LEU:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:245:LYS:O	1:H:269:LYS:HB2	2.01	0.60
1:L:40:GLN:OE1	1:L:40:GLN:O	2.20	0.60
1:A:36:GLU:HG3	1:A:42:ARG:HH21	1.67	0.60
1:A:261:ARG:NH2	1:A:292:GLU:OE2	2.34	0.60
1:B:294:PHE:CE1	1:B:298:HIS:HE1	2.19	0.60
1:D:272:ALA:CB	1:D:314:ILE:HD12	2.31	0.60
1:E:44:ARG:C	1:E:46:ARG:N	2.54	0.60
1:I:397:LEU:HD22	1:K:394:TYR:CE1	2.36	0.60
1:J:44:ARG:HH11	1:J:44:ARG:CG	2.15	0.60
1:E:294:PHE:CE1	1:E:298:HIS:CE1	2.83	0.60
1:F:239:THR:HG21	1:G:428:ILE:CD1	2.20	0.60
1:L:360:PHE:CD1	1:L:365:ILE:HD11	2.37	0.60
1:A:119:ASP:OD2	1:A:459:ARG:NH1	2.33	0.60
1:E:29:VAL:HG22	1:E:43:ASN:H	1.67	0.60
1:F:236:LEU:HB2	1:F:238:MET:HG3	1.83	0.60
1:F:281:TRP:CD1	1:F:282:ASN:HA	2.37	0.60
1:B:240:PRO:HG2	1:B:245:LYS:HZ2	1.66	0.59
1:B:432:PRO:HB3	1:B:436:PHE:CD2	2.37	0.59
1:C:8:ASN:O	1:C:11:LYS:HB2	2.02	0.59
1:F:33:LYS:C	1:F:35:ARG:HB2	2.23	0.59
1:G:17:PHE:CD2	1:G:53:LYS:HD2	2.37	0.59
1:C:274:GLY:N	1:C:314:ILE:HD12	2.17	0.59
1:H:37:THR:CG2	1:H:40:GLN:HA	2.32	0.59
1:H:394:TYR:HB2	1:H:445:GLU:HG3	1.82	0.59
1:I:281:TRP:CD1	1:I:282:ASN:N	2.68	0.59
1:B:394:TYR:CE1	1:F:397:LEU:HD22	2.37	0.59
1:I:44:ARG:O	1:I:44:ARG:HG2	1.91	0.59
1:K:458:GLU:N	1:K:458:GLU:OE1	2.35	0.59
1:L:311:GLU:HG2	1:L:312:GLY:N	2.16	0.59
1:L:346:GLU:OE2	1:L:478:ARG:NH2	2.36	0.59
1:L:432:PRO:HB3	1:L:436:PHE:CD2	2.37	0.59
1:C:9:PHE:CE1	1:C:103:GLU:OE2	2.55	0.59
1:E:173:GLU:HG3	1:E:174:ARG:H	1.67	0.59
1:G:35:ARG:C	1:G:37:THR:H	2.04	0.59
1:A:432:PRO:HB3	1:A:436:PHE:CD2	2.37	0.59
1:B:281:TRP:CD1	1:B:282:ASN:HA	2.37	0.59
1:G:28:LEU:C	1:G:32:LEU:HD22	2.22	0.59
1:G:43:ASN:O	1:G:46:ARG:HD3	2.03	0.59
1:I:432:PRO:HB3	1:I:436:PHE:CD2	2.37	0.59
1:L:281:TRP:HD1	1:L:282:ASN:CA	2.15	0.59
1:B:281:TRP:CD1	1:B:282:ASN:CA	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:ARG:C	1:D:421:PHE:N	2.56	0.59
1:H:243:GLY:O	1:H:245:LYS:N	2.36	0.59
1:I:64:PRO:HB3	1:L:51:ILE:HG12	1.83	0.59
1:I:72:TRP:HB2	1:L:47:GLY:HA3	1.85	0.59
1:I:247:PHE:CD2	1:I:263:LEU:HD23	2.38	0.59
1:I:499:THR:HA	1:L:66:ARG:NH1	2.14	0.59
1:B:236:LEU:HB2	1:B:238:MET:HG3	1.83	0.59
1:A:236:LEU:HB2	1:A:238:MET:HG3	1.84	0.59
1:E:294:PHE:CZ	1:E:298:HIS:CE1	2.91	0.59
1:K:240:PRO:CG	1:K:245:LYS:NZ	2.64	0.59
1:A:240:PRO:CG	1:A:245:LYS:HE2	2.33	0.59
1:A:470:LYS:HE2	1:A:471:TYR:HE2	1.67	0.59
1:F:432:PRO:HB3	1:F:436:PHE:CD2	2.37	0.59
1:K:19:ARG:NE	1:K:479:THR:HG21	2.16	0.59
1:A:34:THR:HB	1:A:35:ARG:HB2	1.85	0.58
1:B:47:GLY:HA3	1:D:72:TRP:HB2	1.84	0.58
1:C:51:ILE:HG12	1:F:64:PRO:HB3	1.85	0.58
1:C:411:MET:HB3	1:E:433:THR:HG21	1.85	0.58
1:J:10:PHE:HA	1:J:106:ALA:HB2	1.83	0.58
1:K:405:SER:O	1:K:409:LEU:HD12	2.02	0.58
1:E:294:PHE:CZ	1:E:304:PHE:HA	2.38	0.58
1:J:34:THR:OG1	1:J:35:ARG:HG2	2.03	0.58
1:K:52:ILE:O	1:K:82:HIS:NE2	2.34	0.58
1:D:346:GLU:OE2	1:D:478:ARG:NH2	2.33	0.58
1:F:38:GLU:O	1:F:39:GLU:HB2	2.04	0.58
1:G:432:PRO:HB3	1:G:436:PHE:CD2	2.39	0.58
1:J:41:LYS:HD2	1:J:44:ARG:NH1	2.18	0.58
1:A:44:ARG:NH1	1:A:44:ARG:HG2	2.17	0.58
1:A:213:SER:HB2	1:A:217:ARG:HD2	1.84	0.58
1:E:432:PRO:HB3	1:E:436:PHE:CD2	2.38	0.58
1:G:30:GLU:O	1:G:34:THR:N	2.37	0.58
1:I:427:THR:HG22	1:I:429:PRO:HD3	1.86	0.58
1:J:410:LEU:HB3	1:J:430:ILE:HA	1.85	0.58
1:A:213:SER:O	1:A:217:ARG:HG3	2.02	0.58
1:C:427:THR:HG22	1:C:429:PRO:HD3	1.85	0.58
1:J:44:ARG:C	1:J:46:ARG:N	2.57	0.58
1:H:427:THR:HG22	1:H:429:PRO:HD3	1.85	0.58
1:I:34:THR:HB	1:I:35:ARG:CG	2.33	0.58
1:J:6:ASP:OD1	1:J:329:LYS:HE3	2.04	0.58
1:F:427:THR:HG22	1:F:429:PRO:HD3	1.85	0.58
1:G:38:GLU:O	1:G:39:GLU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:397:LEU:HD22	1:L:394:TYR:CE1	2.39	0.58
1:I:280:ILE:HG22	1:I:286:ILE:HD11	1.84	0.58
1:J:432:PRO:HB3	1:J:436:PHE:CD2	2.38	0.58
1:L:10:PHE:HA	1:L:106:ALA:HB2	1.85	0.58
1:C:30:GLU:O	1:C:32:LEU:N	2.37	0.58
1:D:427:THR:HG22	1:D:429:PRO:HD3	1.86	0.58
1:B:35:ARG:C	1:B:37:THR:H	2.06	0.58
1:L:294:PHE:HA	1:L:297:GLN:HG3	1.85	0.58
1:A:60:SER:HB3	1:A:78:TYR:HD1	1.69	0.57
1:A:240:PRO:CB	1:A:245:LYS:HE2	2.33	0.57
1:C:38:GLU:O	1:C:39:GLU:HB2	2.02	0.57
1:H:432:PRO:HB3	1:H:436:PHE:CD2	2.38	0.57
1:I:236:LEU:HB2	1:I:238:MET:HG3	1.86	0.57
1:J:281:TRP:HD1	1:J:282:ASN:N	2.01	0.57
1:J:427:THR:HG22	1:J:429:PRO:HD3	1.85	0.57
1:L:414:GLN:O	1:L:418:GLU:HG3	2.04	0.57
1:A:427:THR:HG22	1:A:429:PRO:HD3	1.86	0.57
1:E:314:ILE:O	1:E:316:GLU:N	2.36	0.57
1:F:36:GLU:HG3	1:F:42:ARG:HH21	1.68	0.57
1:I:33:LYS:C	1:I:35:ARG:HB2	2.24	0.57
1:J:35:ARG:O	1:J:37:THR:N	2.37	0.57
1:K:10:PHE:HA	1:K:106:ALA:HB2	1.85	0.57
1:B:294:PHE:CZ	1:B:304:PHE:HA	2.39	0.57
1:D:17:PHE:CE2	1:D:53:LYS:HD2	2.39	0.57
1:E:500:PHE:HZ	1:F:500:PHE:HB3	1.68	0.57
1:G:252:PHE:CD2	1:G:295:LYS:CE	2.87	0.57
1:H:10:PHE:HA	1:H:106:ALA:HB2	1.86	0.57
1:A:189:HIS:C	1:A:189:HIS:HD1	2.07	0.57
1:E:427:THR:HG22	1:E:429:PRO:HD3	1.87	0.57
1:F:10:PHE:HA	1:F:106:ALA:HB2	1.87	0.57
1:J:37:THR:CG2	1:J:40:GLN:HA	2.34	0.57
1:K:427:THR:HG22	1:K:429:PRO:HD3	1.85	0.57
1:K:432:PRO:HB3	1:K:436:PHE:CD2	2.38	0.57
1:L:403:ARG:HG3	1:L:440:ILE:HG23	1.86	0.57
1:A:423:LYS:HZ3	1:H:437:GLN:HE21	1.44	0.57
1:D:44:ARG:C	1:D:46:ARG:N	2.57	0.57
1:B:12:MET:SD	1:B:354:PRO:HD3	2.45	0.57
1:B:209:HIS:HD2	1:B:445:GLU:HB3	1.69	0.57
1:D:19:ARG:NE	1:D:479:THR:HG21	2.18	0.57
1:J:30:GLU:O	1:J:34:THR:N	2.36	0.57
1:L:471:TYR:O	1:L:473:LEU:N	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:C	1:A:46:ARG:N	2.58	0.57
1:F:6:ASP:OD1	1:F:332:THR:HB	2.04	0.57
1:B:469:MET:HE3	1:G:308:LYS:HE2	1.87	0.57
1:C:236:LEU:HB2	1:C:238:MET:HG3	1.86	0.57
1:G:243:GLY:O	1:G:245:LYS:N	2.38	0.57
1:L:405:SER:O	1:L:409:LEU:HD12	2.05	0.57
1:A:314:ILE:C	1:A:316:GLU:H	2.09	0.57
1:B:85:HIS:NE2	2:B:601:ADP:N1	2.44	0.57
1:B:281:TRP:HE1	1:B:283:PRO:N	2.02	0.57
1:B:427:THR:HG22	1:B:429:PRO:HD3	1.85	0.57
1:E:113:TYR:HB2	1:E:371:LEU:HD11	1.86	0.57
1:H:236:LEU:HB3	1:H:342:LYS:HE3	1.86	0.57
1:L:355:GLU:O	1:L:359:ILE:HD12	2.04	0.57
1:G:400:LYS:CD	1:G:403:ARG:HH21	2.18	0.57
1:I:27:LYS:HE3	1:I:470:LYS:CE	2.35	0.57
1:K:410:LEU:HB3	1:K:430:ILE:HA	1.87	0.57
1:L:60:SER:HB3	1:L:78:TYR:HD1	1.69	0.57
1:A:400:LYS:CD	1:A:403:ARG:HH21	2.18	0.56
1:D:290:GLU:O	1:D:294:PHE:N	2.23	0.56
1:E:500:PHE:HZ	1:F:500:PHE:CB	2.18	0.56
1:F:459:ARG:NH2	2:F:601:ADP:O3B	2.38	0.56
1:G:400:LYS:HD3	1:G:403:ARG:HH21	1.70	0.56
1:G:427:THR:HG22	1:G:429:PRO:HD3	1.87	0.56
1:J:37:THR:HG23	1:J:40:GLN:HA	1.86	0.56
1:K:281:TRP:HE1	1:K:283:PRO:N	2.02	0.56
1:K:314:ILE:O	1:K:316:GLU:N	2.38	0.56
1:B:34:THR:CA	1:B:35:ARG:HB3	2.32	0.56
1:C:432:PRO:HB3	1:C:436:PHE:CD2	2.40	0.56
1:D:281:TRP:HD1	1:D:282:ASN:CA	2.18	0.56
1:H:154:LYS:HB3	1:K:189:HIS:NE2	2.20	0.56
1:K:44:ARG:HG3	1:K:44:ARG:O	1.97	0.56
1:K:293:ASP:O	1:K:297:GLN:HB2	2.04	0.56
1:L:44:ARG:C	1:L:46:ARG:N	2.58	0.56
1:F:293:ASP:O	1:F:297:GLN:HB2	2.05	0.56
1:G:44:ARG:C	1:G:46:ARG:N	2.58	0.56
1:G:293:ASP:O	1:G:297:GLN:HB2	2.05	0.56
1:H:274:GLY:N	1:H:314:ILE:HD12	2.21	0.56
1:H:400:LYS:CD	1:H:403:ARG:HH21	2.18	0.56
1:L:236:LEU:HB2	1:L:238:MET:HG3	1.87	0.56
1:A:294:PHE:O	1:A:298:HIS:ND1	2.38	0.56
1:C:47:GLY:HA3	1:F:72:TRP:HB2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:30:GLU:N	1:F:32:LEU:HD12	2.19	0.56
1:J:439:ARG:NH2	1:K:405:SER:OG	2.35	0.56
1:K:281:TRP:HD1	1:K:282:ASN:N	2.03	0.56
1:L:427:THR:HG22	1:L:429:PRO:HD3	1.86	0.56
1:B:32:LEU:HD13	1:B:33:LYS:HG3	1.86	0.56
1:I:117:VAL:HG21	1:I:371:LEU:HG	1.86	0.56
1:J:318:ASP:HA	1:J:340:LYS:HG3	1.88	0.56
1:E:281:TRP:CD1	1:E:282:ASN:CA	2.88	0.56
1:I:446:LYS:O	1:I:450:HIS:HD2	1.89	0.56
1:J:240:PRO:CG	1:J:245:LYS:NZ	2.67	0.56
1:L:290:GLU:CD	1:L:306:LYS:HZ3	2.09	0.56
1:L:315:LEU:O	1:L:339:VAL:HG12	2.05	0.56
1:A:35:ARG:C	1:A:37:THR:H	2.05	0.56
1:B:189:HIS:HD1	1:B:189:HIS:C	2.08	0.56
1:H:150:MET:O	1:H:154:LYS:HG3	2.06	0.56
1:J:189:HIS:HD1	1:J:189:HIS:C	2.09	0.56
1:K:225:ASN:ND2	1:K:458:GLU:OE2	2.38	0.56
1:C:282:ASN:ND2	1:C:306:LYS:O	2.39	0.56
1:D:495:GLU:O	1:E:177:SER:OG	2.20	0.56
1:H:400:LYS:HD3	1:H:403:ARG:HH21	1.71	0.56
1:J:44:ARG:NH1	1:J:44:ARG:HG3	2.21	0.56
1:E:28:LEU:C	1:E:32:LEU:HD11	2.27	0.56
1:E:281:TRP:HE1	1:E:283:PRO:N	2.02	0.56
1:G:10:PHE:HA	1:G:106:ALA:HB2	1.87	0.56
1:H:64:PRO:HB3	1:J:51:ILE:HG12	1.88	0.56
1:I:400:LYS:HD3	1:I:403:ARG:HH21	1.71	0.56
1:B:400:LYS:CD	1:B:403:ARG:HH21	2.18	0.56
1:D:400:LYS:CD	1:D:403:ARG:HH21	2.18	0.56
1:E:294:PHE:CZ	1:E:298:HIS:HE1	2.24	0.56
1:A:51:ILE:HG12	1:E:64:PRO:HB3	1.87	0.55
1:B:10:PHE:HA	1:B:106:ALA:HB2	1.88	0.55
1:C:10:PHE:HA	1:C:106:ALA:HB2	1.89	0.55
1:C:315:LEU:O	1:C:339:VAL:HG12	2.06	0.55
1:D:60:SER:HB3	1:D:78:TYR:HD1	1.70	0.55
1:D:314:ILE:O	1:D:316:GLU:N	2.39	0.55
1:F:37:THR:HB	1:F:40:GLN:HA	1.88	0.55
1:G:419:ARG:C	1:G:421:PHE:N	2.59	0.55
1:H:38:GLU:O	1:H:39:GLU:HB2	2.06	0.55
1:A:34:THR:CA	1:A:35:ARG:HB3	2.32	0.55
1:C:44:ARG:C	1:C:46:ARG:N	2.60	0.55
1:G:132:ASN:C	1:G:134:LYS:H	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:9:PHE:C	1:H:11:LYS:H	2.09	0.55
1:J:402:GLU:HA	1:J:405:SER:HB2	1.87	0.55
1:B:281:TRP:HD1	1:B:282:ASN:HA	1.71	0.55
1:C:419:ARG:C	1:C:421:PHE:N	2.59	0.55
1:F:60:SER:HB3	1:F:78:TYR:CD1	2.41	0.55
1:H:35:ARG:HG3	1:H:36:GLU:N	2.21	0.55
1:I:318:ASP:HA	1:I:340:LYS:HD2	1.87	0.55
1:A:38:GLU:O	1:A:39:GLU:HB2	2.06	0.55
1:B:9:PHE:CZ	1:B:328:GLU:OE2	2.59	0.55
1:B:245:LYS:O	1:B:269:LYS:HG2	2.05	0.55
1:D:281:TRP:CD1	1:D:282:ASN:CA	2.90	0.55
1:D:400:LYS:HD3	1:D:403:ARG:HH21	1.70	0.55
1:H:44:ARG:C	1:H:46:ARG:N	2.60	0.55
1:L:337:PRO:HA	1:L:363:ARG:HE	1.72	0.55
1:D:17:PHE:CD2	1:D:53:LYS:HD2	2.41	0.55
1:G:82:HIS:ND1	1:G:109:SER:HA	2.22	0.55
1:I:217:ARG:NE	1:I:450:HIS:ND1	2.55	0.55
1:C:344:ILE:HD12	1:C:360:PHE:CE2	2.42	0.55
1:D:147:ARG:NH1	1:D:151:GLU:OE2	2.40	0.55
1:G:64:PRO:HB3	1:K:51:ILE:HG12	1.88	0.55
1:J:282:ASN:ND2	1:J:306:LYS:O	2.40	0.55
1:A:10:PHE:HA	1:A:106:ALA:HB2	1.88	0.55
1:D:9:PHE:C	1:D:11:LYS:N	2.54	0.55
1:L:33:LYS:C	1:L:35:ARG:N	2.53	0.55
1:A:482:TYR:O	1:A:486:ILE:HG12	2.07	0.55
1:C:43:ASN:O	1:C:46:ARG:HD3	2.07	0.55
1:E:240:PRO:HB2	1:E:244:ASP:O	2.07	0.55
1:F:499:THR:HG23	1:F:500:PHE:N	2.22	0.55
1:H:501:THR:HG21	1:L:185:SER:OG	2.06	0.55
1:I:51:ILE:HG12	1:L:64:PRO:HB3	1.88	0.55
1:I:147:ARG:NH1	1:I:151:GLU:OE2	2.40	0.55
1:K:281:TRP:CD1	1:K:282:ASN:CA	2.90	0.55
1:A:142:GLU:OE1	1:F:498:VAL:HG12	2.06	0.55
1:A:147:ARG:NH1	1:A:151:GLU:OE2	2.40	0.55
1:A:240:PRO:HG2	1:A:245:LYS:HZ3	1.72	0.55
1:B:400:LYS:HD3	1:B:403:ARG:HH21	1.71	0.55
1:E:281:TRP:CD1	1:E:282:ASN:HA	2.42	0.55
1:G:233:MET:O	1:G:238:MET:N	2.33	0.55
1:H:87:THR:HG22	1:H:88:PRO:HD3	1.89	0.55
1:H:117:VAL:HG21	1:H:371:LEU:HG	1.88	0.55
1:J:294:PHE:CZ	1:J:304:PHE:HA	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:482:TYR:O	1:K:486:ILE:HG12	2.07	0.55
1:L:482:TYR:O	1:L:486:ILE:HG12	2.06	0.55
1:E:82:HIS:ND1	1:E:109:SER:HA	2.22	0.55
1:F:286:ILE:CG2	1:F:291:LEU:HD22	2.37	0.55
1:H:314:ILE:O	1:H:316:GLU:N	2.39	0.55
1:J:147:ARG:NH1	1:J:151:GLU:OE2	2.40	0.55
1:K:36:GLU:HG3	1:K:42:ARG:HH21	1.71	0.55
1:A:281:TRP:HD1	1:A:282:ASN:CA	2.20	0.54
1:A:400:LYS:HD3	1:A:403:ARG:HH21	1.71	0.54
1:D:429:PRO:HA	1:E:416:SER:CB	2.37	0.54
1:E:35:ARG:HB3	1:E:35:ARG:CZ	2.37	0.54
1:G:281:TRP:HD1	1:G:282:ASN:CA	2.20	0.54
1:K:274:GLY:N	1:K:314:ILE:HD13	2.22	0.54
1:B:147:ARG:NH1	1:B:151:GLU:OE2	2.40	0.54
1:D:9:PHE:C	1:D:11:LYS:H	2.09	0.54
1:D:355:GLU:O	1:D:359:ILE:HD12	2.07	0.54
1:I:282:ASN:ND2	1:I:306:LYS:O	2.41	0.54
1:K:355:GLU:O	1:K:359:ILE:HD12	2.06	0.54
1:K:400:LYS:CD	1:K:403:ARG:HH21	2.19	0.54
1:K:419:ARG:C	1:K:421:PHE:N	2.59	0.54
1:L:247:PHE:HB3	1:L:321:ILE:HB	1.89	0.54
1:L:459:ARG:NH2	2:L:601:ADP:O3B	2.38	0.54
1:B:294:PHE:CE1	1:B:298:HIS:CE1	2.94	0.54
1:C:19:ARG:HE	1:C:479:THR:HG21	1.72	0.54
1:C:400:LYS:HD3	1:C:403:ARG:HH21	1.73	0.54
1:D:294:PHE:CZ	1:D:304:PHE:HA	2.42	0.54
1:G:239:THR:HG23	1:G:239:THR:O	2.08	0.54
1:G:281:TRP:CD1	1:G:282:ASN:CA	2.91	0.54
1:L:247:PHE:CD2	1:L:263:LEU:HD23	2.43	0.54
1:D:240:PRO:HG3	1:D:245:LYS:HZ2	1.67	0.54
1:D:318:ASP:HA	1:D:340:LYS:HG2	1.89	0.54
1:F:282:ASN:ND2	1:F:306:LYS:O	2.40	0.54
1:I:439:ARG:HH21	1:J:405:SER:HG	1.53	0.54
1:J:33:LYS:C	1:J:35:ARG:N	2.61	0.54
1:J:34:THR:O	1:J:35:ARG:HB3	2.07	0.54
1:L:85:HIS:HB2	1:L:492:VAL:HG11	1.88	0.54
1:L:147:ARG:NH1	1:L:151:GLU:OE2	2.41	0.54
1:A:47:GLY:HA3	1:E:72:TRP:HB2	1.88	0.54
1:H:233:MET:HB3	1:H:239:THR:N	2.19	0.54
1:I:44:ARG:C	1:I:46:ARG:N	2.60	0.54
1:C:192:ILE:O	1:C:391:HIS:NE2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:MET:O	1:E:239:THR:C	2.46	0.54
1:E:346:GLU:OE2	1:E:478:ARG:NH2	2.38	0.54
1:F:147:ARG:NH1	1:F:151:GLU:OE2	2.41	0.54
1:F:236:LEU:HB3	1:F:342:LYS:HE3	1.89	0.54
1:F:281:TRP:NE1	1:F:283:PRO:HD3	2.22	0.54
1:I:82:HIS:ND1	1:I:109:SER:HA	2.23	0.54
1:I:245:LYS:O	1:I:269:LYS:HB2	2.07	0.54
1:J:240:PRO:HB2	1:J:244:ASP:O	2.07	0.54
1:L:32:LEU:HD21	1:L:490:PHE:HE2	1.73	0.54
1:F:419:ARG:C	1:F:421:PHE:N	2.60	0.54
1:G:147:ARG:NH1	1:G:151:GLU:OE2	2.40	0.54
1:G:383:PHE:HD2	1:G:449:VAL:HG13	1.73	0.54
1:J:239:THR:HG23	1:J:239:THR:O	2.06	0.54
1:K:252:PHE:HD2	1:K:295:LYS:HZ2	1.51	0.54
1:L:310:TYR:CG	1:L:311:GLU:N	2.75	0.54
1:C:328:GLU:HB2	1:C:329:LYS:HG3	1.90	0.54
1:D:239:THR:HG23	1:D:239:THR:O	2.08	0.54
1:L:328:GLU:HB3	1:L:329:LYS:HG3	1.89	0.54
1:A:142:GLU:CD	1:F:499:THR:HB	2.29	0.54
1:A:501:THR:OG1	1:B:185:SER:HB3	2.08	0.54
1:C:147:ARG:NH1	1:C:151:GLU:OE2	2.41	0.54
1:F:281:TRP:HD1	1:F:282:ASN:N	2.06	0.54
1:F:428:ILE:CD1	1:G:239:THR:HG21	2.37	0.54
1:F:294:PHE:CZ	1:F:304:PHE:HA	2.42	0.54
1:I:272:ALA:HB1	1:I:314:ILE:HD11	1.90	0.54
1:I:281:TRP:CD1	1:I:282:ASN:CA	2.90	0.54
1:J:286:ILE:CG2	1:J:291:LEU:HD22	2.38	0.54
1:L:281:TRP:CD1	1:L:282:ASN:CA	2.91	0.54
1:L:282:ASN:ND2	1:L:306:LYS:O	2.41	0.54
1:B:240:PRO:HG2	1:B:245:LYS:CE	2.38	0.53
1:E:419:ARG:C	1:E:421:PHE:N	2.60	0.53
1:I:36:GLU:HG3	1:I:42:ARG:HH21	1.73	0.53
1:J:35:ARG:C	1:J:37:THR:N	2.60	0.53
1:J:82:HIS:ND1	1:J:109:SER:HA	2.24	0.53
1:K:30:GLU:N	1:K:32:LEU:HD12	2.23	0.53
1:C:35:ARG:O	1:C:37:THR:N	2.36	0.53
1:H:47:GLY:HA3	1:J:72:TRP:HB2	1.89	0.53
1:H:147:ARG:NH1	1:H:151:GLU:OE2	2.41	0.53
1:K:147:ARG:NH1	1:K:151:GLU:OE2	2.41	0.53
1:L:37:THR:HG21	1:L:40:GLN:HB2	1.91	0.53
1:L:82:HIS:ND1	1:L:109:SER:HA	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:294:PHE:CZ	1:L:304:PHE:HA	2.43	0.53
1:C:410:LEU:HB3	1:C:430:ILE:HA	1.89	0.53
1:E:10:PHE:HA	1:E:106:ALA:HB2	1.90	0.53
1:G:53:LYS:HB3	1:G:54:PRO:HD3	1.90	0.53
1:H:28:LEU:HD21	1:H:490:PHE:CG	2.43	0.53
1:H:281:TRP:HD1	1:H:282:ASN:CA	2.22	0.53
1:H:286:ILE:CG2	1:H:291:LEU:HD22	2.38	0.53
1:H:419:ARG:C	1:H:421:PHE:N	2.61	0.53
1:K:87:THR:HG22	1:K:88:PRO:HD3	1.89	0.53
1:L:39:GLU:O	1:L:40:GLN:HB3	2.07	0.53
1:C:28:LEU:HD21	1:C:490:PHE:CG	2.43	0.53
1:H:82:HIS:ND1	1:H:109:SER:HA	2.24	0.53
1:I:467:THR:HG21	1:I:484:ASN:HB2	1.90	0.53
1:L:29:VAL:HG12	1:L:42:ARG:HB2	1.91	0.53
1:A:34:THR:HB	1:A:35:ARG:CG	2.38	0.53
1:D:23:ILE:HG22	1:D:471:TYR:CE2	2.43	0.53
1:K:257:LEU:HD11	1:K:292:GLU:CG	2.38	0.53
1:B:203:ILE:HG21	1:B:209:HIS:HE1	1.74	0.53
1:C:281:TRP:CD1	1:C:282:ASN:CA	2.92	0.53
1:D:87:THR:HG22	1:D:88:PRO:HD3	1.90	0.53
1:D:355:GLU:O	1:D:358:LYS:HB3	2.08	0.53
1:E:87:THR:HG22	1:E:88:PRO:HD3	1.90	0.53
1:A:473:LEU:HB3	1:A:476:ASP:HB3	1.90	0.53
1:B:82:HIS:ND1	1:B:109:SER:HA	2.23	0.53
1:H:346:GLU:OE2	1:H:478:ARG:NH2	2.42	0.53
1:I:47:GLY:HA3	1:L:72:TRP:HB2	1.91	0.53
1:K:24:VAL:HG22	1:K:483:VAL:HG13	1.90	0.53
1:K:39:GLU:O	1:K:40:GLN:HB3	2.08	0.53
1:C:41:LYS:CG	1:C:44:ARG:NH1	2.71	0.53
1:C:400:LYS:CD	1:C:403:ARG:HH21	2.22	0.53
1:E:38:GLU:O	1:E:39:GLU:HB2	2.09	0.53
1:F:82:HIS:ND1	1:F:109:SER:HA	2.23	0.53
1:J:44:ARG:HH11	1:J:44:ARG:HG3	1.72	0.53
1:K:82:HIS:ND1	1:K:109:SER:HA	2.24	0.53
1:L:286:ILE:CG2	1:L:291:LEU:HD22	2.37	0.53
1:A:82:HIS:ND1	1:A:109:SER:HA	2.23	0.53
1:E:19:ARG:HH21	1:E:479:THR:HG21	1.72	0.53
1:E:286:ILE:CG2	1:E:291:LEU:HD22	2.38	0.53
1:F:239:THR:HG23	1:F:239:THR:O	2.08	0.53
1:F:240:PRO:HG2	1:F:245:LYS:HZ2	1.69	0.53
1:H:30:GLU:H	1:H:32:LEU:HD12	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:THR:HG22	1:F:88:PRO:HD3	1.90	0.53
1:F:314:ILE:O	1:F:316:GLU:N	2.42	0.53
1:G:482:TYR:O	1:G:486:ILE:HG12	2.09	0.53
1:H:281:TRP:CD1	1:H:282:ASN:CA	2.92	0.53
1:J:281:TRP:CD1	1:J:282:ASN:CA	2.92	0.53
1:K:35:ARG:O	1:K:37:THR:N	2.35	0.53
1:K:36:GLU:HG3	1:K:42:ARG:NH2	2.24	0.53
1:L:28:LEU:HD21	1:L:490:PHE:CG	2.44	0.53
1:D:331:LEU:HD22	1:D:360:PHE:HZ	1.74	0.52
1:E:238:MET:C	1:E:240:PRO:N	2.63	0.52
1:L:37:THR:CG2	1:L:40:GLN:HA	2.38	0.52
1:L:419:ARG:C	1:L:421:PHE:N	2.62	0.52
1:C:33:LYS:HG2	1:C:36:GLU:OE2	2.10	0.52
1:C:360:PHE:CD1	1:C:365:ILE:HD11	2.44	0.52
1:G:32:LEU:HD23	1:G:33:LYS:HG3	1.92	0.52
1:G:36:GLU:CG	1:G:42:ARG:HH21	2.22	0.52
1:G:87:THR:HG22	1:G:88:PRO:HD3	1.91	0.52
1:I:294:PHE:CZ	1:I:304:PHE:HA	2.44	0.52
1:J:499:THR:HG22	1:J:499:THR:O	2.10	0.52
1:A:405:SER:HG	1:F:439:ARG:HH21	1.55	0.52
1:B:355:GLU:O	1:B:359:ILE:HD12	2.09	0.52
1:D:294:PHE:CG	1:D:294:PHE:O	2.61	0.52
1:F:6:ASP:OD1	1:F:353:THR:HG21	2.08	0.52
1:G:240:PRO:HG2	1:G:245:LYS:CE	2.38	0.52
1:C:280:ILE:HG22	1:C:286:ILE:HD11	1.91	0.52
1:F:329:LYS:H	1:F:351:PRO:HA	1.73	0.52
1:H:459:ARG:NH2	2:H:601:ADP:O3B	2.42	0.52
1:I:427:THR:HA	1:J:420:LYS:HE2	1.92	0.52
1:K:286:ILE:CG2	1:K:291:LEU:HD22	2.38	0.52
1:K:466:ARG:O	1:K:469:MET:HB2	2.10	0.52
1:A:24:VAL:HG22	1:A:483:VAL:HG13	1.92	0.52
1:A:282:ASN:ND2	1:A:306:LYS:O	2.42	0.52
1:C:281:TRP:HD1	1:C:282:ASN:CA	2.22	0.52
1:E:281:TRP:HD1	1:E:282:ASN:N	2.05	0.52
1:F:281:TRP:HD1	1:F:282:ASN:HA	1.73	0.52
1:F:355:GLU:O	1:F:359:ILE:HD12	2.09	0.52
1:H:344:ILE:HD12	1:H:360:PHE:CE2	2.45	0.52
1:I:344:ILE:HD12	1:I:360:PHE:CE2	2.45	0.52
1:L:19:ARG:NE	1:L:479:THR:HG21	2.25	0.52
1:D:427:THR:HA	1:E:420:LYS:HE2	1.90	0.52
1:H:355:GLU:O	1:H:359:ILE:HD12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:405:SER:O	1:H:409:LEU:HD12	2.10	0.52
1:I:400:LYS:CD	1:I:403:ARG:HH21	2.22	0.52
1:J:355:GLU:O	1:J:358:LYS:HB3	2.10	0.52
1:K:320:ASP:O	1:K:342:LYS:N	2.39	0.52
1:L:335:ASN:O	1:L:338:ARG:HB2	2.09	0.52
1:A:344:ILE:HD12	1:A:360:PHE:CE2	2.45	0.52
1:B:233:MET:O	1:B:238:MET:N	2.34	0.52
1:B:270:CYS:SG	1:B:273:VAL:HG23	2.50	0.52
1:B:469:MET:HB3	1:G:308:LYS:NZ	2.25	0.52
1:C:82:HIS:ND1	1:C:109:SER:HA	2.24	0.52
1:E:355:GLU:O	1:E:359:ILE:HD12	2.10	0.52
1:F:272:ALA:HB1	1:F:314:ILE:HD11	1.92	0.52
1:G:72:TRP:HZ2	1:K:498:VAL:HG11	1.75	0.52
1:L:25:GLU:OE2	1:L:46:ARG:NH1	2.43	0.52
1:A:286:ILE:CG2	1:A:291:LEU:HD22	2.40	0.52
1:C:294:PHE:CZ	1:C:304:PHE:HA	2.45	0.52
1:E:6:ASP:OD2	1:E:333:LYS:NZ	2.43	0.52
1:H:290:GLU:O	1:H:294:PHE:N	2.19	0.52
1:J:290:GLU:O	1:J:294:PHE:N	2.19	0.52
1:K:37:THR:HB	1:K:40:GLN:HA	1.91	0.52
1:K:308:LYS:O	1:K:310:TYR:N	2.43	0.52
1:A:87:THR:HG22	1:A:88:PRO:HD3	1.90	0.52
1:B:314:ILE:C	1:B:316:GLU:H	2.12	0.52
1:C:482:TYR:O	1:C:486:ILE:HG12	2.09	0.52
1:I:246:THR:HG23	1:I:319:CYS:HA	1.91	0.52
1:I:297:GLN:HG3	1:I:298:HIS:ND1	2.25	0.52
1:J:67:ARG:HB3	1:J:140:GLU:OE2	2.10	0.52
1:J:355:GLU:O	1:J:359:ILE:HD12	2.10	0.52
1:L:290:GLU:O	1:L:294:PHE:N	2.19	0.52
1:A:416:SER:CB	1:F:429:PRO:HA	2.40	0.52
1:A:419:ARG:C	1:A:421:PHE:N	2.63	0.52
1:D:240:PRO:HB2	1:D:244:ASP:O	2.10	0.52
1:E:35:ARG:O	1:E:37:THR:N	2.37	0.52
1:F:270:CYS:SG	1:F:273:VAL:HG23	2.50	0.52
1:J:270:CYS:SG	1:J:273:VAL:HG23	2.50	0.52
1:K:233:MET:O	1:K:238:MET:N	2.34	0.52
1:K:270:CYS:SG	1:K:273:VAL:HG23	2.50	0.52
1:B:281:TRP:HD1	1:B:282:ASN:CA	2.23	0.51
1:D:82:HIS:ND1	1:D:109:SER:HA	2.24	0.51
1:D:305:PRO:O	1:D:306:LYS:HB2	2.10	0.51
1:D:462:ARG:O	1:D:466:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:10:PHE:HA	1:I:106:ALA:CB	2.40	0.51
1:J:245:LYS:HG3	1:J:246:THR:H	1.75	0.51
1:K:33:LYS:C	1:K:35:ARG:N	2.63	0.51
1:K:282:ASN:ND2	1:K:306:LYS:O	2.43	0.51
1:L:33:LYS:HG2	1:L:36:GLU:OE2	2.10	0.51
1:L:344:ILE:HD12	1:L:360:PHE:CE2	2.45	0.51
1:A:346:GLU:OE2	1:A:478:ARG:NH2	2.43	0.51
1:B:87:THR:HG22	1:B:88:PRO:HD3	1.92	0.51
1:B:402:GLU:HA	1:B:405:SER:HB2	1.93	0.51
1:F:344:ILE:HD12	1:F:360:PHE:CE2	2.45	0.51
1:H:294:PHE:CZ	1:H:304:PHE:HA	2.44	0.51
1:I:498:VAL:HG13	1:L:72:TRP:CH2	2.45	0.51
1:D:344:ILE:HD12	1:D:360:PHE:CE2	2.45	0.51
1:G:498:VAL:O	1:G:500:PHE:N	2.38	0.51
1:I:87:THR:HG22	1:I:88:PRO:HD3	1.92	0.51
1:K:213:SER:HB2	1:K:217:ARG:HD2	1.92	0.51
1:L:240:PRO:HB2	1:L:244:ASP:O	2.10	0.51
1:A:36:GLU:HG3	1:A:42:ARG:NH2	2.26	0.51
1:D:247:PHE:HB3	1:D:321:ILE:HB	1.93	0.51
1:E:344:ILE:HD12	1:E:360:PHE:CE2	2.45	0.51
1:F:32:LEU:HD13	1:F:33:LYS:HG3	1.93	0.51
1:H:10:PHE:HA	1:H:106:ALA:CB	2.41	0.51
1:L:85:HIS:HB2	1:L:492:VAL:CG1	2.40	0.51
1:D:281:TRP:HD1	1:D:282:ASN:HA	1.75	0.51
1:J:238:MET:C	1:J:240:PRO:N	2.63	0.51
1:K:281:TRP:CD1	1:K:282:ASN:HA	2.45	0.51
1:C:36:GLU:HG3	1:C:42:ARG:HH21	1.76	0.51
1:D:281:TRP:CD1	1:D:282:ASN:HA	2.46	0.51
1:J:344:ILE:HD12	1:J:360:PHE:CE2	2.45	0.51
1:K:310:TYR:CG	1:K:311:GLU:N	2.79	0.51
1:B:344:ILE:HD12	1:B:360:PHE:CE2	2.45	0.51
1:C:270:CYS:SG	1:C:273:VAL:HG23	2.51	0.51
1:D:31:ASP:OD1	1:D:31:ASP:O	2.29	0.51
1:H:269:LYS:HE2	1:H:284:ASP:O	2.11	0.51
1:H:270:CYS:SG	1:H:273:VAL:HG23	2.51	0.51
1:J:25:GLU:OE2	1:J:46:ARG:NH1	2.43	0.51
1:A:32:LEU:HG	1:A:33:LYS:HG3	1.92	0.51
1:J:87:THR:HG22	1:J:88:PRO:HD3	1.92	0.51
1:A:293:ASP:O	1:A:297:GLN:HB2	2.11	0.51
1:B:30:GLU:N	1:B:32:LEU:HD12	2.26	0.51
1:B:35:ARG:NH1	1:B:35:ARG:HG2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ASP:OD2	1:B:479:THR:OG1	2.29	0.51
1:B:482:TYR:O	1:B:486:ILE:HG12	2.11	0.51
1:C:41:LYS:HG3	1:C:44:ARG:HH11	1.75	0.51
1:G:286:ILE:CG2	1:G:291:LEU:HD22	2.40	0.51
1:K:344:ILE:HD12	1:K:360:PHE:CE2	2.45	0.51
1:A:292:GLU:O	1:A:295:LYS:HB2	2.11	0.51
1:E:280:ILE:HG22	1:E:286:ILE:HD11	1.93	0.51
1:G:344:ILE:HD12	1:G:360:PHE:CE2	2.45	0.51
1:J:10:PHE:HA	1:J:106:ALA:CB	2.40	0.51
1:L:87:THR:HG22	1:L:88:PRO:HD3	1.93	0.51
1:L:239:THR:HG23	1:L:239:THR:O	2.11	0.51
1:A:19:ARG:NH2	1:A:479:THR:HG21	2.22	0.50
1:C:280:ILE:HG23	1:C:307:ALA:HB1	1.93	0.50
1:D:429:PRO:HA	1:E:416:SER:HB3	1.92	0.50
1:E:405:SER:O	1:E:409:LEU:HD12	2.11	0.50
1:J:42:ARG:O	1:J:45:VAL:N	2.44	0.50
1:L:10:PHE:HA	1:L:106:ALA:CB	2.41	0.50
1:L:233:MET:O	1:L:238:MET:N	2.33	0.50
1:L:270:CYS:SG	1:L:273:VAL:HG23	2.50	0.50
1:C:476:ASP:O	1:C:478:ARG:N	2.36	0.50
1:E:281:TRP:HD1	1:E:282:ASN:CA	2.24	0.50
1:F:310:TYR:CG	1:F:311:GLU:N	2.79	0.50
1:F:383:PHE:HD2	1:F:449:VAL:HG13	1.76	0.50
1:G:294:PHE:CZ	1:G:304:PHE:HA	2.47	0.50
1:L:293:ASP:O	1:L:295:LYS:N	2.42	0.50
1:A:60:SER:HB3	1:A:78:TYR:CD1	2.46	0.50
1:B:293:ASP:O	1:B:297:GLN:HB2	2.12	0.50
1:B:310:TYR:CG	1:B:311:GLU:N	2.80	0.50
1:D:10:PHE:HA	1:D:106:ALA:CB	2.39	0.50
1:D:297:GLN:HE21	1:D:298:HIS:CE1	2.29	0.50
1:E:33:LYS:CE	1:E:494:ASN:HD21	2.23	0.50
1:G:25:GLU:OE2	1:G:46:ARG:NH1	2.43	0.50
1:G:429:PRO:HA	1:H:416:SER:CB	2.41	0.50
1:I:328:GLU:HB2	1:I:329:LYS:CG	2.41	0.50
1:C:87:THR:HG22	1:C:88:PRO:HD3	1.92	0.50
1:C:295:LYS:O	1:C:298:HIS:N	2.44	0.50
1:E:114:LYS:HD3	1:E:375:ALA:HA	1.93	0.50
1:F:281:TRP:HD1	1:F:282:ASN:CA	2.23	0.50
1:F:297:GLN:HG3	1:F:298:HIS:ND1	2.26	0.50
1:G:33:LYS:C	1:G:35:ARG:HB3	2.31	0.50
1:A:28:LEU:C	1:A:32:LEU:HD22	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:GLU:O	1:B:358:LYS:HB3	2.11	0.50
1:C:280:ILE:HD12	1:C:301:ILE:HD12	1.94	0.50
1:D:252:PHE:HD2	1:D:295:LYS:HZ2	1.55	0.50
1:I:419:ARG:C	1:I:421:PHE:N	2.65	0.50
1:J:281:TRP:CD1	1:J:282:ASN:HA	2.47	0.50
1:A:239:THR:HG23	1:A:239:THR:O	2.12	0.50
1:E:37:THR:HG22	1:E:40:GLN:HA	1.93	0.50
1:E:281:TRP:HD1	1:E:282:ASN:HA	1.74	0.50
1:G:252:PHE:HD2	1:G:295:LYS:HE3	1.75	0.50
1:G:355:GLU:O	1:G:359:ILE:HD12	2.12	0.50
1:H:29:VAL:HG12	1:H:42:ARG:HB2	1.94	0.50
1:H:437:GLN:OE1	1:H:437:GLN:HA	2.12	0.50
1:K:236:LEU:HB3	1:K:238:MET:HG3	1.94	0.50
1:L:280:ILE:HD11	1:L:301:ILE:O	2.12	0.50
1:A:316:GLU:OE1	1:A:338:ARG:CG	2.60	0.50
1:B:39:GLU:O	1:B:40:GLN:HB3	2.12	0.50
1:F:280:ILE:HG22	1:F:286:ILE:HD11	1.94	0.50
1:H:239:THR:O	1:H:239:THR:HG23	2.12	0.50
1:I:451:SER:OG	1:I:452:GLY:N	2.44	0.50
1:L:295:LYS:N	1:L:297:GLN:HB2	2.26	0.50
1:A:270:CYS:SG	1:A:273:VAL:HG23	2.52	0.50
1:G:270:CYS:SG	1:G:273:VAL:HG23	2.52	0.50
1:K:239:THR:O	1:K:239:THR:HG23	2.12	0.50
1:A:281:TRP:CD1	1:A:282:ASN:CA	2.95	0.50
1:A:281:TRP:NE1	1:A:283:PRO:HD3	2.10	0.50
1:C:25:GLU:OE2	1:C:46:ARG:NH1	2.44	0.50
1:C:394:TYR:HB2	1:C:445:GLU:HG3	1.94	0.50
1:D:36:GLU:HB2	1:D:42:ARG:NH2	2.27	0.50
1:D:462:ARG:HD2	1:D:466:ARG:NH2	2.27	0.50
1:E:272:ALA:HB1	1:E:314:ILE:HD11	1.93	0.50
1:F:44:ARG:C	1:F:46:ARG:N	2.59	0.50
1:K:116:ALA:O	1:K:488:LYS:NZ	2.37	0.50
1:B:469:MET:HB3	1:G:308:LYS:HZ3	1.77	0.49
1:C:245:LYS:O	1:C:269:LYS:HG3	2.12	0.49
1:E:295:LYS:O	1:E:298:HIS:N	2.44	0.49
1:I:280:ILE:HD11	1:I:301:ILE:O	2.12	0.49
1:J:252:PHE:HD2	1:J:295:LYS:HZ2	1.59	0.49
1:J:274:GLY:N	1:J:314:ILE:HD12	2.26	0.49
1:K:294:PHE:CZ	1:K:304:PHE:HA	2.47	0.49
1:L:400:LYS:HD3	1:L:403:ARG:HH21	1.76	0.49
1:D:60:SER:HB3	1:D:78:TYR:CD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:LEU:HD21	1:E:490:PHE:CG	2.47	0.49
1:G:310:TYR:CG	1:G:311:GLU:N	2.80	0.49
1:K:280:ILE:HG22	1:K:286:ILE:HD11	1.93	0.49
1:B:281:TRP:HD1	1:B:282:ASN:N	2.10	0.49
1:C:320:ASP:O	1:C:342:LYS:N	2.36	0.49
1:D:9:PHE:CE1	1:D:328:GLU:OE2	2.65	0.49
1:E:147:ARG:NH1	1:E:151:GLU:OE2	2.45	0.49
1:E:310:TYR:CG	1:E:311:GLU:N	2.79	0.49
1:G:28:LEU:HD21	1:G:490:PHE:CG	2.47	0.49
1:H:30:GLU:N	1:H:32:LEU:HD12	2.27	0.49
1:I:328:GLU:HB2	1:I:329:LYS:HG3	1.95	0.49
1:J:280:ILE:HG22	1:J:286:ILE:HD11	1.94	0.49
1:K:10:PHE:HA	1:K:106:ALA:CB	2.41	0.49
1:K:25:GLU:OE2	1:K:46:ARG:NH1	2.45	0.49
1:K:132:ASN:C	1:K:134:LYS:H	2.16	0.49
1:K:367:VAL:O	1:K:477:LEU:HD23	2.12	0.49
1:D:310:TYR:CG	1:D:311:GLU:N	2.80	0.49
1:D:414:GLN:O	1:D:418:GLU:HG3	2.12	0.49
1:E:270:CYS:SG	1:E:273:VAL:HG23	2.52	0.49
1:G:304:PHE:CD1	1:G:305:PRO:HD2	2.48	0.49
1:K:132:ASN:O	1:K:134:LYS:N	2.41	0.49
1:L:30:GLU:N	1:L:32:LEU:HD12	2.28	0.49
1:A:10:PHE:HA	1:A:106:ALA:CB	2.42	0.49
1:B:239:THR:HG23	1:B:239:THR:O	2.13	0.49
1:B:419:ARG:C	1:B:421:PHE:N	2.66	0.49
1:C:281:TRP:CD1	1:C:282:ASN:HA	2.47	0.49
1:C:310:TYR:CG	1:C:311:GLU:N	2.81	0.49
1:C:335:ASN:O	1:C:338:ARG:HB2	2.12	0.49
1:D:414:GLN:OE1	1:D:428:ILE:HA	2.12	0.49
1:D:422:GLY:O	1:D:423:LYS:HD3	2.13	0.49
1:G:280:ILE:HG22	1:G:286:ILE:HD11	1.94	0.49
1:J:229:GLU:CD	1:J:462:ARG:HH22	2.16	0.49
1:L:60:SER:HB3	1:L:78:TYR:CD1	2.46	0.49
1:C:33:LYS:C	1:C:35:ARG:N	2.66	0.49
1:D:53:LYS:HB3	1:D:54:PRO:CD	2.39	0.49
1:F:290:GLU:OE1	1:F:306:LYS:NZ	2.45	0.49
1:I:35:ARG:HD2	1:I:36:GLU:CA	2.43	0.49
1:J:19:ARG:NE	1:J:479:THR:HG21	2.22	0.49
1:J:245:LYS:O	1:J:269:LYS:HB2	2.12	0.49
1:K:150:MET:O	1:K:154:LYS:HG3	2.11	0.49
1:A:280:ILE:HD11	1:A:301:ILE:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LYS:HB3	1:B:54:PRO:HD3	1.95	0.49
1:B:240:PRO:CG	1:B:245:LYS:HE3	2.43	0.49
1:B:394:TYR:HB2	1:B:445:GLU:HG3	1.95	0.49
1:C:281:TRP:HD1	1:C:282:ASN:HA	1.77	0.49
1:C:382:TYR:OH	1:D:391:HIS:O	2.31	0.49
1:I:201:LYS:HG2	1:I:384:GLU:OE1	2.12	0.49
1:B:44:ARG:C	1:B:46:ARG:N	2.60	0.49
1:D:28:LEU:C	1:D:32:LEU:HD22	2.32	0.49
1:F:304:PHE:CD1	1:F:305:PRO:HD2	2.48	0.49
1:G:19:ARG:NH2	1:G:479:THR:HG21	2.27	0.49
1:G:314:ILE:O	1:G:316:GLU:N	2.46	0.49
1:K:304:PHE:CD1	1:K:305:PRO:HD2	2.48	0.49
1:L:400:LYS:CD	1:L:403:ARG:HH21	2.26	0.49
1:A:55:CYS:HA	1:A:82:HIS:HA	1.95	0.49
1:A:280:ILE:HG22	1:A:286:ILE:HD11	1.94	0.49
1:A:437:GLN:HG2	1:H:423:LYS:NZ	2.28	0.49
1:D:270:CYS:SG	1:D:273:VAL:HG23	2.52	0.49
1:F:10:PHE:HA	1:F:106:ALA:CB	2.42	0.49
1:G:132:ASN:O	1:G:134:LYS:N	2.40	0.49
1:G:281:TRP:CD1	1:G:282:ASN:HA	2.47	0.49
1:A:316:GLU:OE1	1:A:338:ARG:HG2	2.12	0.49
1:B:304:PHE:CD1	1:B:305:PRO:HD2	2.47	0.49
1:C:203:ILE:HG22	2:C:602:ADP:H5'2	1.94	0.49
1:C:239:THR:O	1:C:239:THR:HG23	2.12	0.49
1:C:305:PRO:O	1:C:307:ALA:N	2.46	0.49
1:F:213:SER:O	1:F:217:ARG:HG3	2.13	0.49
1:G:94:ARG:HD3	1:G:99:VAL:HG12	1.95	0.49
1:G:281:TRP:HD1	1:G:282:ASN:HA	1.77	0.49
1:H:281:TRP:CD1	1:H:282:ASN:HA	2.48	0.49
1:A:239:THR:HA	1:A:240:PRO:HD3	1.45	0.48
1:A:437:GLN:HG2	1:H:423:LYS:HZ2	1.76	0.48
1:H:37:THR:HG23	1:H:40:GLN:HA	1.95	0.48
1:H:94:ARG:HD3	1:H:99:VAL:HG12	1.95	0.48
1:J:39:GLU:O	1:J:40:GLN:HB3	2.13	0.48
1:J:53:LYS:HB3	1:J:54:PRO:HD3	1.95	0.48
1:J:280:ILE:HD11	1:J:301:ILE:O	2.13	0.48
1:E:53:LYS:HB3	1:E:54:PRO:HD3	1.95	0.48
1:E:281:TRP:NE1	1:E:283:PRO:HD3	2.26	0.48
1:H:304:PHE:CD1	1:H:305:PRO:HD2	2.49	0.48
1:I:53:LYS:HB3	1:I:54:PRO:HD3	1.95	0.48
1:I:432:PRO:HB3	1:I:436:PHE:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:GLY:HA3	1:C:125:ALA:O	2.14	0.48
1:C:372:TYR:OH	1:C:461:ALA:HB2	2.13	0.48
1:E:30:GLU:C	1:E:32:LEU:N	2.67	0.48
1:F:24:VAL:HG22	1:F:483:VAL:HG13	1.95	0.48
1:G:32:LEU:CD1	1:G:490:PHE:HE2	2.26	0.48
1:H:53:LYS:HB3	1:H:54:PRO:HD3	1.95	0.48
1:H:66:ARG:NH1	1:H:72:TRP:CZ2	2.82	0.48
1:L:94:ARG:HD3	1:L:99:VAL:HG12	1.95	0.48
1:B:10:PHE:HA	1:B:106:ALA:CB	2.42	0.48
1:B:94:ARG:HD3	1:B:99:VAL:HG12	1.95	0.48
1:B:286:ILE:CG2	1:B:291:LEU:HD22	2.42	0.48
1:B:498:VAL:HG23	1:B:498:VAL:O	2.13	0.48
1:E:304:PHE:CD1	1:E:305:PRO:HD2	2.48	0.48
1:F:6:ASP:OD2	1:F:333:LYS:HE3	2.13	0.48
1:G:10:PHE:HA	1:G:106:ALA:CB	2.42	0.48
1:H:315:LEU:O	1:H:339:VAL:HG12	2.12	0.48
1:L:75:ILE:HG23	1:L:131:ILE:HD13	1.96	0.48
1:L:272:ALA:HB1	1:L:314:ILE:HD11	1.94	0.48
1:B:280:ILE:HG22	1:B:286:ILE:HD11	1.94	0.48
1:C:95:TYR:HB3	1:C:133:PRO:HG3	1.95	0.48
1:D:19:ARG:HE	1:D:479:THR:CG2	2.23	0.48
1:D:466:ARG:HG2	1:D:466:ARG:HH11	1.79	0.48
1:E:19:ARG:NE	1:E:479:THR:HG21	2.25	0.48
1:I:446:LYS:O	1:I:450:HIS:CD2	2.66	0.48
1:J:310:TYR:CG	1:J:311:GLU:N	2.80	0.48
1:L:247:PHE:O	1:L:271:VAL:HG23	2.13	0.48
1:A:146:ARG:HD2	1:F:499:THR:HG21	1.96	0.48
1:B:274:GLY:N	1:B:314:ILE:HD13	2.29	0.48
1:C:32:LEU:HD11	1:C:490:PHE:HE2	1.77	0.48
1:E:91:GLY:HA3	1:E:125:ALA:O	2.14	0.48
1:E:174:ARG:HH11	1:E:174:ARG:HG3	1.78	0.48
1:E:328:GLU:HB3	1:E:329:LYS:HG3	1.95	0.48
1:F:233:MET:O	1:F:238:MET:N	2.34	0.48
1:H:482:TYR:O	1:H:486:ILE:HG12	2.14	0.48
1:I:36:GLU:HG3	1:I:42:ARG:NH2	2.29	0.48
1:I:95:TYR:HB3	1:I:133:PRO:HG3	1.96	0.48
1:J:281:TRP:HD1	1:J:282:ASN:CA	2.27	0.48
1:J:315:LEU:O	1:J:339:VAL:HG12	2.13	0.48
1:K:295:LYS:HG3	1:K:296:LEU:N	2.27	0.48
1:L:37:THR:CG2	1:L:40:GLN:HB2	2.44	0.48
1:C:35:ARG:HB3	1:C:35:ARG:NH2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:HH11	1:D:35:ARG:HD3	1.34	0.48
1:E:19:ARG:HE	1:E:479:THR:CG2	2.23	0.48
1:E:37:THR:HG22	1:E:40:GLN:CA	2.42	0.48
1:F:53:LYS:HB3	1:F:54:PRO:HD3	1.95	0.48
1:H:91:GLY:HA3	1:H:125:ALA:O	2.13	0.48
1:H:95:TYR:HB3	1:H:133:PRO:HG3	1.96	0.48
1:I:39:GLU:O	1:I:40:GLN:HB3	2.14	0.48
1:I:482:TYR:O	1:I:486:ILE:HG12	2.14	0.48
1:J:238:MET:O	1:J:239:THR:C	2.52	0.48
1:K:280:ILE:HD11	1:K:301:ILE:O	2.14	0.48
1:A:39:GLU:O	1:A:40:GLN:HB3	2.13	0.48
1:A:95:TYR:HB3	1:A:133:PRO:HG3	1.96	0.48
1:A:315:LEU:O	1:A:339:VAL:HG12	2.13	0.48
1:G:32:LEU:HD11	1:G:490:PHE:HE2	1.79	0.48
1:J:91:GLY:HA3	1:J:125:ALA:O	2.14	0.48
1:L:281:TRP:CD1	1:L:282:ASN:HA	2.49	0.48
1:A:245:LYS:O	1:A:269:LYS:HB2	2.13	0.48
1:D:91:GLY:HA3	1:D:125:ALA:O	2.14	0.48
1:D:233:MET:O	1:D:238:MET:N	2.36	0.48
1:F:91:GLY:HA3	1:F:125:ALA:O	2.14	0.48
1:F:239:THR:HA	1:F:240:PRO:HD3	1.52	0.48
1:G:75:ILE:HG23	1:G:131:ILE:HD13	1.96	0.48
1:G:91:GLY:HA3	1:G:125:ALA:O	2.14	0.48
1:H:498:VAL:HB	1:L:142:GLU:OE2	2.13	0.48
1:I:25:GLU:OE2	1:I:46:ARG:NH1	2.46	0.48
1:I:281:TRP:CD1	1:I:282:ASN:HA	2.48	0.48
1:I:459:ARG:O	1:I:463:GLN:HG3	2.14	0.48
1:K:35:ARG:O	1:K:35:ARG:HG2	1.97	0.48
1:L:280:ILE:HG22	1:L:286:ILE:HD11	1.96	0.48
1:L:281:TRP:HD1	1:L:282:ASN:HA	1.78	0.48
1:A:91:GLY:HA3	1:A:125:ALA:O	2.14	0.48
1:B:9:PHE:CD2	1:B:103:GLU:OE2	2.65	0.48
1:B:91:GLY:HA3	1:B:125:ALA:O	2.14	0.48
1:B:95:TYR:HB3	1:B:133:PRO:HG3	1.95	0.48
1:D:9:PHE:HE1	1:D:328:GLU:CG	2.25	0.48
1:E:94:ARG:HD3	1:E:99:VAL:HG12	1.95	0.48
1:E:167:PRO:HG3	1:E:176:MET:HG3	1.96	0.48
1:H:239:THR:HA	1:H:240:PRO:HD3	1.39	0.48
1:J:75:ILE:HG23	1:J:131:ILE:HD13	1.96	0.48
1:K:366:MET:HG2	1:K:477:LEU:CD2	2.44	0.48
1:L:91:GLY:HA3	1:L:125:ALA:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:HH11	1:B:44:ARG:CG	2.09	0.47
1:D:471:TYR:CE2	1:D:483:VAL:HG11	2.49	0.47
1:D:482:TYR:O	1:D:486:ILE:HG12	2.15	0.47
1:E:75:ILE:HG23	1:E:131:ILE:HD13	1.96	0.47
1:J:290:GLU:OE1	1:J:306:LYS:NZ	2.43	0.47
1:L:252:PHE:CD1	1:L:273:VAL:HG11	2.49	0.47
1:B:315:LEU:O	1:B:339:VAL:HG12	2.15	0.47
1:D:28:LEU:HD21	1:D:490:PHE:CG	2.49	0.47
1:D:95:TYR:HB3	1:D:133:PRO:HG3	1.96	0.47
1:D:432:PRO:HB3	1:D:436:PHE:CD2	2.49	0.47
1:E:282:ASN:ND2	1:E:306:LYS:O	2.47	0.47
1:E:315:LEU:O	1:E:339:VAL:HG12	2.15	0.47
1:E:328:GLU:O	1:E:330:GLN:HG3	2.15	0.47
1:F:208:ILE:HG13	1:F:445:GLU:OE1	2.14	0.47
1:G:24:VAL:HG22	1:G:483:VAL:HG13	1.95	0.47
1:H:310:TYR:CG	1:H:311:GLU:N	2.81	0.47
1:I:34:THR:CA	1:I:35:ARG:HB2	2.44	0.47
1:I:91:GLY:HA3	1:I:125:ALA:O	2.14	0.47
1:I:280:ILE:HA	1:I:308:LYS:O	2.14	0.47
1:I:430:ILE:H	1:I:430:ILE:HG13	1.56	0.47
1:K:32:LEU:HD21	1:K:490:PHE:HE2	1.79	0.47
1:A:305:PRO:C	1:A:306:LYS:HG3	2.34	0.47
1:B:25:GLU:OE2	1:B:46:ARG:NH1	2.47	0.47
1:D:51:ILE:O	1:D:54:PRO:HD2	2.15	0.47
1:D:315:LEU:O	1:D:339:VAL:HG12	2.13	0.47
1:E:28:LEU:O	1:E:32:LEU:HD11	2.15	0.47
1:F:252:PHE:CD1	1:F:273:VAL:HG11	2.49	0.47
1:F:308:LYS:O	1:F:310:TYR:N	2.47	0.47
1:G:32:LEU:CD2	1:G:33:LYS:HG3	2.44	0.47
1:G:167:PRO:HG3	1:G:176:MET:HG3	1.96	0.47
1:H:167:PRO:HG3	1:H:176:MET:HG3	1.96	0.47
1:K:44:ARG:HH11	1:K:44:ARG:HD3	1.47	0.47
1:K:75:ILE:HG23	1:K:131:ILE:HD13	1.96	0.47
1:K:238:MET:C	1:K:240:PRO:N	2.64	0.47
1:L:42:ARG:O	1:L:45:VAL:N	2.46	0.47
1:A:75:ILE:HG23	1:A:131:ILE:HD13	1.96	0.47
1:A:94:ARG:HD2	1:A:99:VAL:HG12	1.97	0.47
1:A:167:PRO:HG3	1:A:176:MET:HG3	1.96	0.47
1:C:405:SER:O	1:C:409:LEU:HD12	2.14	0.47
1:D:75:ILE:HG23	1:D:131:ILE:HD13	1.96	0.47
1:G:38:GLU:O	1:G:40:GLN:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:295:LYS:O	1:G:298:HIS:N	2.47	0.47
1:L:291:LEU:O	1:L:295:LYS:HB3	2.13	0.47
1:L:293:ASP:O	1:L:297:GLN:HB2	2.14	0.47
1:B:75:ILE:HG23	1:B:131:ILE:HD13	1.97	0.47
1:B:150:MET:O	1:B:154:LYS:HG3	2.15	0.47
1:C:35:ARG:O	1:C:37:THR:HG22	2.15	0.47
1:D:94:ARG:HD3	1:D:99:VAL:HG12	1.95	0.47
1:E:308:LYS:O	1:E:310:TYR:N	2.47	0.47
1:G:95:TYR:HB3	1:G:133:PRO:HG3	1.96	0.47
1:H:280:ILE:HG22	1:H:286:ILE:HD11	1.94	0.47
1:J:281:TRP:HD1	1:J:282:ASN:HA	1.79	0.47
1:J:482:TYR:O	1:J:486:ILE:HG12	2.14	0.47
1:K:95:TYR:HB3	1:K:133:PRO:HG3	1.96	0.47
1:K:499:THR:HG22	1:K:500:PHE:N	2.29	0.47
1:B:264:HIS:HA	1:B:268:ALA:O	2.15	0.47
1:D:9:PHE:N	1:D:9:PHE:CD1	2.81	0.47
1:D:208:ILE:HG13	1:D:387:LYS:HD2	1.97	0.47
1:D:304:PHE:CD1	1:D:305:PRO:HD2	2.49	0.47
1:F:432:PRO:HB3	1:F:436:PHE:HD2	1.80	0.47
1:F:482:TYR:O	1:F:486:ILE:HG12	2.14	0.47
1:G:459:ARG:HG2	1:G:463:GLN:HE21	1.80	0.47
1:I:134:LYS:C	1:I:136:TYR:H	2.17	0.47
1:I:320:ASP:O	1:I:342:LYS:N	2.33	0.47
1:J:405:SER:O	1:J:409:LEU:HD12	2.15	0.47
1:K:167:PRO:HG3	1:K:176:MET:HG3	1.97	0.47
1:K:264:HIS:HA	1:K:268:ALA:O	2.14	0.47
1:A:308:LYS:O	1:A:310:TYR:N	2.48	0.47
1:B:280:ILE:HD11	1:B:301:ILE:O	2.15	0.47
1:E:240:PRO:CG	1:E:245:LYS:NZ	2.71	0.47
1:F:305:PRO:O	1:F:307:ALA:N	2.47	0.47
1:G:239:THR:HA	1:G:240:PRO:HD3	1.43	0.47
1:H:75:ILE:HG23	1:H:131:ILE:HD13	1.96	0.47
1:I:416:SER:CB	1:K:429:PRO:HA	2.44	0.47
1:J:233:MET:O	1:J:238:MET:N	2.35	0.47
1:J:414:GLN:O	1:J:418:GLU:HG3	2.15	0.47
1:A:294:PHE:O	1:A:294:PHE:CG	2.68	0.47
1:B:167:PRO:HG3	1:B:176:MET:HG3	1.96	0.47
1:B:294:PHE:C	1:B:297:GLN:HB3	2.35	0.47
1:D:35:ARG:O	1:D:37:THR:HG22	2.14	0.47
1:E:32:LEU:HD21	1:E:490:PHE:HE2	1.80	0.47
1:F:167:PRO:HG3	1:F:176:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:ASP:N	1:I:7:PRO:HD3	2.30	0.47
1:I:75:ILE:HG23	1:I:131:ILE:HD13	1.97	0.47
1:I:240:PRO:HG2	1:I:245:LYS:HZ1	1.76	0.47
1:I:252:PHE:HD2	1:I:295:LYS:HZ2	1.61	0.47
1:K:91:GLY:HA3	1:K:125:ALA:O	2.14	0.47
1:A:134:LYS:C	1:A:136:TYR:H	2.18	0.47
1:C:134:LYS:C	1:C:136:TYR:H	2.17	0.47
1:D:269:LYS:HE2	1:D:284:ASP:O	2.15	0.47
1:E:29:VAL:HG22	1:E:43:ASN:N	2.28	0.47
1:F:94:ARG:HD3	1:F:99:VAL:HG12	1.96	0.47
1:H:189:HIS:NE2	1:K:154:LYS:HB3	2.30	0.47
1:I:448:ILE:HD13	1:J:401:TYR:CE1	2.50	0.47
1:K:368:ILE:HA	1:K:369:PRO:HD3	1.74	0.47
1:A:328:GLU:O	1:A:330:GLN:HG3	2.15	0.47
1:C:280:ILE:HD11	1:C:301:ILE:O	2.14	0.47
1:C:305:PRO:C	1:C:307:ALA:H	2.18	0.47
1:D:25:GLU:OE2	1:D:46:ARG:NH1	2.47	0.47
1:D:247:PHE:CD2	1:D:263:LEU:HD23	2.49	0.47
1:D:308:LYS:O	1:D:310:TYR:N	2.48	0.47
1:E:414:GLN:O	1:E:418:GLU:HG3	2.15	0.47
1:G:315:LEU:O	1:G:339:VAL:HG12	2.15	0.47
1:I:167:PRO:HG3	1:I:176:MET:HG3	1.96	0.47
1:A:246:THR:HA	1:A:269:LYS:HB2	1.97	0.46
1:H:8:ASN:O	1:H:12:MET:HG3	2.15	0.46
1:H:430:ILE:H	1:H:430:ILE:HG13	1.55	0.46
1:I:32:LEU:HD13	1:I:33:LYS:CD	2.19	0.46
1:K:500:PHE:CE2	1:L:500:PHE:HE1	2.33	0.46
1:L:314:ILE:HG21	1:L:314:ILE:HD13	1.51	0.46
1:A:274:GLY:HA3	1:A:314:ILE:HG13	1.96	0.46
1:C:39:GLU:O	1:C:40:GLN:HB3	2.15	0.46
1:F:280:ILE:HD11	1:F:301:ILE:O	2.15	0.46
1:F:315:LEU:O	1:F:339:VAL:HG12	2.15	0.46
1:G:400:LYS:HB2	1:L:455:TYR:HB2	1.97	0.46
1:H:432:PRO:HB3	1:H:436:PHE:HD2	1.80	0.46
1:I:94:ARG:HD2	1:I:99:VAL:HG12	1.97	0.46
1:I:310:TYR:CG	1:I:311:GLU:N	2.83	0.46
1:I:405:SER:OG	1:K:439:ARG:NH2	2.40	0.46
1:I:498:VAL:HG13	1:L:72:TRP:HH2	1.81	0.46
1:L:53:LYS:HB3	1:L:54:PRO:HD3	1.97	0.46
1:B:28:LEU:HD21	1:B:490:PHE:CG	2.51	0.46
1:B:189:HIS:C	1:B:189:HIS:ND1	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ARG:HD3	1:C:99:VAL:HG12	1.95	0.46
1:D:280:ILE:HD11	1:D:291:LEU:HD21	1.97	0.46
1:D:328:GLU:O	1:D:330:GLN:HG3	2.15	0.46
1:E:95:TYR:HB3	1:E:133:PRO:HG3	1.97	0.46
1:H:281:TRP:HD1	1:H:282:ASN:HA	1.79	0.46
1:I:239:THR:HG23	1:I:239:THR:O	2.16	0.46
1:B:432:PRO:HB3	1:B:436:PHE:HD2	1.79	0.46
1:C:53:LYS:HB3	1:C:54:PRO:HD3	1.95	0.46
1:C:88:PRO:HG2	1:C:122:PHE:CE1	2.51	0.46
1:D:167:PRO:HG3	1:D:176:MET:HG3	1.97	0.46
1:E:33:LYS:C	1:E:35:ARG:N	2.66	0.46
1:F:414:GLN:O	1:F:418:GLU:HG3	2.15	0.46
1:H:142:GLU:O	1:H:146:ARG:HG3	2.16	0.46
1:H:280:ILE:HD11	1:H:301:ILE:O	2.15	0.46
1:H:318:ASP:HA	1:H:340:LYS:HG2	1.98	0.46
1:I:48:ILE:HD11	1:I:498:VAL:HG22	1.96	0.46
1:J:94:ARG:HD2	1:J:99:VAL:HG12	1.97	0.46
1:J:274:GLY:CA	1:J:314:ILE:HD12	2.44	0.46
1:L:167:PRO:HG3	1:L:176:MET:HG3	1.96	0.46
1:L:246:THR:HA	1:L:269:LYS:HB2	1.98	0.46
1:A:37:THR:HB	1:A:40:GLN:HA	1.97	0.46
1:C:31:ASP:OD2	1:C:470:LYS:NZ	2.39	0.46
1:C:277:ASP:HB2	1:C:278:GLY:H	1.59	0.46
1:E:29:VAL:HG22	1:E:42:ARG:HB2	1.98	0.46
1:F:75:ILE:HG23	1:F:131:ILE:HD13	1.96	0.46
1:F:95:TYR:HB3	1:F:133:PRO:HG3	1.97	0.46
1:G:405:SER:O	1:G:409:LEU:HD12	2.16	0.46
1:H:414:GLN:O	1:H:418:GLU:HG3	2.16	0.46
1:I:294:PHE:O	1:I:294:PHE:CG	2.68	0.46
1:L:95:TYR:HB3	1:L:133:PRO:HG3	1.96	0.46
1:C:10:PHE:HA	1:C:106:ALA:CB	2.45	0.46
1:C:75:ILE:HG23	1:C:131:ILE:HD13	1.97	0.46
1:C:167:PRO:HG3	1:C:176:MET:HG3	1.97	0.46
1:C:308:LYS:O	1:C:310:TYR:N	2.48	0.46
1:C:430:ILE:H	1:C:430:ILE:HG13	1.61	0.46
1:F:25:GLU:OE2	1:F:46:ARG:NH1	2.48	0.46
1:F:264:HIS:HA	1:F:268:ALA:O	2.16	0.46
1:G:34:THR:HG23	1:G:35:ARG:HG2	1.98	0.46
1:G:280:ILE:HD11	1:G:301:ILE:O	2.15	0.46
1:H:414:GLN:OE1	1:H:428:ILE:HA	2.15	0.46
1:I:281:TRP:HD1	1:I:282:ASN:HA	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:189:HIS:C	1:J:189:HIS:ND1	2.68	0.46
1:K:55:CYS:HA	1:K:82:HIS:HA	1.96	0.46
1:A:150:MET:SD	1:A:186:THR:HG21	2.55	0.46
1:G:36:GLU:CG	1:G:42:ARG:NH2	2.78	0.46
1:G:142:GLU:O	1:G:146:ARG:HG3	2.16	0.46
1:K:430:ILE:H	1:K:430:ILE:HG13	1.48	0.46
1:L:32:LEU:HD13	1:L:33:LYS:HG3	1.98	0.46
1:A:25:GLU:OE2	1:A:46:ARG:NH1	2.48	0.46
1:A:55:CYS:HB2	1:A:105:LYS:HE3	1.98	0.46
1:A:289:LYS:O	1:A:292:GLU:HB2	2.15	0.46
1:B:32:LEU:HD21	1:B:490:PHE:HE2	1.81	0.46
1:E:293:ASP:O	1:E:295:LYS:N	2.47	0.46
1:E:309:ILE:H	1:E:309:ILE:HG12	1.54	0.46
1:G:51:ILE:O	1:G:54:PRO:HD2	2.16	0.46
1:I:331:LEU:HD22	1:I:360:PHE:HZ	1.81	0.46
1:K:44:ARG:C	1:K:46:ARG:N	2.56	0.46
1:L:252:PHE:HD2	1:L:295:LYS:HZ1	1.60	0.46
1:B:142:GLU:O	1:B:146:ARG:HG3	2.15	0.46
1:D:55:CYS:HA	1:D:82:HIS:HA	1.98	0.46
1:E:252:PHE:CD1	1:E:273:VAL:HG11	2.51	0.46
1:E:293:ASP:C	1:E:295:LYS:H	2.19	0.46
1:G:282:ASN:ND2	1:G:306:LYS:O	2.48	0.46
1:H:252:PHE:CD1	1:H:273:VAL:HG11	2.51	0.46
1:I:142:GLU:O	1:I:146:ARG:HG3	2.16	0.46
1:I:315:LEU:O	1:I:339:VAL:HG12	2.16	0.46
1:J:167:PRO:HG3	1:J:176:MET:HG3	1.97	0.46
1:L:38:GLU:O	1:L:39:GLU:HB2	2.16	0.46
1:L:134:LYS:C	1:L:136:TYR:H	2.19	0.46
1:D:35:ARG:O	1:D:37:THR:N	2.39	0.46
1:D:282:ASN:OD1	1:D:283:PRO:HD2	2.16	0.46
1:E:25:GLU:C	1:E:27:LYS:H	2.18	0.46
1:G:252:PHE:CD1	1:G:273:VAL:HG11	2.51	0.46
1:I:35:ARG:HD2	1:I:36:GLU:HA	1.98	0.46
1:I:148:PHE:CE2	1:I:152:LEU:HD11	2.51	0.46
1:J:252:PHE:CD1	1:J:273:VAL:HG11	2.51	0.46
1:L:142:GLU:O	1:L:146:ARG:HG3	2.16	0.46
1:L:294:PHE:O	1:L:294:PHE:CG	2.69	0.46
1:L:331:LEU:HD22	1:L:360:PHE:HZ	1.81	0.46
1:A:414:GLN:O	1:A:418:GLU:HG3	2.16	0.45
1:C:35:ARG:C	1:C:37:THR:N	2.67	0.45
1:F:88:PRO:HG2	1:F:122:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:209:HIS:HB3	1:I:446:LYS:HB2	1.98	0.45
1:J:9:PHE:CZ	1:J:110:LEU:HD22	2.49	0.45
1:J:88:PRO:HG2	1:J:122:PHE:CE1	2.51	0.45
1:J:142:GLU:O	1:J:146:ARG:HG3	2.15	0.45
1:K:414:GLN:OE1	1:K:428:ILE:HA	2.16	0.45
1:A:142:GLU:O	1:A:146:ARG:HG3	2.16	0.45
1:A:432:PRO:HB3	1:A:436:PHE:HD2	1.79	0.45
1:C:142:GLU:O	1:C:146:ARG:HG3	2.16	0.45
1:C:239:THR:HA	1:C:240:PRO:HD3	1.47	0.45
1:E:148:PHE:CE2	1:E:152:LEU:HD11	2.51	0.45
1:E:294:PHE:O	1:E:294:PHE:CG	2.69	0.45
1:H:9:PHE:C	1:H:11:LYS:N	2.70	0.45
1:H:55:CYS:HA	1:H:82:HIS:HA	1.99	0.45
1:J:95:TYR:HB3	1:J:133:PRO:HG3	1.97	0.45
1:L:289:LYS:O	1:L:292:GLU:HB3	2.15	0.45
2:C:601:ADP:H5'2	1:D:203:ILE:HG22	1.98	0.45
1:D:88:PRO:HG2	1:D:122:PHE:CE1	2.52	0.45
1:D:131:ILE:HG13	1:D:136:TYR:CE1	2.52	0.45
1:D:264:HIS:HA	1:D:268:ALA:O	2.16	0.45
1:D:293:ASP:O	1:D:295:LYS:N	2.49	0.45
1:E:88:PRO:HG2	1:E:122:PHE:CE1	2.52	0.45
1:F:134:LYS:C	1:F:136:TYR:H	2.18	0.45
1:F:294:PHE:CG	1:F:294:PHE:O	2.68	0.45
1:G:148:PHE:CE2	1:G:152:LEU:HD11	2.52	0.45
1:J:331:LEU:HD22	1:J:360:PHE:HZ	1.82	0.45
1:J:346:GLU:OE2	1:J:478:ARG:NH2	2.45	0.45
1:K:240:PRO:CG	1:K:245:LYS:HZ2	2.29	0.45
1:L:148:PHE:CE2	1:L:152:LEU:HD11	2.52	0.45
1:L:264:HIS:HA	1:L:268:ALA:O	2.16	0.45
1:C:131:ILE:HG13	1:C:136:TYR:CE1	2.51	0.45
1:E:120:VAL:HG13	1:E:382:TYR:HB2	1.98	0.45
1:F:142:GLU:O	1:F:146:ARG:HG3	2.16	0.45
1:G:429:PRO:HA	1:H:416:SER:HB3	1.97	0.45
1:H:432:PRO:HA	1:L:412:SER:OG	2.16	0.45
1:I:55:CYS:HA	1:I:82:HIS:HA	1.99	0.45
1:J:134:LYS:C	1:J:136:TYR:H	2.19	0.45
1:J:209:HIS:HD2	1:J:445:GLU:HB3	1.81	0.45
1:A:88:PRO:HG2	1:A:122:PHE:CE1	2.52	0.45
1:B:131:ILE:HG13	1:B:136:TYR:CE1	2.52	0.45
1:C:55:CYS:HA	1:C:82:HIS:HA	1.99	0.45
1:C:304:PHE:CD1	1:C:305:PRO:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:LYS:C	1:D:136:TYR:H	2.20	0.45
1:D:148:PHE:CE2	1:D:152:LEU:HD11	2.51	0.45
1:E:142:GLU:O	1:E:146:ARG:HG3	2.16	0.45
1:E:239:THR:HG23	1:E:239:THR:O	2.17	0.45
1:F:148:PHE:CE2	1:F:152:LEU:HD11	2.51	0.45
1:H:88:PRO:HG2	1:H:122:PHE:CE1	2.52	0.45
1:H:148:PHE:CE2	1:H:152:LEU:HD11	2.52	0.45
1:H:263:LEU:HD12	1:H:263:LEU:HA	1.84	0.45
1:H:331:LEU:HD22	1:H:360:PHE:HZ	1.81	0.45
1:I:131:ILE:HG13	1:I:136:TYR:CE1	2.52	0.45
1:I:414:GLN:OE1	1:I:428:ILE:HA	2.16	0.45
1:J:55:CYS:HA	1:J:82:HIS:HA	1.99	0.45
1:K:94:ARG:HD2	1:K:99:VAL:HG12	1.96	0.45
1:L:208:ILE:HG13	1:L:387:LYS:HD2	1.99	0.45
1:B:331:LEU:HD22	1:B:360:PHE:HZ	1.82	0.45
1:C:346:GLU:HG2	1:C:351:PRO:HG2	1.98	0.45
1:E:173:GLU:O	1:E:176:MET:HB2	2.17	0.45
1:F:469:MET:HA	1:F:472:ASN:ND2	2.31	0.45
1:H:35:ARG:HE	1:H:35:ARG:HB2	1.10	0.45
1:I:293:ASP:O	1:I:295:LYS:N	2.50	0.45
1:I:416:SER:HB3	1:K:428:ILE:O	2.17	0.45
1:J:38:GLU:O	1:J:40:GLN:N	2.39	0.45
1:J:148:PHE:CE2	1:J:152:LEU:HD11	2.52	0.45
1:L:55:CYS:HA	1:L:82:HIS:HA	1.99	0.45
1:A:64:PRO:HB3	1:E:51:ILE:HG12	1.97	0.45
1:B:148:PHE:CE2	1:B:152:LEU:HD11	2.52	0.45
1:E:305:PRO:O	1:E:307:ALA:N	2.49	0.45
1:F:131:ILE:HG13	1:F:136:TYR:CE1	2.52	0.45
1:G:72:TRP:HB2	1:K:47:GLY:HA3	1.98	0.45
1:G:272:ALA:HB1	1:G:314:ILE:HD12	1.98	0.45
1:G:338:ARG:HH11	1:G:338:ARG:HD3	1.46	0.45
1:H:131:ILE:HG13	1:H:136:TYR:CE1	2.52	0.45
1:H:294:PHE:O	1:H:294:PHE:CG	2.69	0.45
1:K:414:GLN:O	1:K:418:GLU:HG3	2.16	0.45
1:L:236:LEU:HD21	1:L:475:LEU:HD21	1.99	0.45
1:L:247:PHE:N	1:L:247:PHE:CD1	2.85	0.45
1:A:44:ARG:HB3	1:A:45:VAL:H	1.69	0.45
1:C:414:GLN:O	1:C:418:GLU:HG3	2.16	0.45
1:D:305:PRO:C	1:D:307:ALA:H	2.20	0.45
1:D:368:ILE:HA	1:D:369:PRO:HD3	1.74	0.45
1:E:280:ILE:HD11	1:E:301:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:314:ILE:HG21	1:F:314:ILE:HD13	1.49	0.45
1:F:405:SER:O	1:F:409:LEU:HD12	2.16	0.45
1:G:111:MET:HA	1:G:114:LYS:HB3	1.99	0.45
1:I:236:LEU:HB3	1:I:342:LYS:HE2	1.98	0.45
1:K:148:PHE:CE2	1:K:152:LEU:HD11	2.51	0.45
1:L:88:PRO:HG2	1:L:122:PHE:CE1	2.51	0.45
1:L:414:GLN:OE1	1:L:428:ILE:HA	2.16	0.45
1:A:131:ILE:HG13	1:A:136:TYR:CE1	2.52	0.45
1:C:446:LYS:HG2	1:C:450:HIS:CE1	2.52	0.45
1:D:79:ARG:HH11	1:D:127:ALA:HB2	1.82	0.45
1:D:298:HIS:HB2	1:D:299:GLY:H	1.38	0.45
1:E:131:ILE:HG13	1:E:136:TYR:CE1	2.52	0.45
1:F:55:CYS:HA	1:F:82:HIS:HA	1.99	0.45
1:G:282:ASN:OD1	1:G:283:PRO:HD2	2.17	0.45
1:I:30:GLU:C	1:I:32:LEU:N	2.71	0.45
1:I:277:ASP:HB2	1:I:278:GLY:H	1.56	0.45
1:I:405:SER:O	1:I:409:LEU:HD12	2.17	0.45
1:J:79:ARG:HH11	1:J:127:ALA:HB2	1.82	0.45
1:J:131:ILE:HG13	1:J:136:TYR:CE1	2.52	0.45
1:J:392:VAL:HG21	1:J:397:LEU:CD1	2.46	0.45
1:K:281:TRP:NE1	1:K:283:PRO:HD3	2.26	0.45
1:K:331:LEU:HD22	1:K:360:PHE:HZ	1.82	0.45
1:L:41:LYS:HB3	1:L:44:ARG:NH1	2.30	0.45
1:L:131:ILE:HG13	1:L:136:TYR:CE1	2.52	0.45
1:L:282:ASN:OD1	1:L:283:PRO:HD2	2.17	0.45
1:L:293:ASP:C	1:L:295:LYS:H	2.20	0.45
1:A:293:ASP:O	1:A:295:LYS:N	2.50	0.45
1:A:331:LEU:HD22	1:A:360:PHE:HZ	1.81	0.45
1:B:134:LYS:C	1:B:136:TYR:H	2.20	0.45
1:C:439:ARG:NH2	1:D:405:SER:OG	2.46	0.45
1:D:33:LYS:C	1:D:35:ARG:N	2.66	0.45
1:E:305:PRO:C	1:E:307:ALA:H	2.20	0.45
1:E:432:PRO:HB3	1:E:436:PHE:HD2	1.81	0.45
1:F:293:ASP:O	1:F:295:LYS:N	2.50	0.45
1:G:414:GLN:O	1:G:418:GLU:HG3	2.16	0.45
1:G:501:THR:HG21	1:H:181:ASP:OD2	2.17	0.45
1:H:261:ARG:NH2	1:H:292:GLU:OE2	2.50	0.45
1:H:295:LYS:N	1:H:297:GLN:HB3	2.32	0.45
1:J:51:ILE:O	1:J:54:PRO:HD2	2.17	0.45
1:K:235:ILE:H	1:K:235:ILE:HG12	1.66	0.45
1:L:35:ARG:C	1:L:37:THR:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:HH11	1:A:127:ALA:HB2	1.82	0.44
1:A:148:PHE:CE2	1:A:152:LEU:HD11	2.51	0.44
1:A:420:LYS:HA	1:A:420:LYS:HD3	1.87	0.44
1:B:294:PHE:O	1:B:298:HIS:ND1	2.37	0.44
1:B:308:LYS:O	1:B:310:TYR:N	2.50	0.44
1:B:414:GLN:O	1:B:418:GLU:HG3	2.16	0.44
1:D:142:GLU:O	1:D:146:ARG:HG3	2.16	0.44
1:E:79:ARG:HH11	1:E:127:ALA:HB2	1.82	0.44
1:E:111:MET:HA	1:E:114:LYS:HB3	1.98	0.44
1:G:55:CYS:HA	1:G:82:HIS:HA	1.99	0.44
1:G:88:PRO:HG2	1:G:122:PHE:CE1	2.51	0.44
1:G:305:PRO:O	1:G:306:LYS:CB	2.60	0.44
1:H:294:PHE:C	1:H:297:GLN:HB3	2.37	0.44
1:H:368:ILE:HA	1:H:369:PRO:HD3	1.75	0.44
1:I:212:ILE:H	1:I:212:ILE:HG13	1.54	0.44
1:I:263:LEU:HD12	1:I:263:LEU:HA	1.85	0.44
1:J:150:MET:SD	1:J:186:THR:HG21	2.57	0.44
1:J:280:ILE:HG23	1:J:307:ALA:HB1	1.99	0.44
1:J:414:GLN:OE1	1:J:428:ILE:HA	2.17	0.44
1:K:305:PRO:C	1:K:307:ALA:H	2.21	0.44
1:L:314:ILE:C	1:L:316:GLU:H	2.20	0.44
1:B:363:ARG:HE	1:B:363:ARG:HB3	1.66	0.44
1:B:414:GLN:OE1	1:B:428:ILE:HA	2.17	0.44
1:C:39:GLU:OE1	1:C:41:LYS:HG2	2.17	0.44
1:C:79:ARG:HH11	1:C:127:ALA:HB2	1.82	0.44
1:F:331:LEU:HD22	1:F:360:PHE:HZ	1.81	0.44
1:F:437:GLN:CG	1:G:244:ASP:HB2	2.26	0.44
1:F:467:THR:C	1:F:469:MET:H	2.20	0.44
1:G:174:ARG:HH11	1:G:174:ARG:HD2	1.25	0.44
1:G:294:PHE:HA	1:G:297:GLN:HG2	1.98	0.44
1:H:32:LEU:HD21	1:H:490:PHE:HE1	1.82	0.44
1:H:134:LYS:C	1:H:136:TYR:H	2.19	0.44
1:I:362:GLU:C	1:I:364:ASN:H	2.20	0.44
1:I:396:ARG:NH2	1:K:118:VAL:O	2.47	0.44
1:K:88:PRO:HG2	1:K:122:PHE:CE1	2.52	0.44
1:L:335:ASN:C	1:L:338:ARG:HB2	2.37	0.44
1:A:405:SER:O	1:A:409:LEU:HD12	2.17	0.44
1:B:55:CYS:HA	1:B:82:HIS:HA	1.99	0.44
1:B:79:ARG:HH11	1:B:127:ALA:HB2	1.82	0.44
1:E:10:PHE:HA	1:E:106:ALA:CB	2.47	0.44
1:E:35:ARG:C	1:E:37:THR:N	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:CYS:HA	1:E:82:HIS:HA	1.99	0.44
1:H:7:PRO:O	1:H:329:LYS:NZ	2.50	0.44
1:H:79:ARG:HH11	1:H:127:ALA:HB2	1.82	0.44
1:H:189:HIS:O	1:H:189:HIS:ND1	2.47	0.44
1:I:51:ILE:O	1:I:54:PRO:HD2	2.18	0.44
1:I:314:ILE:O	1:I:316:GLU:N	2.50	0.44
1:J:32:LEU:HD13	1:J:33:LYS:HG3	1.99	0.44
1:K:238:MET:O	1:K:239:THR:C	2.55	0.44
1:L:35:ARG:O	1:L:37:THR:N	2.51	0.44
1:A:495:GLU:OE1	1:B:204:SER:OG	2.29	0.44
1:B:252:PHE:CD1	1:B:273:VAL:HG11	2.52	0.44
1:B:469:MET:C	1:G:308:LYS:HZ1	2.19	0.44
1:C:432:PRO:HB3	1:C:436:PHE:HD2	1.82	0.44
1:D:261:ARG:NH2	1:D:292:GLU:OE2	2.50	0.44
1:H:259:SER:O	1:H:263:LEU:HB2	2.17	0.44
1:I:79:ARG:HH11	1:I:127:ALA:HB2	1.82	0.44
1:K:131:ILE:HG13	1:K:136:TYR:CE1	2.52	0.44
1:L:6:ASP:HA	1:L:7:PRO:HD3	1.66	0.44
1:L:295:LYS:HG3	1:L:296:LEU:H	1.83	0.44
1:B:150:MET:SD	1:B:186:THR:HG21	2.57	0.44
1:C:148:PHE:CE2	1:C:152:LEU:HD11	2.51	0.44
1:E:39:GLU:O	1:E:40:GLN:HB3	2.17	0.44
1:E:331:LEU:HD22	1:E:360:PHE:HZ	1.82	0.44
1:F:36:GLU:HG3	1:F:42:ARG:NH2	2.32	0.44
1:G:26:ASP:O	1:G:29:VAL:HG22	2.18	0.44
1:I:44:ARG:O	1:I:46:ARG:N	2.51	0.44
1:I:88:PRO:HG2	1:I:122:PHE:CE1	2.52	0.44
1:J:282:ASN:OD1	1:J:283:PRO:HD2	2.17	0.44
1:K:12:MET:SD	1:K:354:PRO:HD3	2.58	0.44
1:L:51:ILE:O	1:L:54:PRO:HD2	2.18	0.44
1:L:308:LYS:O	1:L:310:TYR:N	2.50	0.44
1:B:111:MET:HA	1:B:114:LYS:HB3	1.99	0.44
1:C:414:GLN:OE1	1:C:428:ILE:HA	2.18	0.44
1:D:44:ARG:O	1:D:46:ARG:N	2.46	0.44
1:F:12:MET:SD	1:F:354:PRO:HD3	2.57	0.44
1:F:42:ARG:HH11	1:F:42:ARG:HD2	1.48	0.44
1:F:173:GLU:O	1:F:202:PRO:HD3	2.18	0.44
1:H:39:GLU:O	1:H:40:GLN:HB3	2.18	0.44
1:I:111:MET:HA	1:I:114:LYS:HB3	1.99	0.44
1:A:282:ASN:OD1	1:A:283:PRO:HD2	2.17	0.44
1:A:310:TYR:CG	1:A:311:GLU:N	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LEU:HD22	1:B:482:TYR:CD1	2.53	0.44
1:C:51:ILE:O	1:C:54:PRO:HD2	2.17	0.44
1:C:359:ILE:O	1:C:363:ARG:HB2	2.17	0.44
1:D:453:LEU:HD23	1:D:457:MET:HG2	2.00	0.44
1:E:264:HIS:HA	1:E:268:ALA:O	2.17	0.44
1:G:131:ILE:HG13	1:G:136:TYR:CE1	2.52	0.44
1:H:51:ILE:O	1:H:54:PRO:HD2	2.18	0.44
1:H:308:LYS:O	1:H:310:TYR:N	2.50	0.44
1:J:42:ARG:HB2	1:J:43:ASN:H	1.62	0.44
1:K:34:THR:HG22	1:K:35:ARG:CB	2.48	0.44
1:K:79:ARG:HH11	1:K:127:ALA:HB2	1.82	0.44
1:K:141:LEU:HD23	1:K:141:LEU:HA	1.87	0.44
1:K:142:GLU:O	1:K:146:ARG:HG3	2.18	0.44
1:K:282:ASN:OD1	1:K:283:PRO:HD2	2.18	0.44
1:L:247:PHE:N	1:L:247:PHE:HD1	2.15	0.44
1:A:189:HIS:C	1:A:189:HIS:ND1	2.68	0.44
1:A:414:GLN:OE1	1:A:428:ILE:HA	2.18	0.44
1:F:261:ARG:NH2	1:F:292:GLU:OE2	2.51	0.44
1:G:79:ARG:HH11	1:G:127:ALA:HB2	1.82	0.44
1:I:139:ASN:O	1:I:143:LYS:HG3	2.17	0.44
1:J:111:MET:HA	1:J:114:LYS:HB3	2.00	0.44
1:K:19:ARG:HH11	1:K:19:ARG:HD2	1.43	0.44
1:K:315:LEU:O	1:K:339:VAL:HG12	2.17	0.44
1:L:150:MET:SD	1:L:186:THR:HG21	2.58	0.44
1:L:247:PHE:CE1	1:L:269:LYS:C	2.91	0.44
1:A:281:TRP:CD1	1:A:282:ASN:HA	2.52	0.44
1:A:313:SER:CB	1:A:315:LEU:HD12	2.48	0.44
1:A:424:HIS:CE1	1:H:407:TYR:CE2	3.05	0.44
1:B:280:ILE:HD13	1:B:280:ILE:HG21	1.76	0.44
1:C:497:GLY:HA3	1:C:501:THR:HB	2.00	0.44
1:H:111:MET:HA	1:H:114:LYS:HB3	2.00	0.44
1:I:414:GLN:O	1:I:418:GLU:HG3	2.18	0.44
1:L:30:GLU:O	1:L:34:THR:N	2.50	0.44
1:A:26:ASP:O	1:A:29:VAL:HG22	2.18	0.43
1:A:51:ILE:O	1:A:54:PRO:HD2	2.17	0.43
1:A:150:MET:O	1:A:154:LYS:HG3	2.18	0.43
1:B:479:THR:HA	1:B:482:TYR:HB2	1.99	0.43
2:B:601:ADP:O3B	1:F:393:SER:OG	2.27	0.43
1:D:173:GLU:O	1:D:202:PRO:HD3	2.18	0.43
1:D:252:PHE:CD1	1:D:273:VAL:HG11	2.52	0.43
1:D:291:LEU:CD2	1:D:291:LEU:HB3	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:LYS:C	1:E:136:TYR:H	2.21	0.43
1:F:79:ARG:HH11	1:F:127:ALA:HB2	1.82	0.43
1:F:245:LYS:O	1:F:269:LYS:HG3	2.18	0.43
1:G:331:LEU:HD22	1:G:360:PHE:HZ	1.82	0.43
1:H:173:GLU:O	1:H:202:PRO:HD3	2.18	0.43
1:I:455:TYR:O	1:I:459:ARG:HB2	2.16	0.43
1:J:294:PHE:O	1:J:294:PHE:CG	2.71	0.43
1:K:35:ARG:HH11	1:K:35:ARG:HD3	1.31	0.43
1:K:44:ARG:O	1:K:46:ARG:N	2.50	0.43
1:L:34:THR:H	1:L:34:THR:HG23	1.47	0.43
1:L:132:ASN:HA	1:L:133:PRO:HD3	1.82	0.43
1:L:238:MET:C	1:L:240:PRO:N	2.71	0.43
1:L:410:LEU:HB3	1:L:430:ILE:HA	2.01	0.43
1:A:146:ARG:CD	1:F:499:THR:HG21	2.48	0.43
1:B:88:PRO:HG2	1:B:122:PHE:CE1	2.53	0.43
1:C:26:ASP:O	1:C:29:VAL:HG22	2.19	0.43
1:C:368:ILE:HA	1:C:369:PRO:HD3	1.74	0.43
1:E:42:ARG:HA	1:E:45:VAL:CG2	2.48	0.43
1:F:305:PRO:C	1:F:307:ALA:H	2.19	0.43
1:H:282:ASN:OD1	1:H:283:PRO:HD2	2.18	0.43
1:H:293:ASP:C	1:H:295:LYS:H	2.22	0.43
1:H:293:ASP:O	1:H:295:LYS:N	2.50	0.43
1:J:24:VAL:HG22	1:J:483:VAL:HG13	2.00	0.43
1:J:274:GLY:HA3	1:J:314:ILE:HD12	1.99	0.43
1:K:9:PHE:CE2	1:K:350:GLY:HA3	2.53	0.43
1:K:471:TYR:O	1:K:473:LEU:N	2.51	0.43
1:A:335:ASN:O	1:A:338:ARG:HB3	2.17	0.43
1:B:42:ARG:O	1:B:45:VAL:N	2.52	0.43
1:B:247:PHE:CE1	1:B:269:LYS:C	2.91	0.43
1:C:287:ASP:HA	1:C:288:PRO:HD2	1.85	0.43
1:D:42:ARG:HH11	1:D:42:ARG:HD2	1.53	0.43
1:F:51:ILE:O	1:F:54:PRO:HD2	2.17	0.43
1:F:233:MET:HB3	1:F:239:THR:N	2.22	0.43
1:H:260:MET:HG2	1:H:288:PRO:HG3	2.00	0.43
1:I:240:PRO:CG	1:I:245:LYS:NZ	2.73	0.43
1:J:132:ASN:O	1:J:134:LYS:N	2.51	0.43
1:A:252:PHE:CD1	1:A:273:VAL:HG11	2.53	0.43
1:A:271:VAL:HG12	1:A:283:PRO:HA	2.00	0.43
1:B:173:GLU:O	1:B:202:PRO:HD3	2.18	0.43
1:B:368:ILE:HA	1:B:369:PRO:HD3	1.75	0.43
1:B:430:ILE:H	1:B:430:ILE:HG13	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:ARG:NH2	1:C:292:GLU:OE2	2.51	0.43
1:G:173:GLU:O	1:G:202:PRO:HD3	2.18	0.43
1:L:174:ARG:HH11	1:L:174:ARG:HD3	1.56	0.43
1:L:432:PRO:HB3	1:L:436:PHE:HD2	1.80	0.43
1:A:35:ARG:O	1:A:37:THR:N	2.44	0.43
1:C:252:PHE:HB3	1:C:275:GLU:OE2	2.17	0.43
1:D:287:ASP:HA	1:D:288:PRO:HD2	1.85	0.43
1:G:30:GLU:O	1:G:33:LYS:N	2.51	0.43
1:L:111:MET:HA	1:L:114:LYS:HB3	2.01	0.43
1:A:410:LEU:HB3	1:A:430:ILE:HA	2.01	0.43
1:A:470:LYS:HG2	1:A:471:TYR:HD2	1.83	0.43
1:B:320:ASP:O	1:B:342:LYS:N	2.33	0.43
1:B:410:LEU:HB3	1:B:430:ILE:HA	2.00	0.43
1:C:346:GLU:HG2	1:C:351:PRO:CG	2.49	0.43
1:D:42:ARG:O	1:D:45:VAL:N	2.51	0.43
1:E:150:MET:SD	1:E:186:THR:HG21	2.58	0.43
1:F:42:ARG:HA	1:F:45:VAL:HG22	2.00	0.43
1:F:467:THR:HA	1:F:470:LYS:HG3	2.00	0.43
1:G:320:ASP:O	1:G:342:LYS:N	2.38	0.43
1:I:355:GLU:HA	1:I:358:LYS:HB3	2.00	0.43
1:J:261:ARG:NH2	1:J:292:GLU:OE2	2.51	0.43
1:L:79:ARG:HH11	1:L:127:ALA:HB2	1.82	0.43
1:A:397:LEU:HD22	1:F:394:TYR:CE1	2.53	0.43
1:C:501:THR:HG21	1:D:181:ASP:OD1	2.18	0.43
1:E:24:VAL:HG22	1:E:483:VAL:HG13	2.01	0.43
1:F:25:GLU:C	1:F:27:LYS:H	2.21	0.43
1:F:189:HIS:HB3	1:F:190:TYR:HD1	1.84	0.43
1:F:414:GLN:OE1	1:F:428:ILE:HA	2.18	0.43
1:G:414:GLN:OE1	1:G:428:ILE:HA	2.19	0.43
1:H:150:MET:SD	1:H:186:THR:HG21	2.58	0.43
1:H:238:MET:O	1:H:239:THR:C	2.56	0.43
1:H:436:PHE:CG	1:L:408:HIS:HB3	2.53	0.43
1:I:175:GLU:O	1:I:179:ILE:HG13	2.19	0.43
1:I:335:ASN:HA	1:I:338:ARG:HD3	2.01	0.43
1:J:432:PRO:HB3	1:J:436:PHE:HD2	1.80	0.43
1:A:304:PHE:CD1	1:A:305:PRO:HD2	2.53	0.43
1:B:51:ILE:O	1:B:54:PRO:HD2	2.18	0.43
1:C:46:ARG:HH11	1:C:46:ARG:HD2	1.61	0.43
1:C:252:PHE:CD1	1:C:273:VAL:HG11	2.54	0.43
1:D:111:MET:HA	1:D:114:LYS:HB3	2.00	0.43
1:E:140:GLU:O	1:E:144:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:ASP:O	1:F:342:LYS:N	2.38	0.43
1:F:368:ILE:HA	1:F:369:PRO:HD3	1.74	0.43
1:I:410:LEU:HB3	1:I:430:ILE:HA	2.01	0.43
1:K:30:GLU:H	1:K:32:LEU:HD12	1.83	0.43
1:K:111:MET:HA	1:K:114:LYS:HB3	2.01	0.43
1:K:438:ASP:HA	1:K:441:SER:HB3	2.01	0.43
1:A:408:HIS:HB3	1:F:436:PHE:CD1	2.54	0.43
1:B:296:LEU:HB2	1:B:297:GLN:H	1.35	0.43
1:D:39:GLU:O	1:D:40:GLN:HB3	2.19	0.43
1:F:282:ASN:OD1	1:F:283:PRO:HD2	2.18	0.43
1:G:65:ILE:HD13	1:G:144:ILE:HG12	2.01	0.43
1:G:242:PHE:HD1	1:G:242:PHE:HA	1.70	0.43
1:I:192:ILE:O	1:I:391:HIS:NE2	2.51	0.43
1:I:368:ILE:HA	1:I:369:PRO:HD3	1.75	0.43
1:A:65:ILE:HD13	1:A:144:ILE:HG12	2.01	0.43
1:A:174:ARG:H	1:A:174:ARG:HG3	1.52	0.43
1:A:293:ASP:C	1:A:295:LYS:H	2.23	0.43
1:A:332:THR:CB	1:A:333:LYS:HB2	2.49	0.43
1:A:455:TYR:HB2	1:B:400:LYS:HB2	2.01	0.43
1:B:231:SER:HG	1:G:281:TRP:HH2	1.65	0.43
1:D:12:MET:SD	1:D:354:PRO:HD3	2.58	0.43
1:D:238:MET:O	1:D:239:THR:C	2.57	0.43
1:E:368:ILE:HA	1:E:369:PRO:HD3	1.74	0.43
1:F:111:MET:HA	1:F:114:LYS:HB3	2.00	0.43
1:H:65:ILE:HD13	1:H:144:ILE:HG12	2.01	0.43
1:J:264:HIS:HA	1:J:268:ALA:O	2.18	0.43
1:K:281:TRP:HD1	1:K:282:ASN:CA	2.29	0.43
1:K:289:LYS:HB3	1:K:290:GLU:H	1.22	0.43
1:L:189:HIS:HB3	1:L:190:TYR:HD1	1.83	0.43
1:A:280:ILE:HG21	1:A:280:ILE:HD13	1.85	0.42
1:B:135:ASN:OD1	1:B:135:ASN:N	2.52	0.42
1:B:305:PRO:C	1:B:307:ALA:H	2.23	0.42
1:C:173:GLU:O	1:C:202:PRO:HD3	2.19	0.42
1:C:397:LEU:HD22	1:E:394:TYR:CE1	2.54	0.42
1:D:27:LYS:NZ	1:D:31:ASP:HB2	2.35	0.42
1:F:141:LEU:HD23	1:F:141:LEU:HA	1.87	0.42
1:G:132:ASN:HA	1:G:133:PRO:HD3	1.83	0.42
1:G:135:ASN:N	1:G:135:ASN:OD1	2.51	0.42
1:G:264:HIS:HA	1:G:268:ALA:O	2.19	0.42
1:H:175:GLU:O	1:H:179:ILE:HG13	2.19	0.42
1:I:173:GLU:O	1:I:202:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:208:ILE:HG12	1:I:449:VAL:HG21	2.01	0.42
1:K:150:MET:SD	1:K:186:THR:HG21	2.59	0.42
1:K:280:ILE:HG21	1:K:280:ILE:HD13	1.79	0.42
1:L:309:ILE:H	1:L:309:ILE:HG13	1.60	0.42
1:B:233:MET:HB3	1:B:239:THR:N	2.22	0.42
1:C:175:GLU:O	1:C:179:ILE:HG13	2.19	0.42
1:C:500:PHE:O	1:C:500:PHE:CG	2.72	0.42
1:D:9:PHE:O	1:D:10:PHE:C	2.57	0.42
1:D:239:THR:HA	1:D:240:PRO:HD2	1.66	0.42
1:G:44:ARG:HG2	1:G:44:ARG:NH1	2.24	0.42
1:G:208:ILE:HG13	1:G:445:GLU:OE1	2.19	0.42
1:H:499:THR:HG1	1:L:142:GLU:CD	2.20	0.42
2:H:601:ADP:H5'2	1:L:203:ILE:O	2.19	0.42
1:I:65:ILE:HD13	1:I:144:ILE:HG12	2.01	0.42
1:K:65:ILE:HD13	1:K:144:ILE:HG12	2.01	0.42
1:A:8:ASN:OD1	1:A:11:LYS:HB2	2.19	0.42
1:A:12:MET:SD	1:A:354:PRO:HD3	2.59	0.42
1:B:65:ILE:HD13	1:B:144:ILE:HG12	2.01	0.42
1:D:150:MET:SD	1:D:186:THR:HG21	2.58	0.42
1:D:247:PHE:N	1:D:247:PHE:CD1	2.86	0.42
1:E:51:ILE:O	1:E:54:PRO:HD2	2.18	0.42
1:E:132:ASN:O	1:E:134:LYS:N	2.51	0.42
1:E:175:GLU:O	1:E:179:ILE:HG13	2.19	0.42
1:E:186:THR:HB	1:E:187:ILE:H	1.61	0.42
1:E:238:MET:O	1:E:240:PRO:N	2.52	0.42
1:F:140:GLU:O	1:F:144:ILE:HG13	2.20	0.42
1:G:261:ARG:NH2	1:G:292:GLU:OE2	2.51	0.42
1:G:410:LEU:HB3	1:G:430:ILE:HA	2.01	0.42
1:I:357:ASP:OD2	1:I:478:ARG:NE	2.52	0.42
1:L:305:PRO:C	1:L:307:ALA:H	2.23	0.42
1:L:363:ARG:HH11	1:L:363:ARG:HD3	1.23	0.42
1:A:173:GLU:O	1:A:202:PRO:HD3	2.19	0.42
1:C:150:MET:SD	1:C:186:THR:HG21	2.58	0.42
1:D:371:LEU:HD22	1:D:482:TYR:CD2	2.54	0.42
1:E:35:ARG:CZ	1:E:35:ARG:CB	2.84	0.42
1:E:35:ARG:HH21	1:E:35:ARG:HD2	1.23	0.42
1:F:240:PRO:CG	1:F:245:LYS:NZ	2.73	0.42
1:G:140:GLU:O	1:G:144:ILE:HG13	2.19	0.42
1:G:141:LEU:HD23	1:G:141:LEU:HA	1.87	0.42
1:H:7:PRO:HB2	1:H:8:ASN:H	1.56	0.42
1:J:85:HIS:HB3	1:J:493:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:175:GLU:O	1:J:179:ILE:HG13	2.19	0.42
1:K:51:ILE:O	1:K:54:PRO:HD2	2.19	0.42
1:K:173:GLU:O	1:K:202:PRO:HD3	2.19	0.42
1:K:281:TRP:HD1	1:K:282:ASN:HA	1.81	0.42
1:B:140:GLU:O	1:B:144:ILE:HG13	2.19	0.42
1:B:469:MET:CE	1:G:308:LYS:HE2	2.50	0.42
1:C:192:ILE:O	1:C:391:HIS:CE1	2.73	0.42
1:C:280:ILE:CG2	1:C:307:ALA:HB1	2.49	0.42
1:D:189:HIS:HB3	1:D:190:TYR:HD1	1.84	0.42
1:G:46:ARG:HH11	1:G:46:ARG:HD2	1.66	0.42
1:G:314:ILE:H	1:G:314:ILE:HG22	1.56	0.42
1:H:293:ASP:O	1:H:297:GLN:HB2	2.20	0.42
1:H:322:LEU:HB2	1:H:341:ALA:CB	2.50	0.42
1:I:150:MET:SD	1:I:186:THR:HG21	2.60	0.42
1:J:34:THR:C	1:J:35:ARG:HG2	2.40	0.42
1:K:140:GLU:O	1:K:144:ILE:HG13	2.20	0.42
1:K:173:GLU:O	1:K:176:MET:HB2	2.20	0.42
1:L:175:GLU:O	1:L:179:ILE:HG13	2.20	0.42
1:A:174:ARG:HH11	1:A:174:ARG:HD3	1.56	0.42
1:A:281:TRP:HD1	1:A:282:ASN:HA	1.85	0.42
1:B:282:ASN:ND2	1:B:306:LYS:O	2.52	0.42
1:C:111:MET:HA	1:C:114:LYS:HB3	2.01	0.42
1:D:65:ILE:HD13	1:D:144:ILE:HG12	2.01	0.42
1:D:140:GLU:O	1:D:144:ILE:HG13	2.19	0.42
1:F:41:LYS:CD	1:F:44:ARG:HH12	2.31	0.42
1:H:252:PHE:CD2	1:H:295:LYS:NZ	2.86	0.42
1:I:189:HIS:HB3	1:I:190:TYR:HD1	1.85	0.42
1:I:294:PHE:CG	1:I:304:PHE:CD1	3.07	0.42
1:I:451:SER:O	1:I:454:ALA:N	2.43	0.42
1:J:28:LEU:HD21	1:J:490:PHE:CG	2.54	0.42
1:J:235:ILE:H	1:J:235:ILE:HG12	1.69	0.42
1:J:280:ILE:CG2	1:J:307:ALA:HB1	2.50	0.42
1:K:35:ARG:C	1:K:37:THR:N	2.69	0.42
1:L:238:MET:O	1:L:239:THR:C	2.58	0.42
1:L:372:TYR:OH	1:L:461:ALA:HB2	2.19	0.42
1:A:140:GLU:O	1:A:144:ILE:HG13	2.20	0.42
1:A:233:MET:O	1:A:238:MET:N	2.33	0.42
1:A:294:PHE:CZ	1:A:298:HIS:CE1	3.08	0.42
1:B:141:LEU:HD23	1:B:141:LEU:HA	1.88	0.42
1:B:280:ILE:HA	1:B:308:LYS:O	2.20	0.42
1:B:282:ASN:OD1	1:B:283:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ILE:HD13	1:C:144:ILE:HG12	2.01	0.42
1:C:174:ARG:HH11	1:C:174:ARG:HD3	1.57	0.42
1:C:416:SER:HB3	1:E:428:ILE:O	2.19	0.42
1:E:414:GLN:OE1	1:E:428:ILE:HA	2.19	0.42
1:F:289:LYS:HB3	1:F:290:GLU:H	1.19	0.42
1:H:140:GLU:O	1:H:144:ILE:HG13	2.20	0.42
1:J:132:ASN:HA	1:J:133:PRO:HD3	1.83	0.42
1:J:140:GLU:O	1:J:144:ILE:HG13	2.19	0.42
1:J:498:VAL:HG12	1:J:499:THR:N	2.35	0.42
1:K:335:ASN:O	1:K:338:ARG:HB3	2.20	0.42
1:K:371:LEU:HD22	1:K:482:TYR:CD1	2.55	0.42
1:K:394:TYR:HB2	1:K:445:GLU:HG3	2.01	0.42
1:L:30:GLU:H	1:L:32:LEU:HD12	1.83	0.42
1:L:287:ASP:HA	1:L:288:PRO:HD2	1.79	0.42
1:A:315:LEU:HD22	1:A:331:LEU:HG	2.01	0.42
1:C:185:SER:CB	1:E:501:THR:HB	2.49	0.42
1:D:423:LYS:HB3	1:D:424:HIS:H	1.15	0.42
1:E:263:LEU:HD12	1:E:263:LEU:HA	1.85	0.42
1:E:294:PHE:CG	1:E:304:PHE:CD1	3.07	0.42
1:F:7:PRO:HB2	1:F:8:ASN:H	1.68	0.42
1:F:65:ILE:HD13	1:F:144:ILE:HG12	2.02	0.42
1:F:163:ASP:O	1:F:165:PRO:HD3	2.20	0.42
1:G:150:MET:SD	1:G:186:THR:HG21	2.59	0.42
1:G:280:ILE:HA	1:G:308:LYS:O	2.19	0.42
1:I:26:ASP:O	1:I:29:VAL:HG22	2.20	0.42
1:I:48:ILE:HD11	1:I:498:VAL:CG2	2.50	0.42
1:I:140:GLU:O	1:I:144:ILE:HG13	2.20	0.42
1:I:290:GLU:OE1	1:I:306:LYS:CE	2.67	0.42
1:J:33:LYS:HB3	1:J:36:GLU:HB2	2.01	0.42
1:K:209:HIS:CD2	1:K:445:GLU:OE1	2.72	0.42
1:K:277:ASP:HB2	1:K:278:GLY:H	1.65	0.42
1:K:294:PHE:CG	1:K:304:PHE:CD1	3.08	0.42
1:L:24:VAL:HG22	1:L:483:VAL:HG13	2.01	0.42
1:L:65:ILE:HD13	1:L:144:ILE:HG12	2.01	0.42
1:A:111:MET:HA	1:A:114:LYS:HB3	2.01	0.42
1:A:407:TYR:CD2	1:H:424:HIS:CE1	3.08	0.42
1:B:6:ASP:HA	1:B:7:PRO:HD2	1.50	0.42
1:B:132:ASN:O	1:B:134:LYS:N	2.53	0.42
1:B:369:PRO:HG3	1:B:478:ARG:HA	2.01	0.42
1:C:132:ASN:HA	1:C:133:PRO:HD3	1.80	0.42
1:D:277:ASP:HB2	1:D:278:GLY:H	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:GLU:O	1:F:179:ILE:HG13	2.20	0.42
1:G:35:ARG:HH11	1:G:35:ARG:HD3	1.01	0.42
1:H:66:ARG:NH1	1:J:498:VAL:HG13	2.35	0.42
1:H:240:PRO:CB	1:H:245:LYS:HE2	2.50	0.42
1:J:294:PHE:CG	1:J:304:PHE:CD1	3.08	0.42
1:L:318:ASP:HA	1:L:340:LYS:HG2	2.02	0.42
1:L:438:ASP:HA	1:L:441:SER:HB3	2.02	0.42
1:B:163:ASP:O	1:B:165:PRO:HD3	2.20	0.42
1:C:233:MET:HB3	1:C:239:THR:N	2.21	0.42
1:D:212:ILE:H	1:D:212:ILE:HG13	1.56	0.42
1:D:428:ILE:O	1:E:416:SER:HB3	2.20	0.42
2:D:601:ADP:O2A	1:E:209:HIS:NE2	2.53	0.42
1:F:150:MET:SD	1:F:186:THR:HG21	2.59	0.42
1:G:44:ARG:NH1	1:G:44:ARG:CG	2.82	0.42
1:H:282:ASN:ND2	1:H:306:LYS:O	2.53	0.42
1:I:174:ARG:HH11	1:I:174:ARG:HD3	1.53	0.42
1:I:240:PRO:CG	1:I:245:LYS:CE	2.97	0.42
1:J:245:LYS:HG3	1:J:246:THR:N	2.35	0.42
1:A:34:THR:CB	1:A:35:ARG:HB3	2.46	0.41
1:A:294:PHE:C	1:A:297:GLN:HB3	2.41	0.41
1:A:295:LYS:N	1:A:297:GLN:HB3	2.35	0.41
1:A:424:HIS:CE1	1:H:407:TYR:CD2	3.08	0.41
1:C:247:PHE:CE2	1:C:263:LEU:HD23	2.55	0.41
1:C:311:GLU:HG2	1:C:312:GLY:N	2.35	0.41
1:D:383:PHE:CD1	1:E:397:LEU:HD21	2.55	0.41
1:E:410:LEU:HB3	1:E:430:ILE:HA	2.02	0.41
1:F:277:ASP:HB2	1:F:278:GLY:H	1.57	0.41
1:G:9:PHE:C	1:G:11:LYS:H	2.23	0.41
1:G:189:HIS:HB3	1:G:190:TYR:HD1	1.85	0.41
1:I:411:MET:HB3	1:K:433:THR:HG21	2.01	0.41
1:J:139:ASN:O	1:J:143:LYS:HG3	2.20	0.41
1:J:362:GLU:C	1:J:364:ASN:H	2.21	0.41
1:L:173:GLU:O	1:L:202:PRO:HD3	2.19	0.41
1:L:289:LYS:HB2	1:L:290:GLU:H	1.18	0.41
1:A:295:LYS:O	1:A:298:HIS:N	2.54	0.41
1:B:295:LYS:O	1:B:298:HIS:N	2.53	0.41
1:D:132:ASN:O	1:D:134:LYS:N	2.54	0.41
1:E:65:ILE:HD13	1:E:144:ILE:HG12	2.02	0.41
1:E:95:TYR:OH	1:E:145:THR:HG23	2.20	0.41
1:E:233:MET:O	1:E:238:MET:N	2.32	0.41
1:E:296:LEU:HB3	1:E:297:GLN:H	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:LEU:O	1:F:32:LEU:HD11	2.20	0.41
1:H:305:PRO:C	1:H:307:ALA:H	2.23	0.41
1:I:34:THR:N	1:I:35:ARG:HB2	2.35	0.41
1:I:173:GLU:O	1:I:176:MET:HB2	2.20	0.41
1:K:175:GLU:O	1:K:179:ILE:HG13	2.20	0.41
1:K:252:PHE:CD1	1:K:273:VAL:HG11	2.55	0.41
1:L:82:HIS:HD2	1:L:83:SER:HB2	1.85	0.41
1:L:304:PHE:CD1	1:L:305:PRO:HD2	2.55	0.41
1:L:355:GLU:HA	1:L:358:LYS:HB3	2.01	0.41
1:D:9:PHE:CE1	1:D:328:GLU:CG	3.04	0.41
1:D:129:VAL:HG12	1:D:131:ILE:HB	2.02	0.41
1:F:247:PHE:CE1	1:F:269:LYS:C	2.94	0.41
1:J:30:GLU:N	1:J:32:LEU:HD12	2.35	0.41
1:K:163:ASP:O	1:K:165:PRO:HD3	2.20	0.41
1:K:225:ASN:OD1	1:K:458:GLU:HG3	2.19	0.41
1:K:432:PRO:HB3	1:K:436:PHE:HD2	1.81	0.41
1:L:140:GLU:O	1:L:144:ILE:HG13	2.19	0.41
1:A:175:GLU:O	1:A:179:ILE:HG13	2.20	0.41
1:B:129:VAL:HG12	1:B:131:ILE:HB	2.03	0.41
1:C:322:LEU:HB2	1:C:341:ALA:CB	2.51	0.41
1:C:355:GLU:O	1:C:359:ILE:HD12	2.21	0.41
1:C:462:ARG:O	1:C:466:ARG:HG3	2.19	0.41
1:E:129:VAL:HG12	1:E:131:ILE:HB	2.03	0.41
1:E:435:GLU:H	1:E:435:GLU:HG3	1.68	0.41
1:F:129:VAL:HG12	1:F:131:ILE:HB	2.03	0.41
1:F:189:HIS:HB3	1:F:190:TYR:CD1	2.56	0.41
1:I:7:PRO:HB2	1:I:8:ASN:H	1.54	0.41
1:I:233:MET:HB3	1:I:239:THR:N	2.21	0.41
1:J:163:ASP:O	1:J:165:PRO:HD3	2.20	0.41
1:J:263:LEU:HD12	1:J:263:LEU:HA	1.86	0.41
1:B:132:ASN:HA	1:B:133:PRO:HD3	1.83	0.41
1:C:140:GLU:O	1:C:144:ILE:HG13	2.19	0.41
1:C:314:ILE:HG21	1:C:314:ILE:HD13	1.74	0.41
1:D:238:MET:C	1:D:240:PRO:N	2.67	0.41
1:E:135:ASN:OD1	1:E:135:ASN:N	2.54	0.41
1:F:410:LEU:HB3	1:F:430:ILE:HA	2.02	0.41
1:G:432:PRO:HB3	1:G:436:PHE:HD2	1.82	0.41
1:I:264:HIS:HA	1:I:268:ALA:O	2.20	0.41
1:J:65:ILE:HD13	1:J:144:ILE:HG12	2.01	0.41
1:J:173:GLU:O	1:J:176:MET:HB2	2.21	0.41
1:J:395:GLY:O	1:J:399:PHE:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:9:PHE:C	1:L:11:LYS:H	2.23	0.41
1:A:416:SER:HB3	1:F:428:ILE:O	2.21	0.41
1:B:37:THR:OG1	1:B:40:GLN:CA	2.66	0.41
1:B:47:GLY:O	1:B:51:ILE:HG13	2.21	0.41
1:B:501:THR:HG21	1:F:181:ASP:OD2	2.19	0.41
1:C:453:LEU:O	1:C:457:MET:HG2	2.20	0.41
1:C:473:LEU:HB3	1:C:476:ASP:HB3	2.02	0.41
1:D:236:LEU:HD21	1:D:475:LEU:HD21	2.03	0.41
1:D:500:PHE:HD2	1:E:146:ARG:HD3	1.85	0.41
1:F:201:LYS:HG2	1:F:384:GLU:OE1	2.20	0.41
1:F:293:ASP:C	1:F:295:LYS:H	2.24	0.41
1:J:281:TRP:NE1	1:J:283:PRO:HD3	2.23	0.41
1:J:305:PRO:O	1:J:307:ALA:N	2.54	0.41
1:J:333:LYS:HB2	1:J:334:SER:H	1.44	0.41
1:J:422:GLY:O	1:J:423:LYS:HD3	2.20	0.41
1:L:37:THR:HG22	1:L:40:GLN:CA	2.51	0.41
1:L:86:ARG:HD2	1:L:86:ARG:HA	1.95	0.41
1:A:29:VAL:HG12	1:A:42:ARG:HB2	2.02	0.41
1:A:402:GLU:HA	1:A:405:SER:HB2	2.02	0.41
1:C:282:ASN:OD1	1:C:283:PRO:HD2	2.19	0.41
1:D:175:GLU:O	1:D:179:ILE:HG13	2.20	0.41
1:D:282:ASN:ND2	1:D:306:LYS:O	2.53	0.41
1:F:308:LYS:HE3	1:F:308:LYS:HB2	1.90	0.41
1:I:186:THR:HB	1:I:187:ILE:H	1.61	0.41
1:I:247:PHE:CE1	1:I:270:CYS:N	2.89	0.41
1:I:453:LEU:O	1:I:457:MET:HG2	2.20	0.41
1:K:294:PHE:CG	1:K:294:PHE:O	2.74	0.41
1:A:305:PRO:C	1:A:307:ALA:H	2.24	0.41
1:B:57:HIS:NE2	1:D:151:GLU:OE1	2.53	0.41
1:B:117:VAL:HG21	1:B:371:LEU:HG	2.03	0.41
1:C:32:LEU:CD1	1:C:490:PHE:HE2	2.34	0.41
1:C:294:PHE:CG	1:C:304:PHE:CD1	3.09	0.41
1:E:282:ASN:OD1	1:E:283:PRO:HD2	2.21	0.41
1:E:362:GLU:C	1:E:364:ASN:H	2.23	0.41
1:G:8:ASN:O	1:G:12:MET:HG3	2.21	0.41
1:J:132:ASN:C	1:J:134:LYS:H	2.23	0.41
1:K:263:LEU:HD12	1:K:263:LEU:HA	1.84	0.41
1:L:129:VAL:HG12	1:L:131:ILE:HB	2.03	0.41
1:A:163:ASP:O	1:A:165:PRO:HD3	2.20	0.41
1:A:322:LEU:HB2	1:A:341:ALA:CB	2.51	0.41
1:A:501:THR:HG22	1:E:147:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ASP:OD1	1:C:6:ASP:N	2.54	0.41
1:C:42:ARG:HH11	1:C:42:ARG:HD2	1.59	0.41
1:C:173:GLU:O	1:C:176:MET:HB2	2.21	0.41
1:C:185:SER:HB3	1:E:501:THR:HB	2.03	0.41
1:C:259:SER:O	1:C:263:LEU:HB2	2.21	0.41
1:C:289:LYS:HB3	1:C:290:GLU:H	1.20	0.41
1:D:247:PHE:O	1:D:271:VAL:HG23	2.21	0.41
1:E:163:ASP:O	1:E:165:PRO:HD3	2.21	0.41
1:E:280:ILE:HG21	1:E:280:ILE:HD13	1.76	0.41
1:F:39:GLU:HB3	1:F:41:LYS:HG3	2.03	0.41
1:F:280:ILE:HD13	1:F:280:ILE:HG21	1.75	0.41
1:G:129:VAL:HG12	1:G:131:ILE:HB	2.03	0.41
1:G:163:ASP:O	1:G:165:PRO:HD3	2.21	0.41
1:H:65:ILE:HG21	1:H:144:ILE:HG12	2.03	0.41
1:I:30:GLU:HB3	1:I:31:ASP:H	1.46	0.41
1:I:135:ASN:N	1:I:135:ASN:OD1	2.54	0.41
1:I:247:PHE:CE1	1:I:269:LYS:C	2.95	0.41
1:I:259:SER:O	1:I:263:LEU:HB2	2.21	0.41
1:I:305:PRO:C	1:I:307:ALA:H	2.25	0.41
1:I:446:LYS:HG2	1:I:450:HIS:CD2	2.56	0.41
1:J:129:VAL:HG12	1:J:131:ILE:HB	2.03	0.41
1:K:143:LYS:H	1:K:143:LYS:HG2	1.58	0.41
1:K:233:MET:HB3	1:K:239:THR:N	2.24	0.41
1:L:41:LYS:CB	1:L:44:ARG:NH1	2.84	0.41
1:B:9:PHE:CZ	1:B:328:GLU:OE1	2.73	0.41
1:B:175:GLU:O	1:B:179:ILE:HG13	2.20	0.41
1:C:141:LEU:HD23	1:C:141:LEU:HA	1.87	0.41
1:E:294:PHE:O	1:E:298:HIS:ND1	2.53	0.41
1:F:173:GLU:O	1:F:176:MET:HB2	2.20	0.41
1:G:41:LYS:C	1:G:44:ARG:HB2	2.41	0.41
1:G:65:ILE:HG21	1:G:144:ILE:HG12	2.03	0.41
1:H:163:ASP:O	1:H:165:PRO:HD3	2.20	0.41
1:H:280:ILE:HG21	1:H:280:ILE:HD13	1.75	0.41
1:I:143:LYS:HG3	1:I:143:LYS:H	1.59	0.41
1:I:189:HIS:HB3	1:I:190:TYR:CD1	2.56	0.41
1:I:241:GLY:O	1:I:242:PHE:CB	2.34	0.41
1:K:129:VAL:HG12	1:K:131:ILE:HB	2.03	0.41
1:K:314:ILE:C	1:K:316:GLU:H	2.25	0.41
1:L:263:LEU:HD12	1:L:263:LEU:HA	1.88	0.41
1:A:35:ARG:C	1:A:37:THR:N	2.74	0.40
1:A:129:VAL:HG12	1:A:131:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:HB2	1:A:245:LYS:HE3	1.89	0.40
1:A:287:ASP:OD1	1:A:288:PRO:HD2	2.21	0.40
1:B:277:ASP:HB2	1:B:278:GLY:H	1.57	0.40
1:B:280:ILE:HG22	1:B:286:ILE:CD1	2.52	0.40
1:B:362:GLU:C	1:B:364:ASN:H	2.24	0.40
1:C:163:ASP:O	1:C:165:PRO:HD3	2.20	0.40
1:D:19:ARG:HH21	1:D:479:THR:HG21	1.84	0.40
1:D:293:ASP:C	1:D:295:LYS:H	2.24	0.40
1:D:400:LYS:HD2	1:D:403:ARG:HH21	1.86	0.40
1:E:39:GLU:HB3	1:E:41:LYS:HG2	2.02	0.40
1:F:44:ARG:NH1	1:F:44:ARG:HG2	2.36	0.40
1:F:338:ARG:HH11	1:F:338:ARG:HD3	1.44	0.40
1:I:129:VAL:HG12	1:I:131:ILE:HB	2.03	0.40
1:J:360:PHE:CG	1:J:365:ILE:HD11	2.56	0.40
1:K:134:LYS:C	1:K:136:TYR:H	2.24	0.40
1:L:305:PRO:O	1:L:307:ALA:N	2.53	0.40
1:A:287:ASP:HA	1:A:288:PRO:HD3	1.82	0.40
1:A:293:ASP:O	1:A:297:GLN:CB	2.69	0.40
1:A:470:LYS:HG2	1:A:471:TYR:CD2	2.56	0.40
1:C:294:PHE:CA	1:C:297:GLN:HG3	2.47	0.40
1:C:412:SER:HB3	1:E:432:PRO:HA	2.03	0.40
1:E:280:ILE:HA	1:E:308:LYS:O	2.21	0.40
1:F:118:VAL:HA	1:F:460:SER:OG	2.22	0.40
1:F:192:ILE:O	1:F:391:HIS:NE2	2.46	0.40
1:H:25:GLU:OE2	1:H:46:ARG:NH1	2.54	0.40
1:H:35:ARG:HH11	1:H:35:ARG:HD3	0.99	0.40
1:I:305:PRO:O	1:I:306:LYS:HG2	2.21	0.40
1:I:400:LYS:HE3	1:K:454:ALA:HB3	2.04	0.40
1:J:259:SER:O	1:J:263:LEU:HB2	2.22	0.40
1:K:466:ARG:C	1:K:469:MET:HB2	2.42	0.40
1:L:212:ILE:H	1:L:212:ILE:HG13	1.56	0.40
1:L:294:PHE:CG	1:L:304:PHE:CD1	3.09	0.40
1:B:201:LYS:HG2	1:B:384:GLU:OE1	2.21	0.40
1:B:261:ARG:NH2	1:B:292:GLU:OE2	2.54	0.40
1:C:150:MET:O	1:C:154:LYS:HG3	2.21	0.40
1:D:163:ASP:O	1:D:165:PRO:HD3	2.21	0.40
1:D:305:PRO:O	1:D:307:ALA:N	2.55	0.40
1:D:362:GLU:C	1:D:364:ASN:H	2.24	0.40
1:D:372:TYR:OH	1:D:461:ALA:HB2	2.21	0.40
1:E:65:ILE:HG21	1:E:144:ILE:HG12	2.03	0.40
1:F:238:MET:C	1:F:240:PRO:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:SER:O	1:F:263:LEU:HB2	2.22	0.40
1:G:322:LEU:HB2	1:G:341:ALA:CB	2.52	0.40
1:I:134:LYS:C	1:I:136:TYR:N	2.75	0.40
1:J:47:GLY:O	1:J:51:ILE:HG13	2.22	0.40
1:J:346:GLU:CD	1:J:478:ARG:HH22	2.22	0.40
1:K:360:PHE:CG	1:K:365:ILE:HD11	2.57	0.40
1:K:457:MET:HB2	1:K:458:GLU:OE1	2.21	0.40
1:L:328:GLU:O	1:L:330:GLN:HG3	2.21	0.40
1:L:368:ILE:HA	1:L:369:PRO:HD3	1.74	0.40
1:B:65:ILE:HG21	1:B:144:ILE:HG12	2.03	0.40
1:C:264:HIS:HA	1:C:268:ALA:O	2.22	0.40
1:C:294:PHE:CG	1:C:294:PHE:O	2.74	0.40
1:D:47:GLY:O	1:D:51:ILE:HG13	2.21	0.40
1:E:24:VAL:HG12	1:E:28:LEU:HB2	2.03	0.40
1:E:150:MET:O	1:E:154:LYS:HG3	2.22	0.40
1:G:373:LEU:HD12	1:G:373:LEU:HA	1.92	0.40
1:G:400:LYS:HD2	1:G:403:ARG:HH21	1.86	0.40
1:H:66:ARG:NH1	1:H:72:TRP:CH2	2.90	0.40
1:H:72:TRP:HB2	1:J:47:GLY:HA3	2.02	0.40
1:H:132:ASN:O	1:H:134:LYS:N	2.54	0.40
1:I:233:MET:O	1:I:238:MET:N	2.33	0.40
1:I:281:TRP:HE1	1:I:283:PRO:N	2.19	0.40
1:J:82:HIS:HD2	1:J:83:SER:HB2	1.87	0.40
1:J:473:LEU:HB3	1:J:476:ASP:HB3	2.03	0.40
1:K:150:MET:HE1	1:K:186:THR:HG21	2.03	0.40
1:L:44:ARG:N	1:L:46:ARG:HG2	2.37	0.40
1:A:32:LEU:CD2	1:A:33:LYS:HG3	2.52	0.40
1:A:292:GLU:HB2	1:A:293:ASP:H	1.65	0.40
1:B:24:VAL:HG23	1:B:483:VAL:HG22	2.04	0.40
1:B:322:LEU:HB2	1:B:341:ALA:CB	2.50	0.40
1:C:212:ILE:H	1:C:212:ILE:HG13	1.42	0.40
1:D:189:HIS:HB3	1:D:190:TYR:CD1	2.55	0.40
1:F:186:THR:HB	1:F:187:ILE:H	1.61	0.40
1:G:47:GLY:O	1:G:51:ILE:HG13	2.21	0.40
1:G:189:HIS:HB3	1:G:190:TYR:CD1	2.56	0.40
1:H:129:VAL:HG12	1:H:131:ILE:HB	2.03	0.40
1:H:402:GLU:HA	1:H:405:SER:HB2	2.04	0.40
1:I:65:ILE:HG21	1:I:144:ILE:HG12	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ARG:NH2	1:E:297:GLN:O[1_455]	1.76	0.44
1:C:338:ARG:NH1	1:E:297:GLN:O[1_455]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	494/496 (100%)	404 (82%)	59 (12%)	31 (6%)	1	14
1	B	494/496 (100%)	404 (82%)	60 (12%)	30 (6%)	1	15
1	C	494/496 (100%)	410 (83%)	54 (11%)	30 (6%)	1	15
1	D	494/496 (100%)	404 (82%)	58 (12%)	32 (6%)	1	14
1	E	494/496 (100%)	410 (83%)	50 (10%)	34 (7%)	1	12
1	F	494/496 (100%)	407 (82%)	56 (11%)	31 (6%)	1	14
1	G	494/496 (100%)	407 (82%)	57 (12%)	30 (6%)	1	15
1	H	494/496 (100%)	407 (82%)	53 (11%)	34 (7%)	1	12
1	I	494/496 (100%)	400 (81%)	61 (12%)	33 (7%)	1	13
1	J	494/496 (100%)	407 (82%)	52 (10%)	35 (7%)	1	12
1	K	494/496 (100%)	403 (82%)	57 (12%)	34 (7%)	1	12
1	L	494/496 (100%)	408 (83%)	54 (11%)	32 (6%)	1	14
All	All	5928/5952 (100%)	4871 (82%)	671 (11%)	386 (6%)	1	14

All (386) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	34	THR
1	A	35	ARG
1	A	43	ASN
1	A	45	VAL
1	A	240	PRO

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Mol	Chain	Res	Type
1	A	242	PHE
1	A	277	ASP
1	A	288	PRO
1	A	289	LYS
1	A	297	GLN
1	A	333	LYS
1	A	420	LYS
1	A	421	PHE
1	B	9	PHE
1	B	34	THR
1	B	35	ARG
1	B	43	ASN
1	B	240	PRO
1	B	242	PHE
1	B	288	PRO
1	B	289	LYS
1	B	297	GLN
1	B	333	LYS
1	B	420	LYS
1	B	421	PHE
1	C	9	PHE
1	C	34	THR
1	C	35	ARG
1	C	43	ASN
1	C	240	PRO
1	C	242	PHE
1	C	288	PRO
1	C	297	GLN
1	C	333	LYS
1	C	420	LYS
1	C	421	PHE
1	D	34	THR
1	D	35	ARG
1	D	43	ASN
1	D	240	PRO
1	D	242	PHE
1	D	288	PRO
1	D	289	LYS
1	D	309	ILE
1	D	333	LYS
1	D	420	LYS
1	D	421	PHE

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Mol	Chain	Res	Type
1	E	31	ASP
1	E	34	THR
1	E	35	ARG
1	E	36	GLU
1	E	37	THR
1	E	43	ASN
1	E	45	VAL
1	E	174	ARG
1	E	240	PRO
1	E	242	PHE
1	E	244	ASP
1	E	288	PRO
1	E	297	GLN
1	E	309	ILE
1	E	333	LYS
1	E	420	LYS
1	E	421	PHE
1	F	34	THR
1	F	43	ASN
1	F	240	PRO
1	F	242	PHE
1	F	288	PRO
1	F	297	GLN
1	F	333	LYS
1	F	420	LYS
1	F	421	PHE
1	F	500	PHE
1	G	31	ASP
1	G	34	THR
1	G	35	ARG
1	G	43	ASN
1	G	45	VAL
1	G	240	PRO
1	G	242	PHE
1	G	288	PRO
1	G	289	LYS
1	G	297	GLN
1	G	327	SER
1	G	333	LYS
1	G	421	PHE
1	G	499	THR
1	H	31	ASP

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Mol	Chain	Res	Type
1	H	34	THR
1	H	35	ARG
1	H	37	THR
1	H	43	ASN
1	H	45	VAL
1	H	240	PRO
1	H	242	PHE
1	H	288	PRO
1	H	289	LYS
1	H	297	GLN
1	H	333	LYS
1	H	420	LYS
1	H	421	PHE
1	I	31	ASP
1	I	34	THR
1	I	35	ARG
1	I	43	ASN
1	I	45	VAL
1	I	240	PRO
1	I	288	PRO
1	I	297	GLN
1	I	333	LYS
1	I	420	LYS
1	I	421	PHE
1	J	34	THR
1	J	36	GLU
1	J	37	THR
1	J	43	ASN
1	J	240	PRO
1	J	242	PHE
1	J	288	PRO
1	J	289	LYS
1	J	297	GLN
1	J	333	LYS
1	J	420	LYS
1	K	31	ASP
1	K	34	THR
1	K	35	ARG
1	K	43	ASN
1	K	45	VAL
1	K	240	PRO
1	K	242	PHE

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Mol	Chain	Res	Type
1	K	276	SER
1	K	288	PRO
1	K	297	GLN
1	K	333	LYS
1	K	421	PHE
1	K	472	ASN
1	K	477	LEU
1	L	31	ASP
1	L	34	THR
1	L	35	ARG
1	L	37	THR
1	L	43	ASN
1	L	240	PRO
1	L	242	PHE
1	L	288	PRO
1	L	289	LYS
1	L	297	GLN
1	L	309	ILE
1	L	333	LYS
1	L	420	LYS
1	L	421	PHE
1	A	32	LEU
1	A	244	ASP
1	A	309	ILE
1	A	315	LEU
1	A	472	ASN
1	B	31	ASP
1	B	32	LEU
1	B	244	ASP
1	B	276	SER
1	B	294	PHE
1	B	315	LEU
1	B	422	GLY
1	B	496	ALA
1	C	7	PRO
1	C	31	ASP
1	C	32	LEU
1	C	36	GLU
1	C	45	VAL
1	C	244	ASP
1	C	289	LYS
1	C	315	LEU

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Mol	Chain	Res	Type
1	C	422	GLY
1	D	32	LEU
1	D	36	GLU
1	D	37	THR
1	D	45	VAL
1	D	244	ASP
1	D	276	SER
1	D	294	PHE
1	D	422	GLY
1	D	474	GLY
1	E	32	LEU
1	E	276	SER
1	E	289	LYS
1	E	315	LEU
1	E	422	GLY
1	F	7	PRO
1	F	31	ASP
1	F	32	LEU
1	F	35	ARG
1	F	244	ASP
1	F	294	PHE
1	F	309	ILE
1	F	315	LEU
1	F	422	GLY
1	G	32	LEU
1	G	37	THR
1	G	244	ASP
1	G	309	ILE
1	G	420	LYS
1	G	422	GLY
1	H	10	PHE
1	H	32	LEU
1	H	244	ASP
1	H	294	PHE
1	H	309	ILE
1	H	422	GLY
1	H	474	GLY
1	I	32	LEU
1	I	37	THR
1	I	242	PHE
1	I	244	ASP
1	I	276	SER

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Mol	Chain	Res	Type
1	I	277	ASP
1	I	289	LYS
1	I	294	PHE
1	I	309	ILE
1	I	422	GLY
1	I	452	GLY
1	I	467	THR
1	I	474	GLY
1	I	499	THR
1	J	31	ASP
1	J	32	LEU
1	J	35	ARG
1	J	244	ASP
1	J	315	LEU
1	J	422	GLY
1	K	32	LEU
1	K	244	ASP
1	K	289	LYS
1	K	309	ILE
1	K	422	GLY
1	K	474	GLY
1	K	499	THR
1	L	32	LEU
1	L	244	ASP
1	L	294	PHE
1	L	315	LEU
1	L	422	GLY
1	A	7	PRO
1	A	294	PHE
1	A	299	GLY
1	A	422	GLY
1	A	446	LYS
1	A	496	ALA
1	B	277	ASP
1	B	299	GLY
1	C	276	SER
1	C	299	GLY
1	D	39	GLU
1	D	277	ASP
1	D	299	GLY
1	D	315	LEU
1	E	277	ASP

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Mol	Chain	Res	Type
1	E	294	PHE
1	E	298	HIS
1	E	299	GLY
1	F	44	ARG
1	F	45	VAL
1	F	276	SER
1	F	277	ASP
1	F	289	LYS
1	F	299	GLY
1	F	338	ARG
1	F	472	ASN
1	G	7	PRO
1	G	133	PRO
1	G	276	SER
1	G	299	GLY
1	G	315	LEU
1	H	7	PRO
1	H	276	SER
1	H	277	ASP
1	H	299	GLY
1	H	315	LEU
1	H	338	ARG
1	H	446	LYS
1	I	7	PRO
1	I	299	GLY
1	J	7	PRO
1	J	276	SER
1	J	299	GLY
1	K	36	GLU
1	K	133	PRO
1	K	299	GLY
1	K	315	LEU
1	K	420	LYS
1	L	277	ASP
1	L	296	LEU
1	L	299	GLY
1	L	472	ASN
1	B	338	ARG
1	C	44	ARG
1	C	277	ASP
1	C	294	PHE
1	C	309	ILE

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Mol	Chain	Res	Type
1	D	7	PRO
1	D	338	ARG
1	E	7	PRO
1	E	239	THR
1	E	424	HIS
1	E	496	ALA
1	F	130	LYS
1	G	277	ASP
1	G	338	ARG
1	H	40	GLN
1	I	39	GLU
1	I	315	LEU
1	I	338	ARG
1	J	45	VAL
1	J	174	ARG
1	J	277	ASP
1	J	294	PHE
1	J	306	LYS
1	J	309	ILE
1	J	338	ARG
1	J	421	PHE
1	J	446	LYS
1	J	474	GLY
1	J	498	VAL
1	K	338	ARG
1	K	430	ILE
1	L	45	VAL
1	A	82	HIS
1	A	276	SER
1	A	306	LYS
1	A	338	ARG
1	B	45	VAL
1	B	82	HIS
1	B	309	ILE
1	C	82	HIS
1	C	340	LYS
1	D	10	PHE
1	D	44	ARG
1	D	82	HIS
1	D	500	PHE
1	E	82	HIS
1	E	133	PRO

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Mol	Chain	Res	Type
1	F	82	HIS
1	G	82	HIS
1	H	39	GLU
1	H	82	HIS
1	H	264	HIS
1	I	82	HIS
1	J	82	HIS
1	J	133	PRO
1	K	82	HIS
1	K	277	ASP
1	K	298	HIS
1	L	44	ARG
1	L	82	HIS
1	L	340	LYS
1	L	496	ALA
1	B	133	PRO
1	C	37	THR
1	E	306	LYS
1	J	239	THR
1	K	7	PRO
1	K	294	PHE
1	L	7	PRO
1	B	7	PRO
1	B	88	PRO
1	D	133	PRO
1	G	498	VAL
1	H	88	PRO
1	I	133	PRO
1	J	88	PRO
1	L	88	PRO
1	L	339	VAL
1	A	88	PRO
1	C	88	PRO
1	D	88	PRO
1	E	88	PRO
1	F	88	PRO
1	F	133	PRO
1	G	88	PRO
1	H	133	PRO
1	I	88	PRO
1	K	88	PRO
1	B	474	GLY

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Mol	Chain	Res	Type
1	A	133	PRO
1	L	133	PRO

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	413/413 (100%)	375 (91%)	38 (9%)	9	36
1	B	413/413 (100%)	372 (90%)	41 (10%)	8	33
1	C	413/413 (100%)	379 (92%)	34 (8%)	11	40
1	D	413/413 (100%)	371 (90%)	42 (10%)	7	32
1	E	413/413 (100%)	372 (90%)	41 (10%)	8	33
1	F	413/413 (100%)	382 (92%)	31 (8%)	13	43
1	G	413/413 (100%)	375 (91%)	38 (9%)	9	36
1	H	413/413 (100%)	374 (91%)	39 (9%)	8	35
1	I	413/413 (100%)	364 (88%)	49 (12%)	5	25
1	J	413/413 (100%)	376 (91%)	37 (9%)	9	37
1	K	413/413 (100%)	363 (88%)	50 (12%)	5	24
1	L	413/413 (100%)	376 (91%)	37 (9%)	9	37
All	All	4956/4956 (100%)	4479 (90%)	477 (10%)	8	34

All (477) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	8	ASN
1	A	32	LEU
1	A	35	ARG
1	A	38	GLU
1	A	42	ARG
1	A	44	ARG
1	A	45	VAL

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Mol	Chain	Res	Type
1	A	50	ARG
1	A	60	SER
1	A	105	LYS
1	A	112	THR
1	A	134	LYS
1	A	145	THR
1	A	189	HIS
1	A	212	ILE
1	A	213	SER
1	A	242	PHE
1	A	271	VAL
1	A	275	GLU
1	A	277	ASP
1	A	281	TRP
1	A	289	LYS
1	A	306	LYS
1	A	308	LYS
1	A	313	SER
1	A	315	LEU
1	A	320	ASP
1	A	332	THR
1	A	334	SER
1	A	342	LYS
1	A	355	GLU
1	A	409	LEU
1	A	421	PHE
1	A	423	LYS
1	A	430	ILE
1	A	431	VAL
1	A	446	LYS
1	B	11	LYS
1	B	32	LEU
1	B	34	THR
1	B	35	ARG
1	B	36	GLU
1	B	38	GLU
1	B	42	ARG
1	B	44	ARG
1	B	45	VAL
1	B	60	SER
1	B	98	ASP
1	B	103	GLU

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Mol	Chain	Res	Type
1	B	112	THR
1	B	135	ASN
1	B	145	THR
1	B	169	MET
1	B	174	ARG
1	B	189	HIS
1	B	213	SER
1	B	235	ILE
1	B	242	PHE
1	B	269	LYS
1	B	271	VAL
1	B	275	GLU
1	B	281	TRP
1	B	295	LYS
1	B	297	GLN
1	B	308	LYS
1	B	314	ILE
1	B	327	SER
1	B	330	GLN
1	B	332	THR
1	B	333	LYS
1	B	334	SER
1	B	338	ARG
1	B	340	LYS
1	B	363	ARG
1	B	402	GLU
1	B	409	LEU
1	B	421	PHE
1	B	430	ILE
1	C	6	ASP
1	C	30	GLU
1	C	34	THR
1	C	38	GLU
1	C	41	LYS
1	C	42	ARG
1	C	45	VAL
1	C	60	SER
1	C	69	ASP
1	C	87	THR
1	C	112	THR
1	C	134	LYS
1	C	145	THR

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Mol	Chain	Res	Type
1	C	212	ILE
1	C	213	SER
1	C	242	PHE
1	C	265	ARG
1	C	271	VAL
1	C	281	TRP
1	C	289	LYS
1	C	295	LYS
1	C	298	HIS
1	C	300	THR
1	C	306	LYS
1	C	308	LYS
1	C	327	SER
1	C	339	VAL
1	C	352	THR
1	C	363	ARG
1	C	403	ARG
1	C	409	LEU
1	C	421	PHE
1	C	430	ILE
1	C	435	GLU
1	D	11	LYS
1	D	31	ASP
1	D	32	LEU
1	D	34	THR
1	D	38	GLU
1	D	39	GLU
1	D	42	ARG
1	D	44	ARG
1	D	45	VAL
1	D	60	SER
1	D	105	LYS
1	D	112	THR
1	D	145	THR
1	D	174	ARG
1	D	212	ILE
1	D	213	SER
1	D	234	SER
1	D	242	PHE
1	D	247	PHE
1	D	265	ARG
1	D	269	LYS

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Mol	Chain	Res	Type
1	D	271	VAL
1	D	280	ILE
1	D	281	TRP
1	D	286	ILE
1	D	289	LYS
1	D	290	GLU
1	D	295	LYS
1	D	298	HIS
1	D	308	LYS
1	D	309	ILE
1	D	311	GLU
1	D	328	GLU
1	D	331	LEU
1	D	332	THR
1	D	334	SER
1	D	338	ARG
1	D	409	LEU
1	D	421	PHE
1	D	430	ILE
1	D	439	ARG
1	D	470	LYS
1	E	6	ASP
1	E	8	ASN
1	E	29	VAL
1	E	32	LEU
1	E	34	THR
1	E	35	ARG
1	E	38	GLU
1	E	44	ARG
1	E	45	VAL
1	E	46	ARG
1	E	50	ARG
1	E	60	SER
1	E	112	THR
1	E	145	THR
1	E	169	MET
1	E	174	ARG
1	E	213	SER
1	E	235	ILE
1	E	242	PHE
1	E	261	ARG
1	E	269	LYS

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Mol	Chain	Res	Type
1	E	271	VAL
1	E	281	TRP
1	E	289	LYS
1	E	297	GLN
1	E	306	LYS
1	E	309	ILE
1	E	311	GLU
1	E	314	ILE
1	E	320	ASP
1	E	332	THR
1	E	333	LYS
1	E	334	SER
1	E	340	LYS
1	E	358	LYS
1	E	420	LYS
1	E	421	PHE
1	E	423	LYS
1	E	430	ILE
1	E	446	LYS
1	E	472	ASN
1	F	6	ASP
1	F	11	LYS
1	F	32	LEU
1	F	35	ARG
1	F	38	GLU
1	F	40	GLN
1	F	42	ARG
1	F	44	ARG
1	F	45	VAL
1	F	60	SER
1	F	112	THR
1	F	145	THR
1	F	212	ILE
1	F	235	ILE
1	F	242	PHE
1	F	269	LYS
1	F	271	VAL
1	F	281	TRP
1	F	289	LYS
1	F	295	LYS
1	F	306	LYS
1	F	309	ILE

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Mol	Chain	Res	Type
1	F	329	LYS
1	F	332	THR
1	F	333	LYS
1	F	400	LYS
1	F	409	LEU
1	F	420	LYS
1	F	421	PHE
1	F	423	LYS
1	F	430	ILE
1	G	19	ARG
1	G	27	LYS
1	G	32	LEU
1	G	33	LYS
1	G	34	THR
1	G	35	ARG
1	G	38	GLU
1	G	42	ARG
1	G	44	ARG
1	G	45	VAL
1	G	46	ARG
1	G	50	ARG
1	G	60	SER
1	G	112	THR
1	G	134	LYS
1	G	135	ASN
1	G	145	THR
1	G	174	ARG
1	G	212	ILE
1	G	213	SER
1	G	242	PHE
1	G	245	LYS
1	G	271	VAL
1	G	281	TRP
1	G	289	LYS
1	G	295	LYS
1	G	306	LYS
1	G	309	ILE
1	G	314	ILE
1	G	327	SER
1	G	333	LYS
1	G	409	LEU
1	G	420	LYS

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Mol	Chain	Res	Type
1	G	421	PHE
1	G	423	LYS
1	G	424	HIS
1	G	430	ILE
1	G	431	VAL
1	H	6	ASP
1	H	11	LYS
1	H	19	ARG
1	H	32	LEU
1	H	34	THR
1	H	35	ARG
1	H	36	GLU
1	H	38	GLU
1	H	45	VAL
1	H	46	ARG
1	H	50	ARG
1	H	60	SER
1	H	69	ASP
1	H	112	THR
1	H	145	THR
1	H	189	HIS
1	H	212	ILE
1	H	213	SER
1	H	231	SER
1	H	238	MET
1	H	239	THR
1	H	242	PHE
1	H	246	THR
1	H	269	LYS
1	H	271	VAL
1	H	281	TRP
1	H	295	LYS
1	H	302	LEU
1	H	309	ILE
1	H	311	GLU
1	H	332	THR
1	H	334	SER
1	H	340	LYS
1	H	342	LYS
1	H	363	ARG
1	H	420	LYS
1	H	431	VAL

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Mol	Chain	Res	Type
1	H	446	LYS
1	H	501	THR
1	I	9	PHE
1	I	12	MET
1	I	19	ARG
1	I	30	GLU
1	I	32	LEU
1	I	35	ARG
1	I	38	GLU
1	I	42	ARG
1	I	44	ARG
1	I	45	VAL
1	I	46	ARG
1	I	60	SER
1	I	98	ASP
1	I	112	THR
1	I	145	THR
1	I	212	ILE
1	I	213	SER
1	I	217	ARG
1	I	242	PHE
1	I	246	THR
1	I	261	ARG
1	I	269	LYS
1	I	271	VAL
1	I	280	ILE
1	I	281	TRP
1	I	289	LYS
1	I	291	LEU
1	I	295	LYS
1	I	298	HIS
1	I	302	LEU
1	I	311	GLU
1	I	313	SER
1	I	314	ILE
1	I	316	GLU
1	I	319	CYS
1	I	322	LEU
1	I	327	SER
1	I	328	GLU
1	I	332	THR
1	I	334	SER

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Mol	Chain	Res	Type
1	I	340	LYS
1	I	355	GLU
1	I	362	GLU
1	I	409	LEU
1	I	421	PHE
1	I	423	LYS
1	I	430	ILE
1	I	451	SER
1	I	479	THR
1	J	11	LYS
1	J	27	LYS
1	J	32	LEU
1	J	38	GLU
1	J	42	ARG
1	J	44	ARG
1	J	45	VAL
1	J	46	ARG
1	J	50	ARG
1	J	60	SER
1	J	67	ARG
1	J	87	THR
1	J	112	THR
1	J	145	THR
1	J	189	HIS
1	J	212	ILE
1	J	213	SER
1	J	242	PHE
1	J	245	LYS
1	J	269	LYS
1	J	271	VAL
1	J	281	TRP
1	J	289	LYS
1	J	295	LYS
1	J	297	GLN
1	J	308	LYS
1	J	311	GLU
1	J	314	ILE
1	J	332	THR
1	J	334	SER
1	J	338	ARG
1	J	363	ARG
1	J	400	LYS

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Mol	Chain	Res	Type
1	J	402	GLU
1	J	421	PHE
1	J	430	ILE
1	J	431	VAL
1	K	11	LYS
1	K	19	ARG
1	K	27	LYS
1	K	30	GLU
1	K	32	LEU
1	K	34	THR
1	K	35	ARG
1	K	38	GLU
1	K	45	VAL
1	K	46	ARG
1	K	50	ARG
1	K	60	SER
1	K	112	THR
1	K	134	LYS
1	K	135	ASN
1	K	143	LYS
1	K	145	THR
1	K	189	HIS
1	K	212	ILE
1	K	213	SER
1	K	235	ILE
1	K	236	LEU
1	K	242	PHE
1	K	246	THR
1	K	250	GLN
1	K	269	LYS
1	K	271	VAL
1	K	276	SER
1	K	277	ASP
1	K	281	TRP
1	K	289	LYS
1	K	292	GLU
1	K	297	GLN
1	K	308	LYS
1	K	314	ILE
1	K	316	GLU
1	K	327	SER
1	K	328	GLU

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Mol	Chain	Res	Type
1	K	332	THR
1	K	334	SER
1	K	338	ARG
1	K	340	LYS
1	K	355	GLU
1	K	358	LYS
1	K	363	ARG
1	K	400	LYS
1	K	421	PHE
1	K	430	ILE
1	K	431	VAL
1	K	477	LEU
1	L	19	ARG
1	L	32	LEU
1	L	38	GLU
1	L	40	GLN
1	L	42	ARG
1	L	44	ARG
1	L	45	VAL
1	L	46	ARG
1	L	50	ARG
1	L	60	SER
1	L	69	ASP
1	L	87	THR
1	L	112	THR
1	L	145	THR
1	L	190	TYR
1	L	212	ILE
1	L	213	SER
1	L	231	SER
1	L	242	PHE
1	L	245	LYS
1	L	246	THR
1	L	247	PHE
1	L	269	LYS
1	L	271	VAL
1	L	281	TRP
1	L	295	LYS
1	L	296	LEU
1	L	311	GLU
1	L	332	THR
1	L	334	SER

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Mol	Chain	Res	Type
1	L	338	ARG
1	L	355	GLU
1	L	403	ARG
1	L	420	LYS
1	L	424	HIS
1	L	430	ILE
1	L	439	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	298	HIS
1	A	437	GLN
1	A	494	ASN
1	B	43	ASN
1	B	209	HIS
1	C	43	ASN
1	C	450	HIS
1	D	43	ASN
1	D	297	GLN
1	E	43	ASN
1	E	258	HIS
1	E	298	HIS
1	E	391	HIS
1	F	43	ASN
1	F	408	HIS
1	F	472	ASN
1	G	43	ASN
1	H	43	ASN
1	H	408	HIS
1	H	424	HIS
1	H	437	GLN
1	H	494	ASN
1	I	43	ASN
1	I	209	HIS
1	I	472	ASN
1	J	43	ASN
1	J	406	ASN
1	J	408	HIS
1	J	494	ASN
1	K	43	ASN

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Mol	Chain	Res	Type
1	K	209	HIS
1	L	43	ASN
1	L	472	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

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	$\# Z > 2$
2	ADP	H	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.27	3 (10%)
2	ADP	L	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.27	3 (10%)
2	ADP	D	601	-	24,29,29	0.90	0	29,45,45	1.40	4 (13%)
2	ADP	I	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.16	2 (6%)
2	ADP	K	601	-	24,29,29	0.88	0	29,45,45	1.29	3 (10%)
2	ADP	C	602	-	24,29,29	0.91	0	29,45,45	1.16	2 (6%)
2	ADP	B	601	-	24,29,29	0.93	1 (4%)	29,45,45	1.26	2 (6%)
2	ADP	F	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.27	3 (10%)
2	ADP	A	601	-	24,29,29	0.91	1 (4%)	29,45,45	1.44	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	C	601	-	24,29,29	0.90	0	29,45,45	1.28	2 (6%)
2	ADP	G	601	-	24,29,29	0.94	1 (4%)	29,45,45	1.18	2 (6%)
2	ADP	J	601	-	24,29,29	0.95	1 (4%)	29,45,45	1.16	2 (6%)

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
2	ADP	H	601	-	-	3/12/32/32	0/3/3/3
2	ADP	L	601	-	-	6/12/32/32	0/3/3/3
2	ADP	D	601	-	-	2/12/32/32	0/3/3/3
2	ADP	I	601	-	-	1/12/32/32	0/3/3/3
2	ADP	K	601	-	-	6/12/32/32	0/3/3/3
2	ADP	C	602	-	-	2/12/32/32	0/3/3/3
2	ADP	B	601	-	-	5/12/32/32	0/3/3/3
2	ADP	F	601	-	-	7/12/32/32	0/3/3/3
2	ADP	A	601	-	-	4/12/32/32	0/3/3/3
2	ADP	C	601	-	-	1/12/32/32	0/3/3/3
2	ADP	G	601	-	-	3/12/32/32	0/3/3/3
2	ADP	J	601	-	-	4/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	601	ADP	PA-O3A	2.23	1.61	1.59
2	F	601	ADP	PA-O3A	2.21	1.61	1.59
2	B	601	ADP	PA-O3A	2.17	1.61	1.59
2	G	601	ADP	PA-O3A	2.16	1.61	1.59
2	L	601	ADP	PA-O3A	2.10	1.61	1.59
2	H	601	ADP	PA-O3A	2.05	1.61	1.59
2	A	601	ADP	PA-O3A	2.04	1.61	1.59
2	I	601	ADP	PA-O3A	2.03	1.61	1.59

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	ADP	N3-C2-N1	-3.71	123.64	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	ADP	N3-C2-N1	-3.70	123.65	128.67
2	C	601	ADP	N3-C2-N1	-3.68	123.67	128.67
2	B	601	ADP	N3-C2-N1	-3.67	123.69	128.67
2	A	601	ADP	C4'-O4'-C1'	-3.64	106.59	109.92
2	J	601	ADP	N3-C2-N1	-3.61	123.78	128.67
2	A	601	ADP	N3-C2-N1	-3.60	123.79	128.67
2	F	601	ADP	N3-C2-N1	-3.59	123.80	128.67
2	K	601	ADP	N3-C2-N1	-3.58	123.82	128.67
2	C	602	ADP	N3-C2-N1	-3.58	123.82	128.67
2	L	601	ADP	N3-C2-N1	-3.57	123.83	128.67
2	I	601	ADP	N3-C2-N1	-3.54	123.86	128.67
2	G	601	ADP	N3-C2-N1	-3.37	124.10	128.67
2	D	601	ADP	O4'-C1'-N9	3.07	112.82	108.75
2	A	601	ADP	C4-C5-N7	-2.90	106.28	109.34
2	A	601	ADP	O4'-C1'-N9	2.89	112.58	108.75
2	D	601	ADP	C4-C5-N7	-2.86	106.31	109.34
2	C	601	ADP	C4-C5-N7	-2.86	106.32	109.34
2	K	601	ADP	C4-C5-N7	-2.84	106.34	109.34
2	L	601	ADP	C4-C5-N7	-2.83	106.35	109.34
2	B	601	ADP	C4-C5-N7	-2.74	106.45	109.34
2	H	601	ADP	C4-C5-N7	-2.73	106.45	109.34
2	J	601	ADP	C4-C5-N7	-2.72	106.46	109.34
2	F	601	ADP	C4-C5-N7	-2.72	106.47	109.34
2	G	601	ADP	C4-C5-N7	-2.71	106.47	109.34
2	F	601	ADP	O4'-C1'-N9	2.68	112.30	108.75
2	I	601	ADP	C4-C5-N7	-2.67	106.52	109.34
2	C	602	ADP	C4-C5-N7	-2.51	106.68	109.34
2	K	601	ADP	O4'-C1'-N9	2.40	111.92	108.75
2	D	601	ADP	C4'-O4'-C1'	-2.25	107.86	109.92
2	L	601	ADP	O4'-C1'-N9	2.25	111.73	108.75
2	H	601	ADP	O4'-C1'-N9	2.11	111.54	108.75

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ADP	C5'-O5'-PA-O2A
2	A	601	ADP	C5'-O5'-PA-O3A
2	B	601	ADP	C5'-O5'-PA-O3A
2	C	601	ADP	PB-O3A-PA-O5'
2	F	601	ADP	C5'-O5'-PA-O1A
2	F	601	ADP	C5'-O5'-PA-O2A

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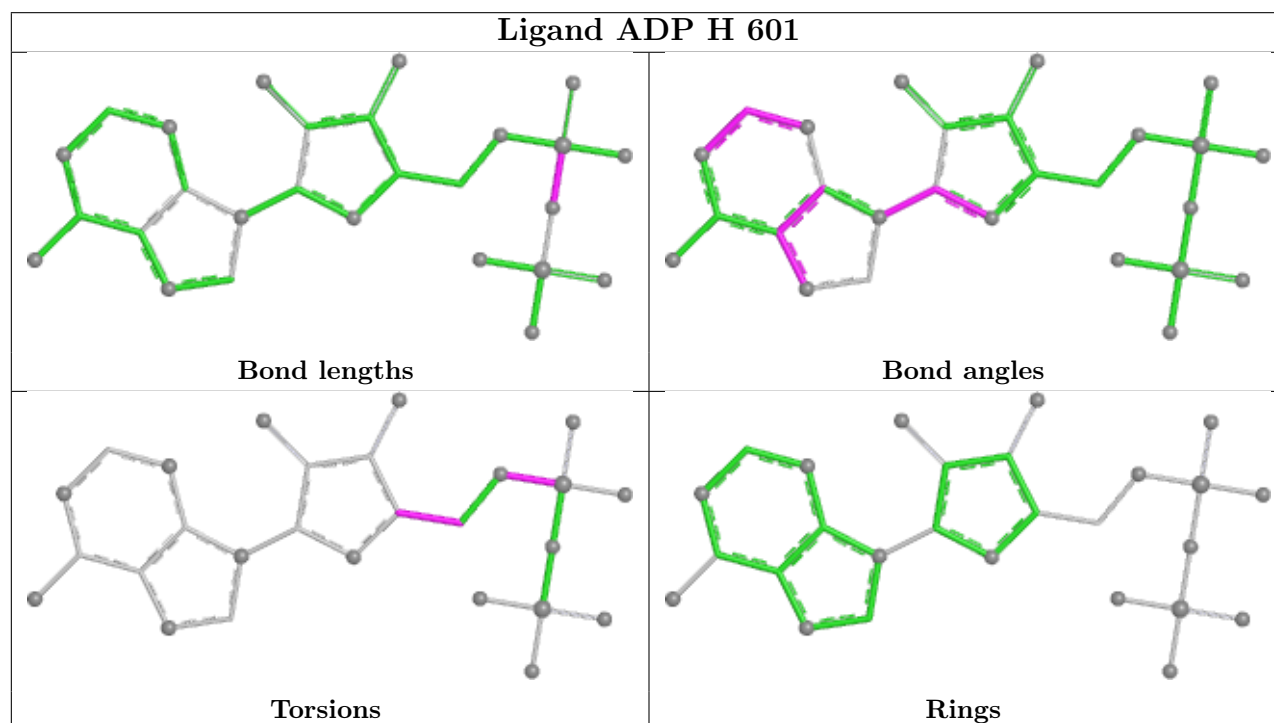
Mol	Chain	Res	Type	Atoms
2	F	601	ADP	C5'-O5'-PA-O3A
2	H	601	ADP	C5'-O5'-PA-O1A
2	I	601	ADP	C5'-O5'-PA-O1A
2	J	601	ADP	C5'-O5'-PA-O2A
2	J	601	ADP	C5'-O5'-PA-O3A
2	K	601	ADP	C5'-O5'-PA-O1A
2	K	601	ADP	C5'-O5'-PA-O3A
2	K	601	ADP	O4'-C4'-C5'-O5'
2	L	601	ADP	C5'-O5'-PA-O1A
2	L	601	ADP	C5'-O5'-PA-O2A
2	L	601	ADP	C5'-O5'-PA-O3A
2	J	601	ADP	O4'-C4'-C5'-O5'
2	K	601	ADP	C3'-C4'-C5'-O5'
2	B	601	ADP	O4'-C4'-C5'-O5'
2	J	601	ADP	C3'-C4'-C5'-O5'
2	L	601	ADP	O4'-C4'-C5'-O5'
2	H	601	ADP	O4'-C4'-C5'-O5'
2	F	601	ADP	O4'-C4'-C5'-O5'
2	L	601	ADP	C3'-C4'-C5'-O5'
2	A	601	ADP	C3'-C4'-C5'-O5'
2	A	601	ADP	O4'-C4'-C5'-O5'
2	B	601	ADP	C3'-C4'-C5'-O5'
2	C	602	ADP	O4'-C4'-C5'-O5'
2	D	601	ADP	PB-O3A-PA-O5'
2	F	601	ADP	C3'-C4'-C5'-O5'
2	H	601	ADP	C3'-C4'-C5'-O5'
2	G	601	ADP	O4'-C4'-C5'-O5'
2	F	601	ADP	PB-O3A-PA-O2A
2	C	602	ADP	C3'-C4'-C5'-O5'
2	B	601	ADP	C5'-O5'-PA-O1A
2	D	601	ADP	C5'-O5'-PA-O2A
2	G	601	ADP	C5'-O5'-PA-O1A
2	F	601	ADP	PB-O3A-PA-O1A
2	G	601	ADP	C3'-C4'-C5'-O5'
2	K	601	ADP	PB-O3A-PA-O1A
2	K	601	ADP	PB-O3A-PA-O2A
2	B	601	ADP	PB-O3A-PA-O2A
2	L	601	ADP	PB-O3A-PA-O2A

There are no ring outliers.

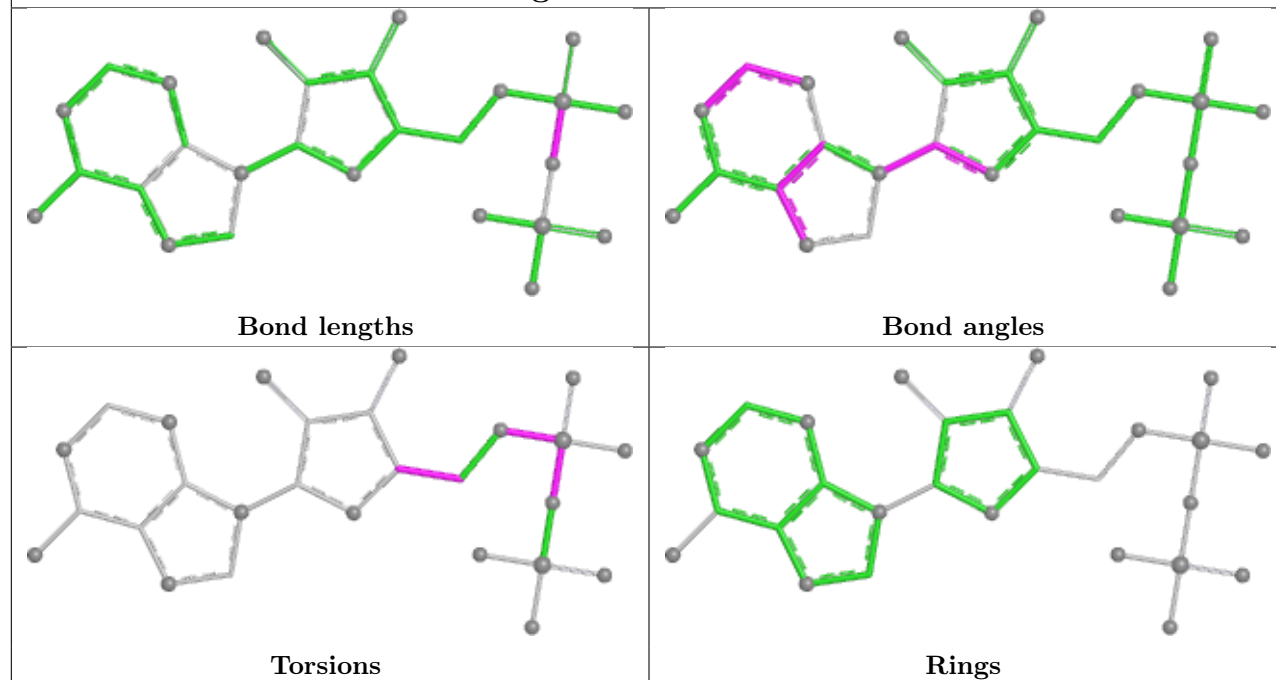
7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	601	ADP	2	0
2	L	601	ADP	1	0
2	D	601	ADP	1	0
2	C	602	ADP	1	0
2	B	601	ADP	2	0
2	F	601	ADP	1	0
2	C	601	ADP	1	0

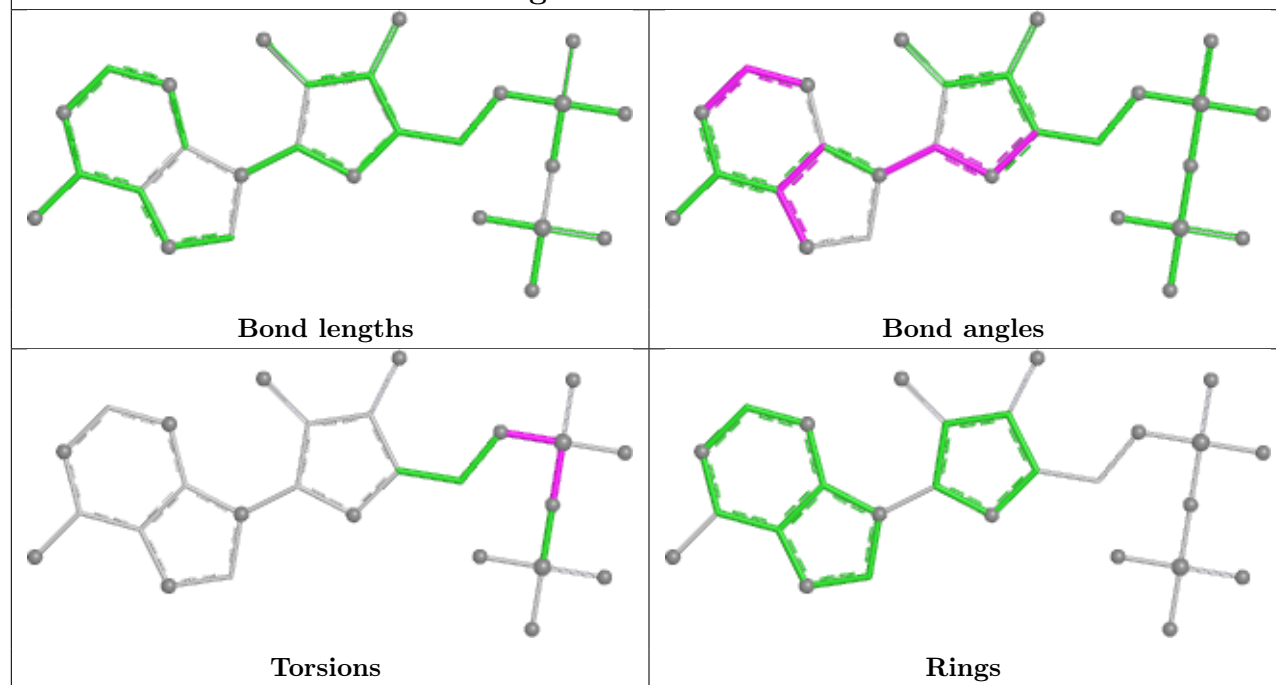
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



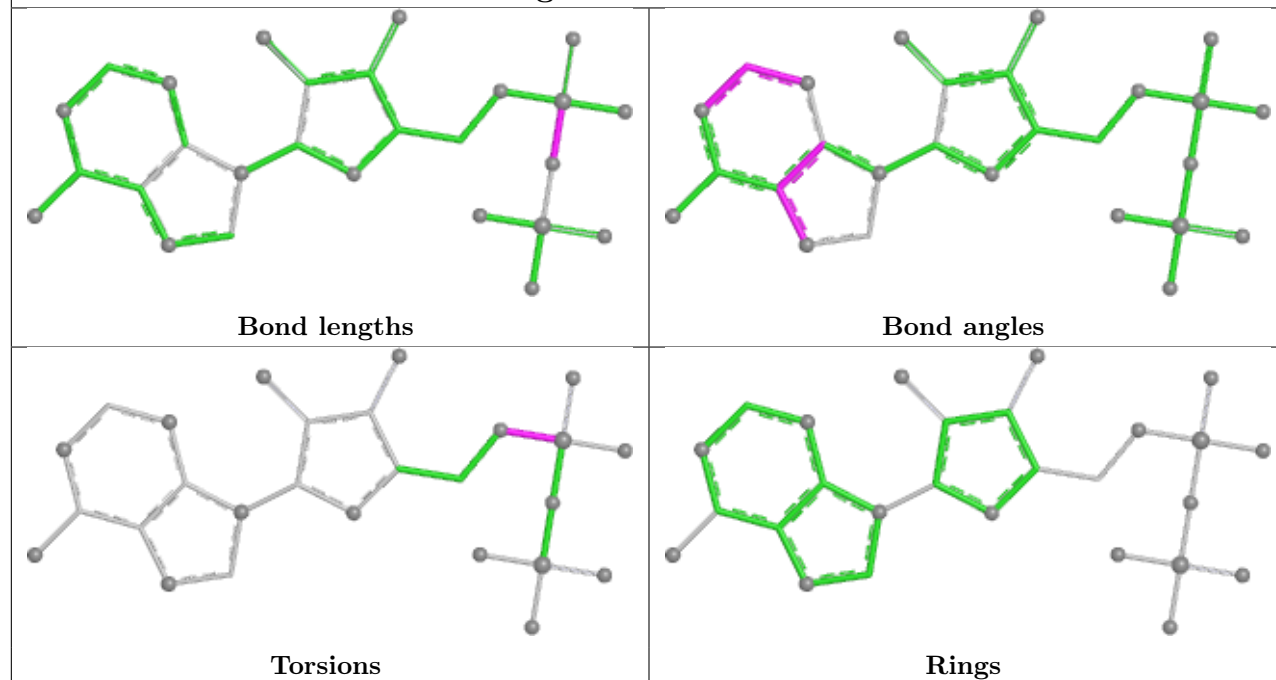
Ligand ADP L 601



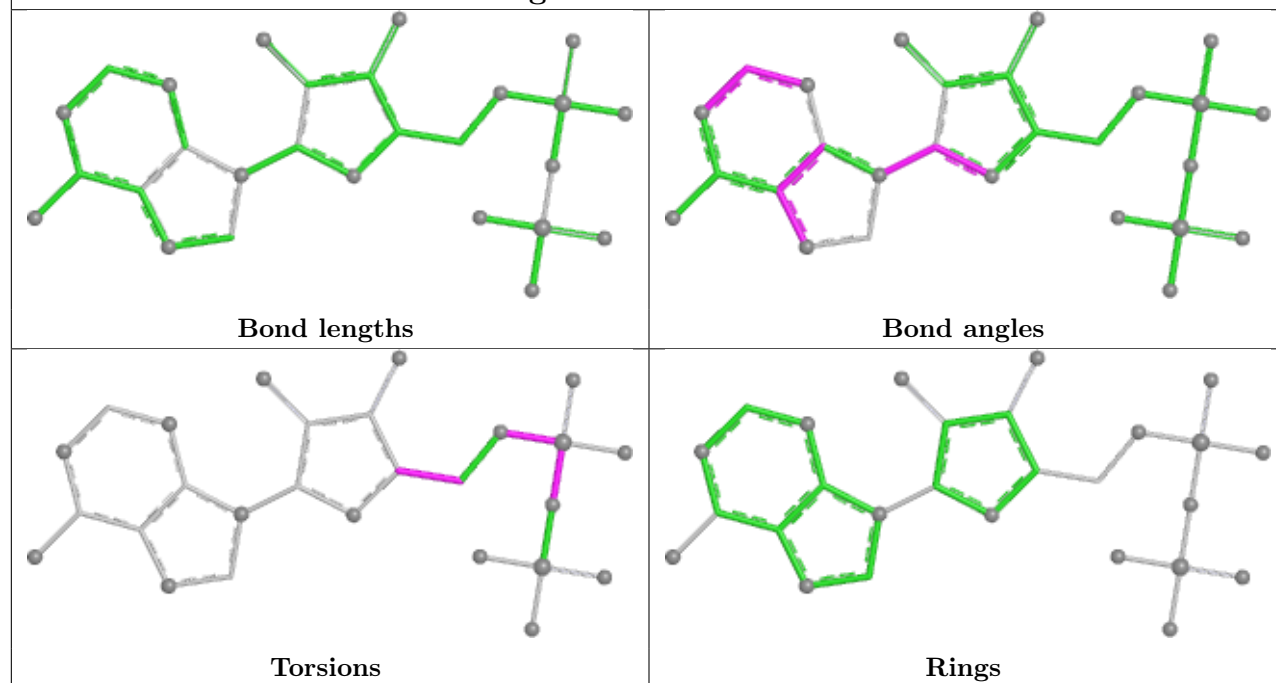
Ligand ADP D 601

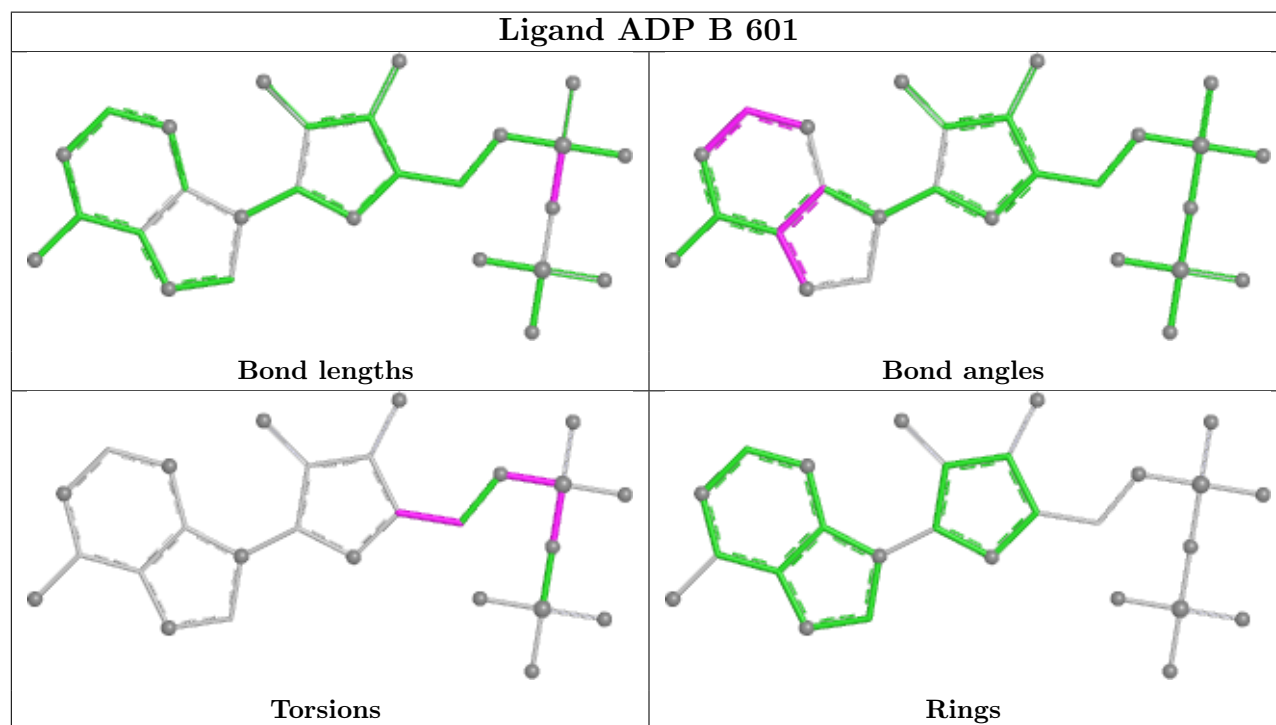
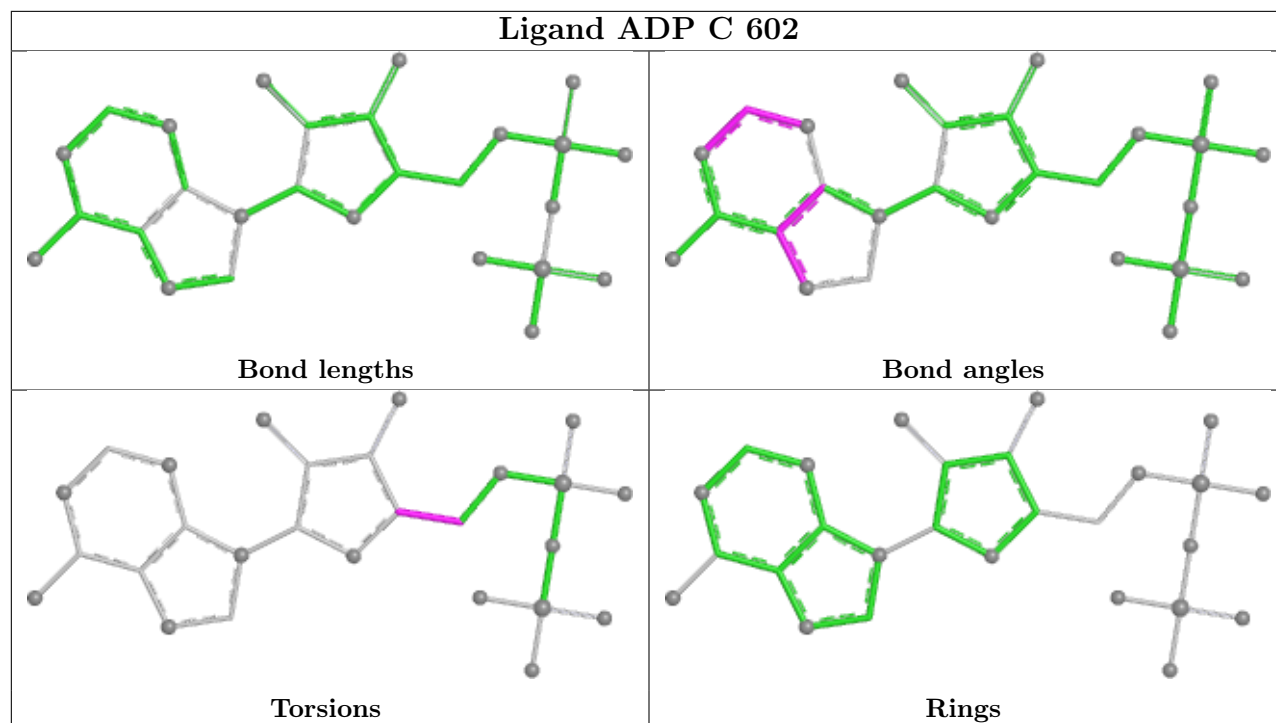


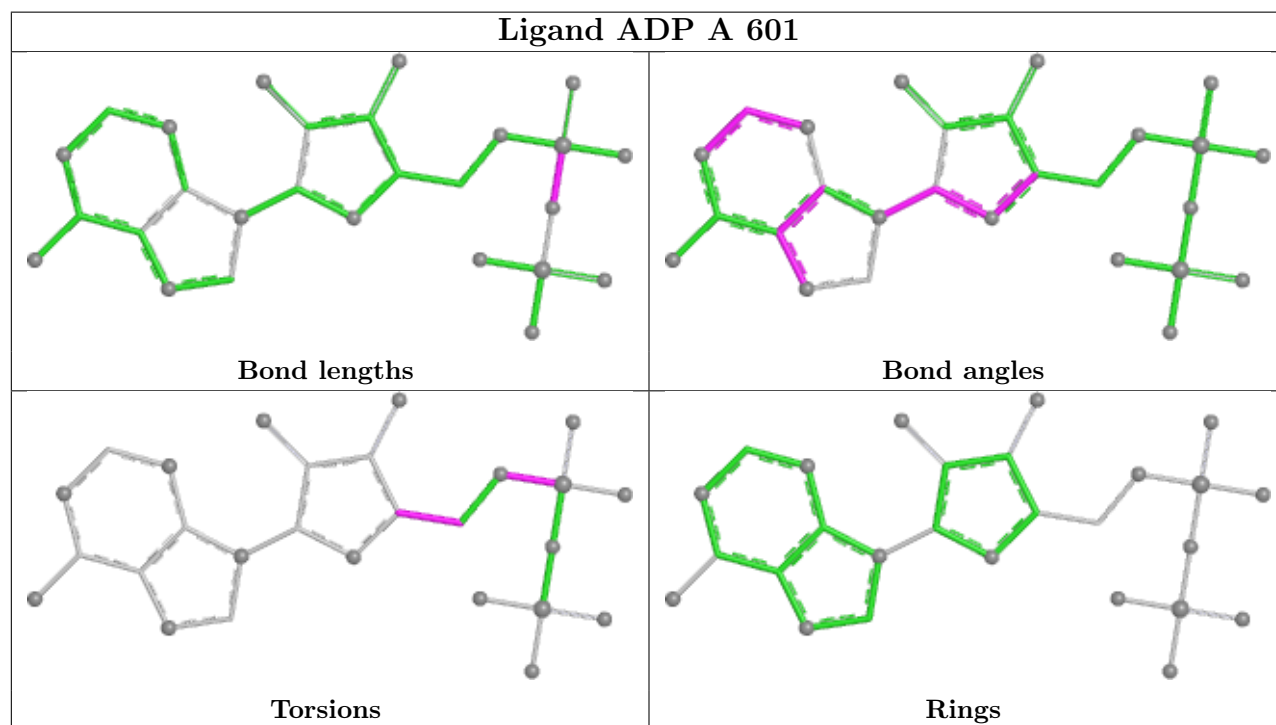
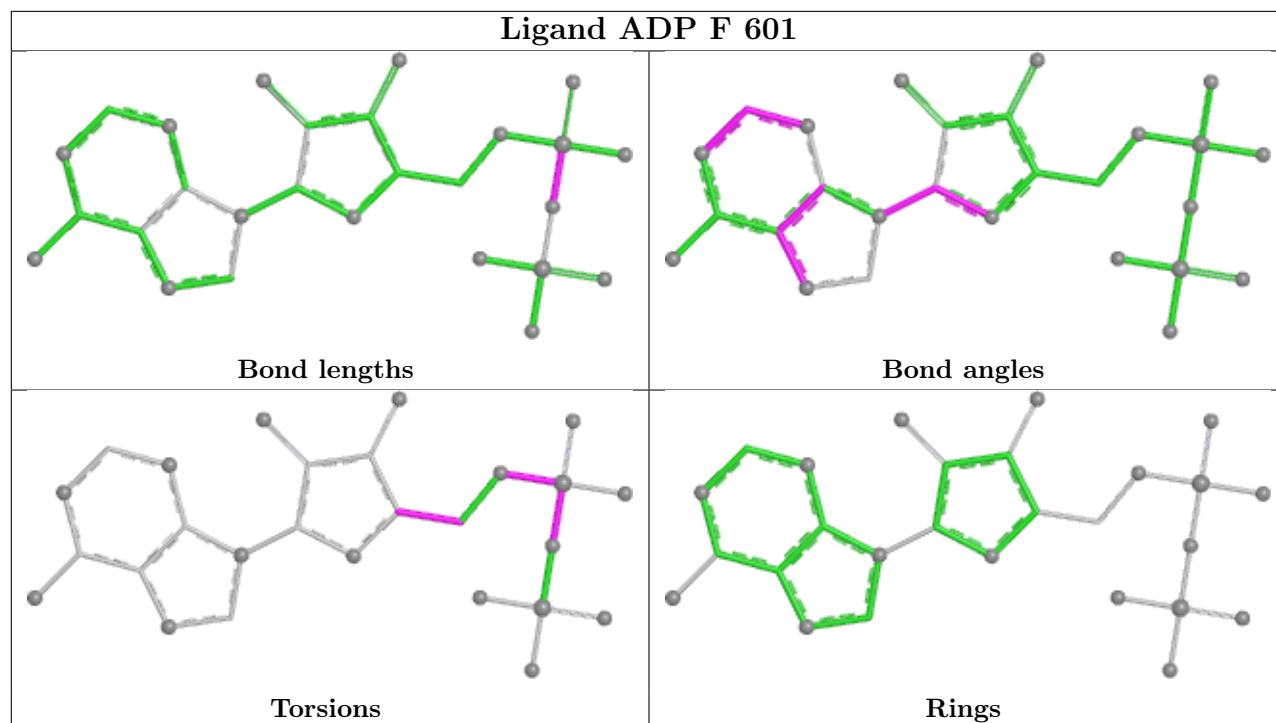
Ligand ADP I 601

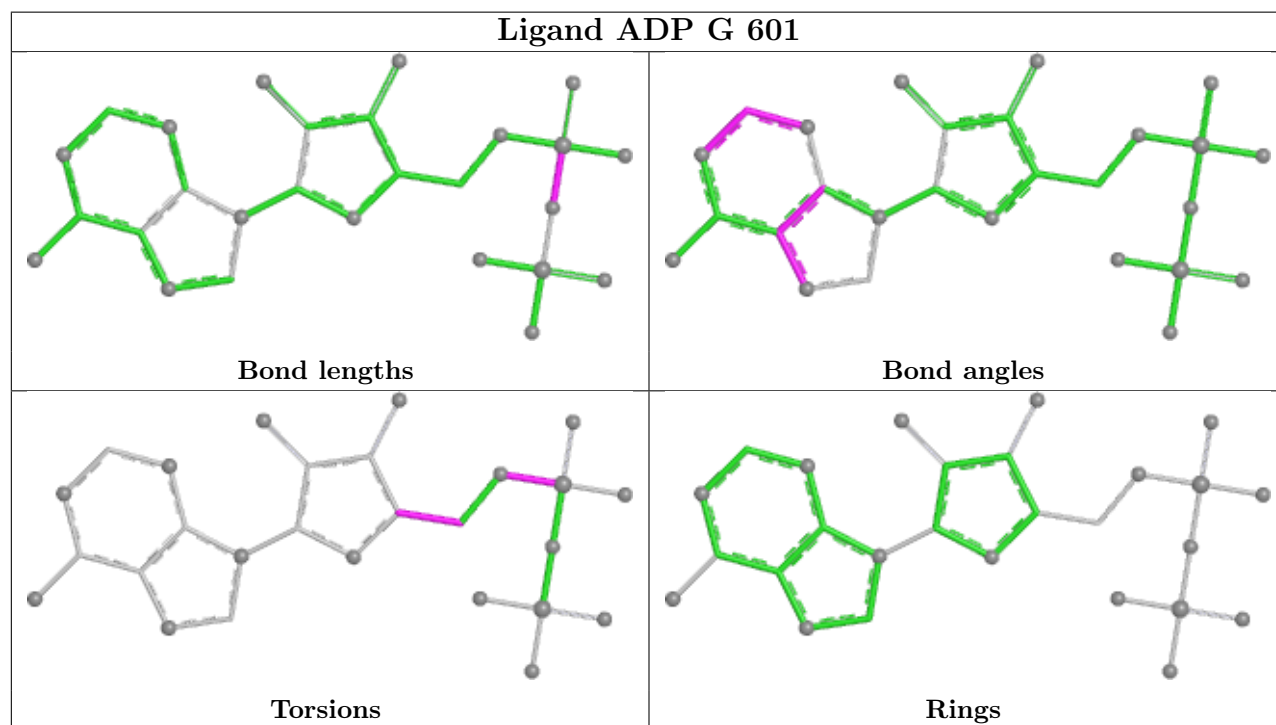
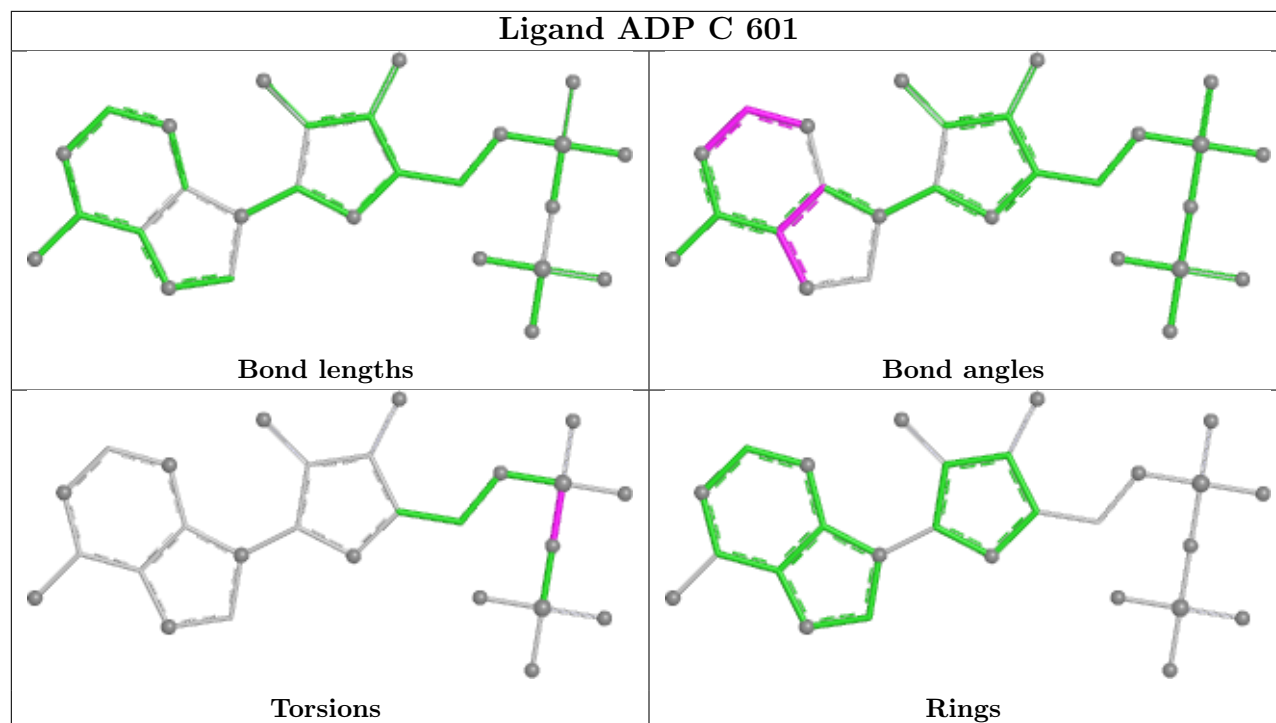


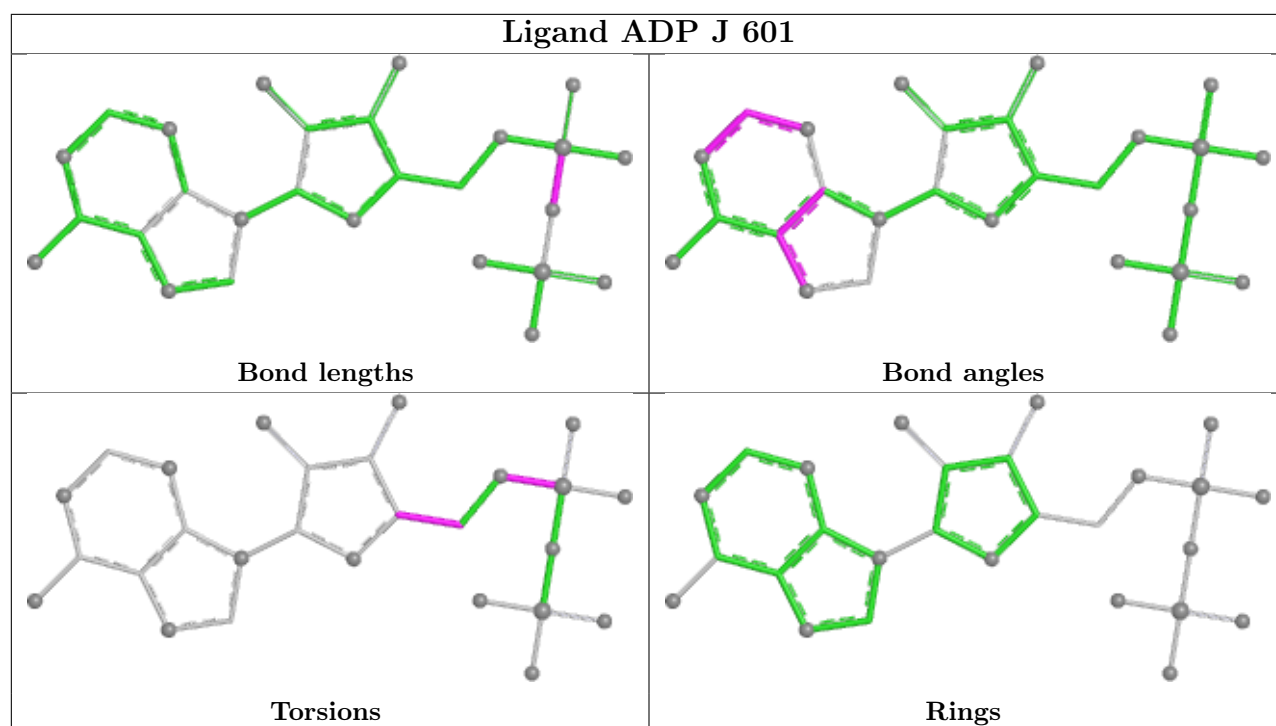
Ligand ADP K 601











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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, 95th 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 ²)	Q < 0.9
1	A	496/496 (100%)	-0.14	20 (4%)	38 33	40, 88, 150, 185	0
1	B	496/496 (100%)	-0.26	13 (2%)	56 49	44, 76, 135, 170	0
1	C	496/496 (100%)	-0.10	19 (3%)	40 36	43, 85, 152, 179	0
1	D	496/496 (100%)	-0.15	13 (2%)	56 49	42, 87, 147, 184	0
1	E	496/496 (100%)	-0.30	6 (1%)	79 73	47, 75, 128, 175	0
1	F	496/496 (100%)	-0.28	14 (2%)	53 47	39, 73, 132, 191	0
1	G	496/496 (100%)	-0.25	11 (2%)	62 56	37, 70, 130, 175	0
1	H	496/496 (100%)	-0.20	16 (3%)	47 42	38, 77, 137, 180	0
1	I	496/496 (100%)	0.01	31 (6%)	20 18	49, 92, 154, 184	0
1	J	496/496 (100%)	-0.29	7 (1%)	75 69	39, 76, 131, 172	0
1	K	496/496 (100%)	-0.07	15 (3%)	50 44	41, 90, 150, 194	0
1	L	496/496 (100%)	-0.14	19 (3%)	40 36	40, 81, 151, 181	0
All	All	5952/5952 (100%)	-0.18	184 (3%)	49 43	37, 80, 146, 194	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	243	GLY	11.1
1	B	243	GLY	6.8
1	J	243	GLY	6.8
1	L	243	GLY	6.8
1	A	242	PHE	6.4
1	I	31	ASP	6.1
1	I	241	GLY	6.0
1	C	241	GLY	5.9
1	J	241	GLY	5.9
1	I	34	THR	5.4
1	K	242	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	34	THR	5.3
1	I	312	GLY	5.3
1	D	243	GLY	5.3
1	B	242	PHE	5.2
1	A	241	GLY	5.0
1	L	241	GLY	5.0
1	C	242	PHE	4.9
1	J	242	PHE	4.9
1	C	424	HIS	4.7
1	A	37	THR	4.6
1	I	424	HIS	4.5
1	K	241	GLY	4.5
1	D	34	THR	4.4
1	L	242	PHE	4.4
1	I	311	GLU	4.4
1	C	243	GLY	4.4
1	I	43	ASN	4.3
1	F	424	HIS	4.3
1	K	31	ASP	4.2
1	C	43	ASN	4.2
1	B	7	PRO	4.1
1	L	32	LEU	4.0
1	C	31	ASP	4.0
1	I	42	ARG	4.0
1	E	242	PHE	4.0
1	D	35	ARG	4.0
1	I	278	GLY	3.8
1	F	35	ARG	3.8
1	I	335	ASN	3.8
1	I	32	LEU	3.8
1	B	43	ASN	3.7
1	A	243	GLY	3.7
1	K	312	GLY	3.7
1	H	35	ARG	3.7
1	C	35	ARG	3.7
1	D	424	HIS	3.6
1	L	501	THR	3.6
1	J	43	ASN	3.6
1	F	6	ASP	3.6
1	A	35	ARG	3.6
1	A	42	ARG	3.6
1	L	35	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	35	ARG	3.5
1	G	34	THR	3.5
1	G	424	HIS	3.5
1	C	34	THR	3.5
1	L	43	ASN	3.4
1	I	499	THR	3.4
1	G	243	GLY	3.4
1	D	31	ASP	3.4
1	C	303	GLY	3.3
1	L	308	LYS	3.3
1	L	34	THR	3.3
1	H	243	GLY	3.3
1	B	241	GLY	3.3
1	G	43	ASN	3.3
1	K	335	ASN	3.3
1	I	37	THR	3.2
1	L	37	THR	3.2
1	D	278	GLY	3.2
1	H	241	GLY	3.2
1	I	329	LYS	3.2
1	H	34	THR	3.1
1	F	243	GLY	3.1
1	L	31	ASP	3.1
1	I	7	PRO	3.1
1	K	303	GLY	3.1
1	D	425	GLY	3.1
1	K	43	ASN	3.1
1	L	285	GLY	3.1
1	A	34	THR	3.0
1	K	35	ARG	3.0
1	E	34	THR	3.0
1	D	43	ASN	3.0
1	E	241	GLY	3.0
1	K	311	GLU	2.9
1	I	35	ARG	2.9
1	E	43	ASN	2.9
1	G	37	THR	2.9
1	H	501	THR	2.9
1	H	242	PHE	2.9
1	F	34	THR	2.8
1	D	242	PHE	2.8
1	K	302	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	6	ASP	2.8
1	A	7	PRO	2.8
1	C	37	THR	2.8
1	C	6	ASP	2.7
1	I	498	VAL	2.7
1	K	244	ASP	2.7
1	B	6	ASP	2.7
1	A	499	THR	2.7
1	B	424	HIS	2.7
1	A	31	ASP	2.7
1	D	37	THR	2.7
1	F	37	THR	2.7
1	A	277	ASP	2.7
1	F	31	ASP	2.6
1	B	35	ARG	2.6
1	I	243	GLY	2.6
1	F	43	ASN	2.6
1	I	313	SER	2.6
1	C	423	LYS	2.6
1	A	6	ASP	2.6
1	G	42	ARG	2.5
1	I	423	LYS	2.5
1	L	298	HIS	2.5
1	I	296	LEU	2.5
1	K	37	THR	2.5
1	A	266	PHE	2.5
1	K	424	HIS	2.5
1	I	332	THR	2.5
1	H	310	TYR	2.5
1	I	501	THR	2.4
1	A	309	ILE	2.4
1	L	309	ILE	2.4
1	F	279	SER	2.4
1	A	302	LEU	2.4
1	H	303	GLY	2.4
1	A	43	ASN	2.4
1	A	497	GLY	2.4
1	F	242	PHE	2.4
1	C	330	GLN	2.4
1	D	285	GLY	2.4
1	I	279	SER	2.4
1	B	31	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	34	THR	2.4
1	K	422	GLY	2.3
1	B	42	ARG	2.3
1	C	327	SER	2.3
1	H	39	GLU	2.3
1	F	241	GLY	2.3
1	G	241	GLY	2.3
1	I	302	LEU	2.3
1	D	332	THR	2.3
1	B	37	THR	2.3
1	C	29	VAL	2.2
1	I	308	LYS	2.2
1	J	31	ASP	2.2
1	E	243	GLY	2.2
1	E	35	ARG	2.2
1	I	10	PHE	2.2
1	I	310	TYR	2.2
1	F	422	GLY	2.2
1	H	10	PHE	2.2
1	G	6	ASP	2.2
1	H	302	LEU	2.2
1	L	6	ASP	2.2
1	G	31	ASP	2.2
1	J	499	THR	2.2
1	L	297	GLN	2.2
1	L	303	GLY	2.2
1	B	298	HIS	2.2
1	C	133	PRO	2.1
1	A	301	ILE	2.1
1	F	42	ARG	2.1
1	A	296	LEU	2.1
1	D	42	ARG	2.1
1	C	36	GLU	2.1
1	H	313	SER	2.1
1	L	425	GLY	2.1
1	H	311	GLU	2.1
1	C	309	ILE	2.1
1	F	329	LYS	2.1
1	H	309	ILE	2.1
1	L	42	ARG	2.1
1	G	36	GLU	2.1
1	H	276	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	337	PRO	2.0
1	C	307	ALA	2.0
1	I	33	LYS	2.0
1	H	31	ASP	2.0
1	I	303	GLY	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 monosaccharides in this entry.

6.4 Ligands [i](#)

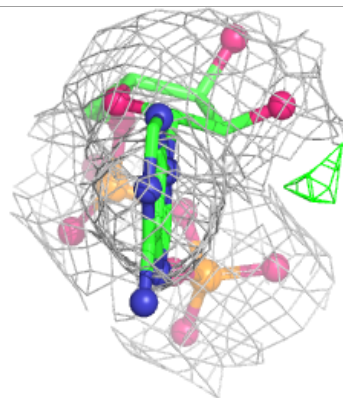
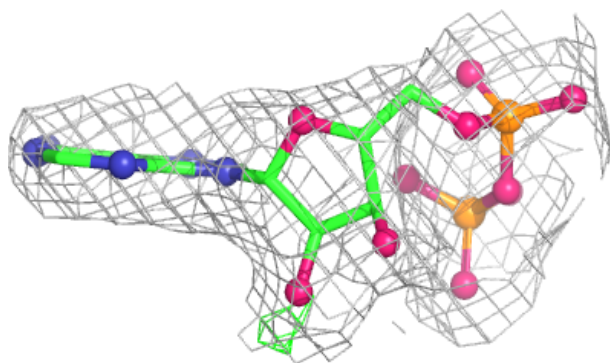
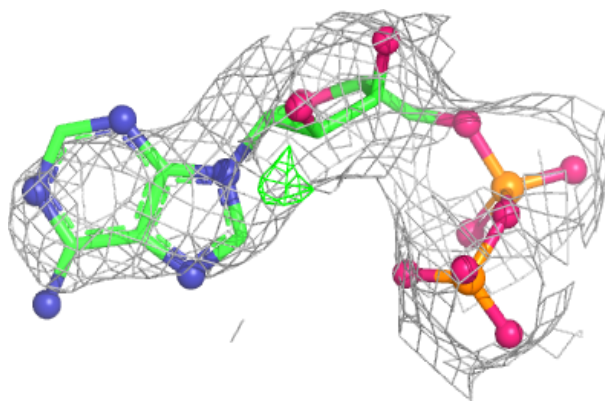
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ADP	F	601	27/27	0.89	0.23	65,97,122,132	0
2	ADP	K	601	27/27	0.90	0.22	57,92,109,121	0
2	ADP	C	602	27/27	0.91	0.36	66,91,120,126	0
2	ADP	B	601	27/27	0.91	0.29	64,79,106,120	0
2	ADP	J	601	27/27	0.91	0.29	64,96,124,149	0
2	ADP	C	601	27/27	0.91	0.21	55,86,112,117	0
2	ADP	H	601	27/27	0.92	0.25	65,80,108,121	0
2	ADP	I	601	27/27	0.92	0.21	66,92,124,130	0
2	ADP	D	601	27/27	0.92	0.21	69,90,116,117	0
2	ADP	A	601	27/27	0.92	0.20	75,97,123,125	0
2	ADP	G	601	27/27	0.93	0.26	66,94,113,122	0
2	ADP	L	601	27/27	0.93	0.28	56,85,105,113	0

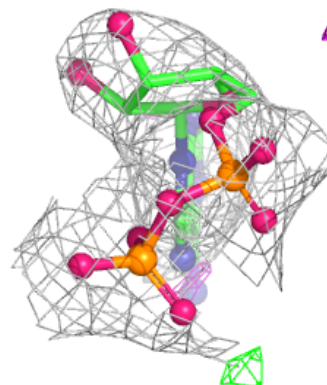
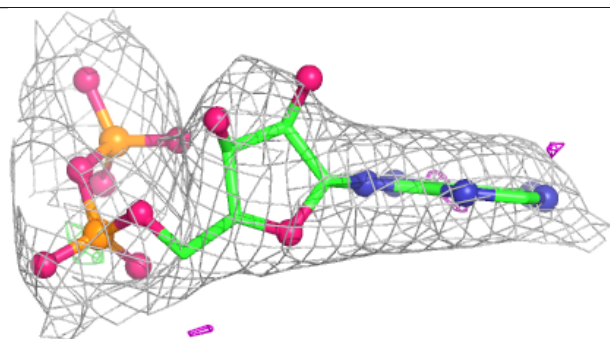
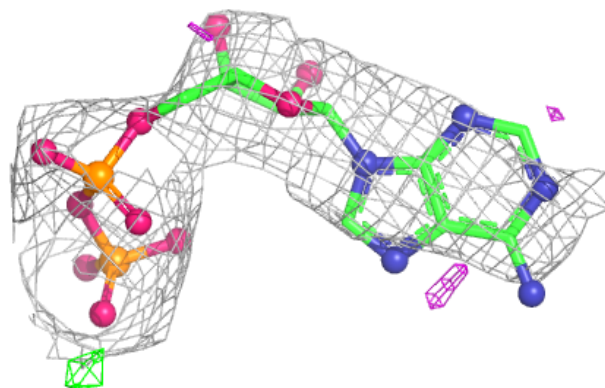
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP F 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

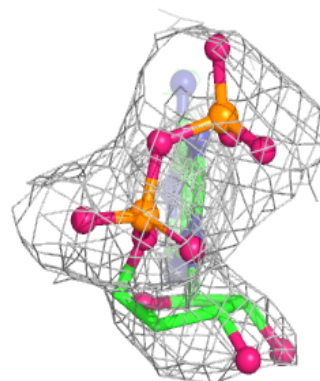
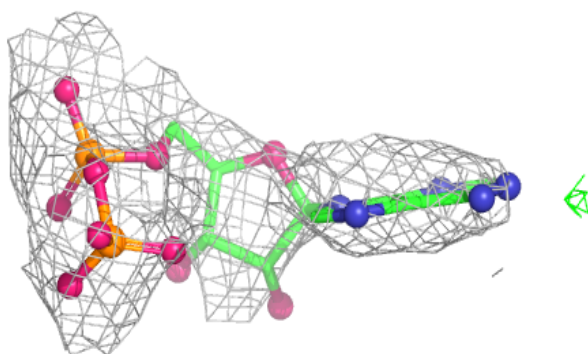
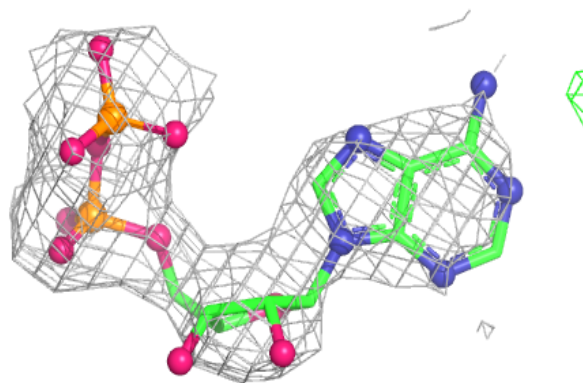
**Electron density around ADP K 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

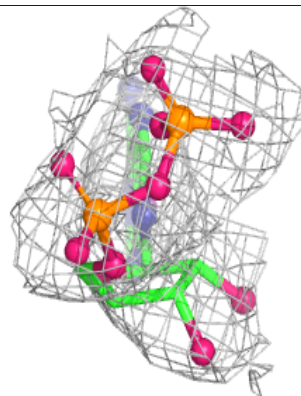
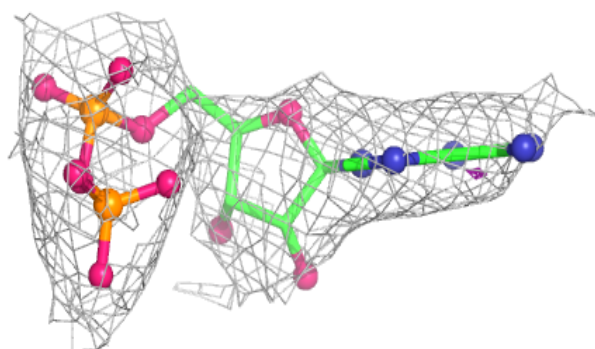
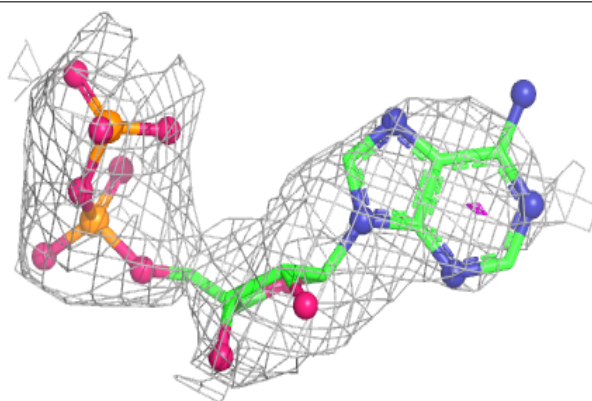


Electron density around ADP C 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

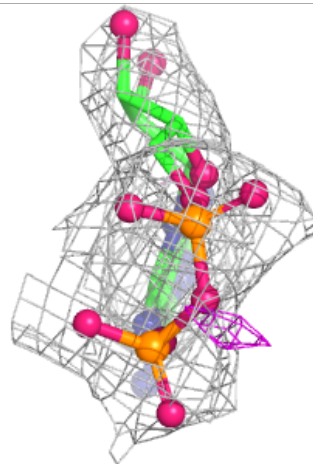
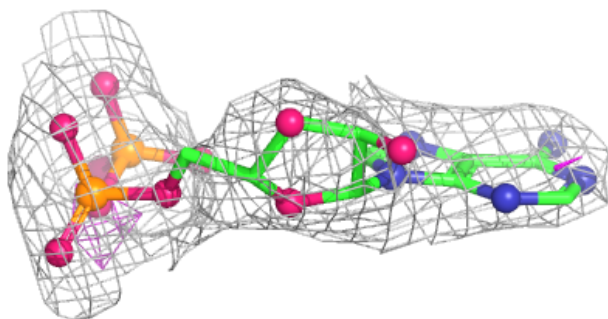
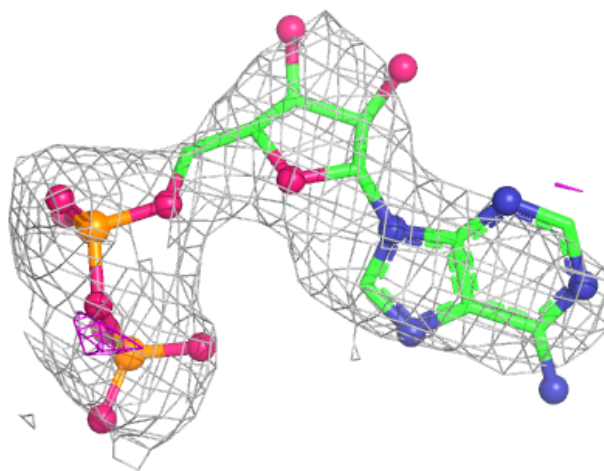
**Electron density around ADP B 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



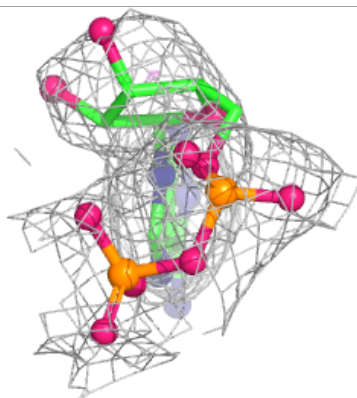
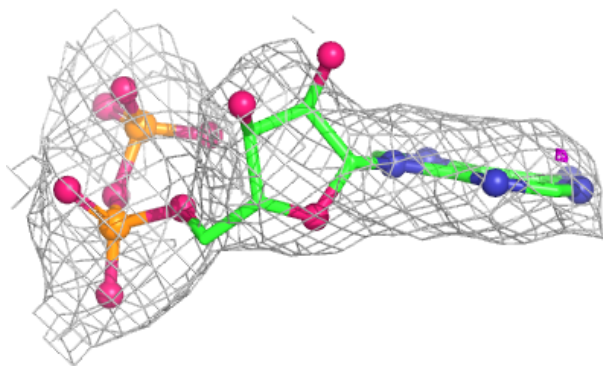
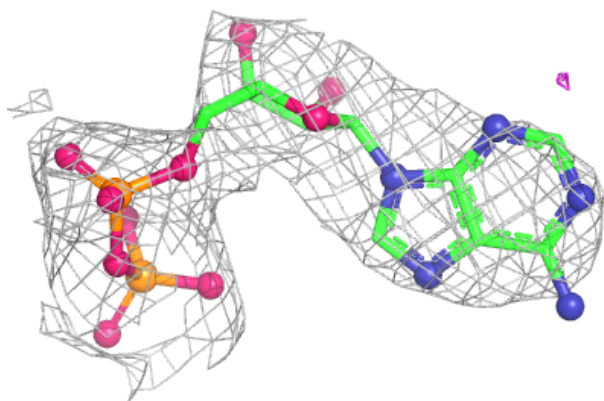
Electron density around ADP J 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

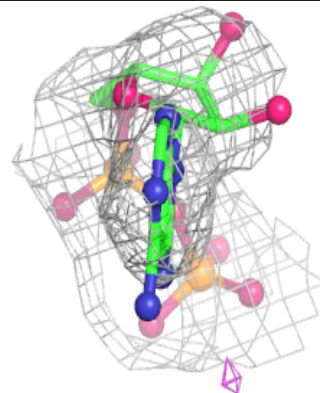
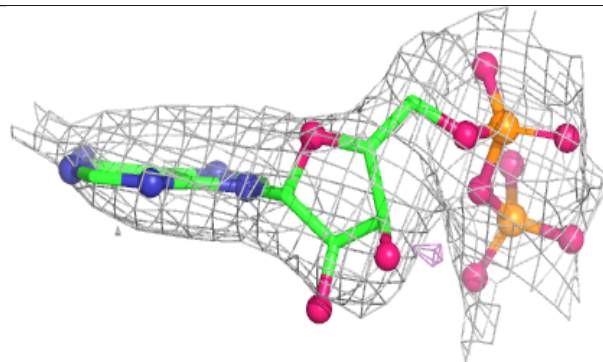
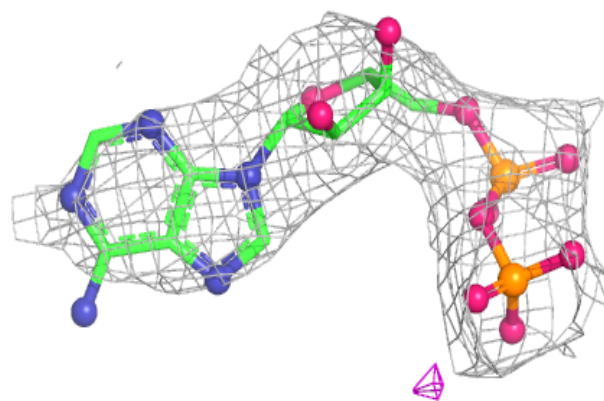


Electron density around ADP C 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

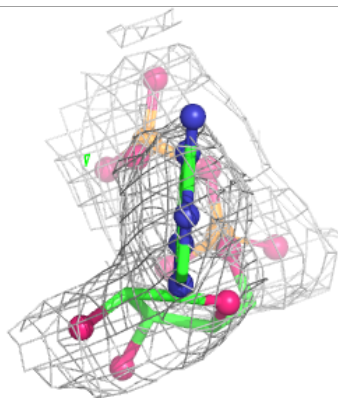
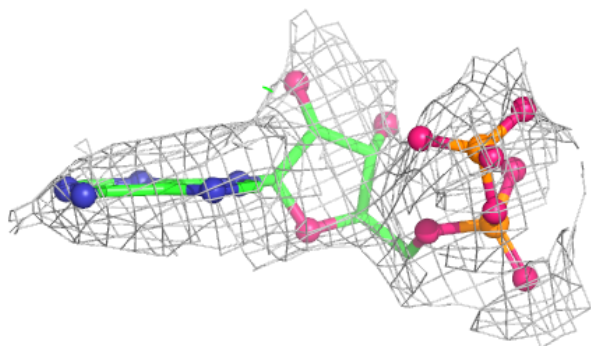
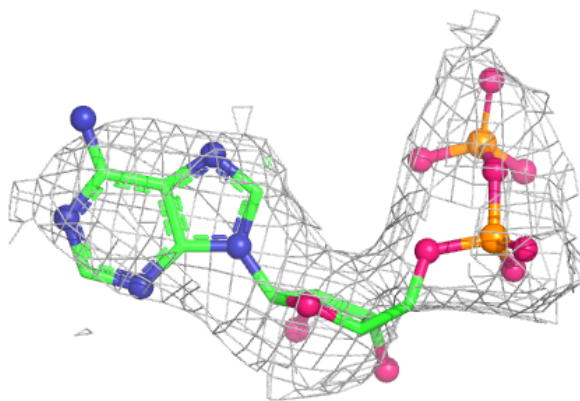
**Electron density around ADP H 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

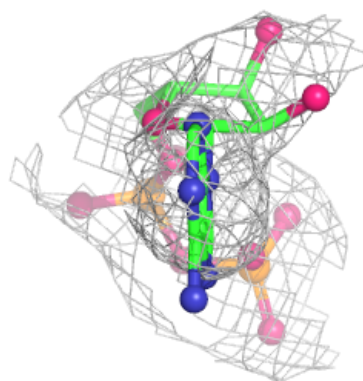
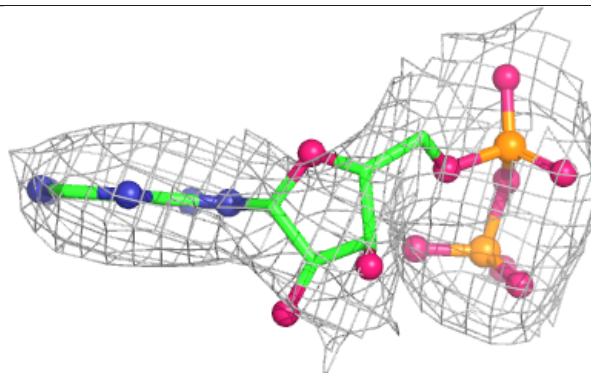
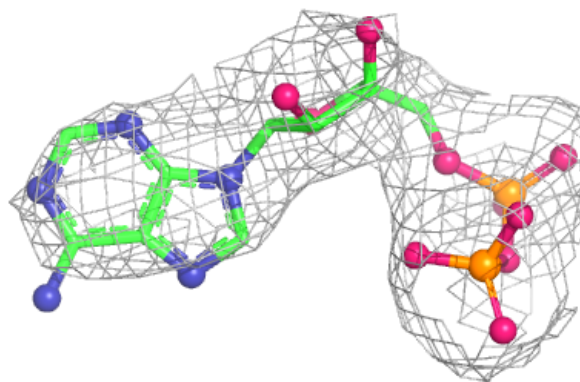


Electron density around ADP I 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

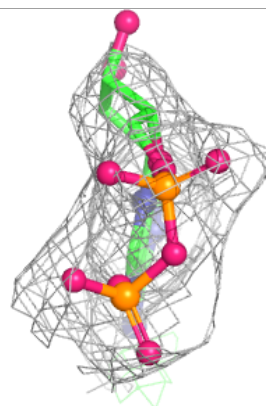
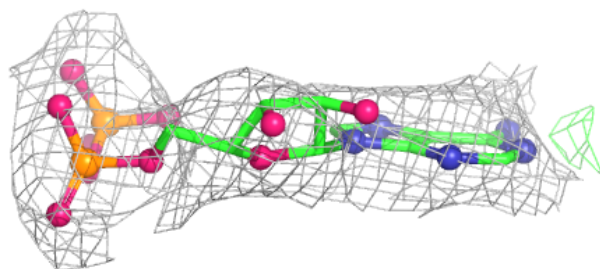
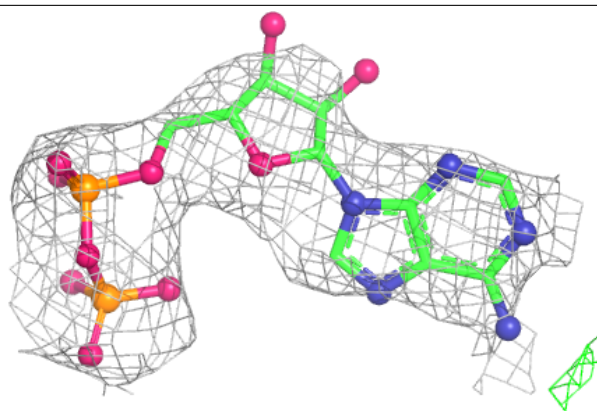
**Electron density around ADP D 601:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

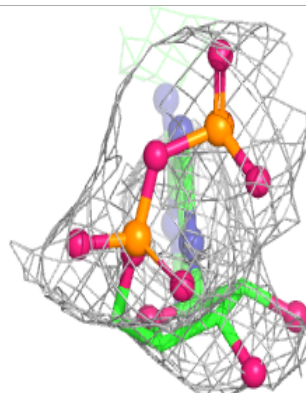
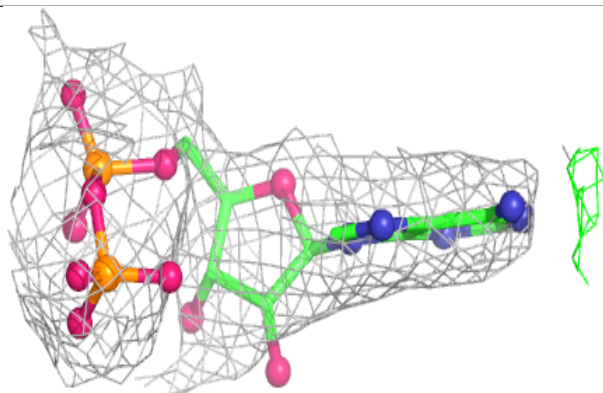
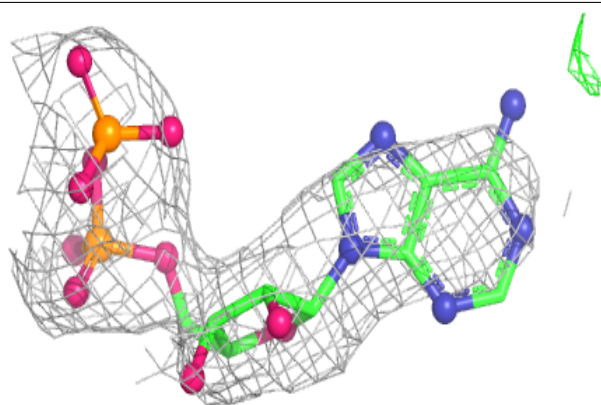


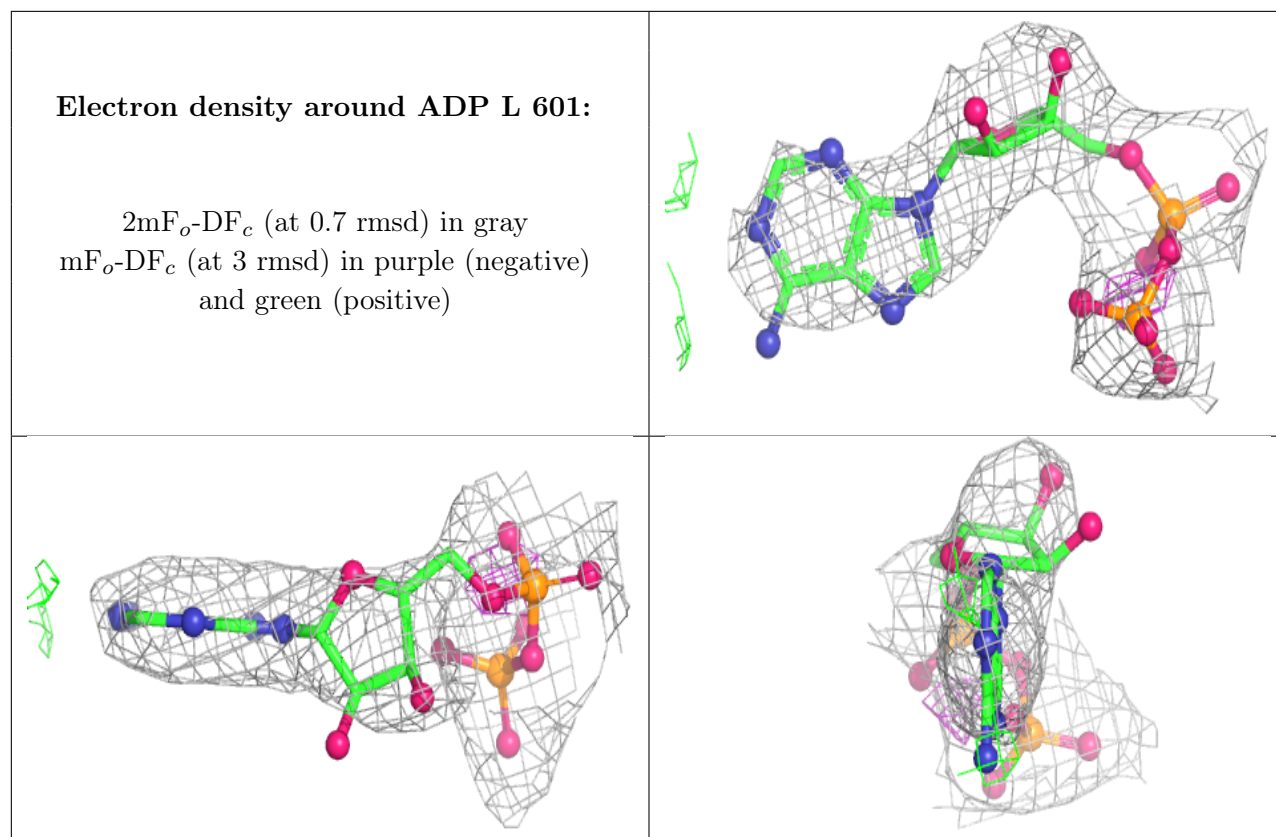
Electron density around ADP A 601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP G 601:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.