



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:26 PM UTC

PDB ID : 6DHK / pdb_00006dhk
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

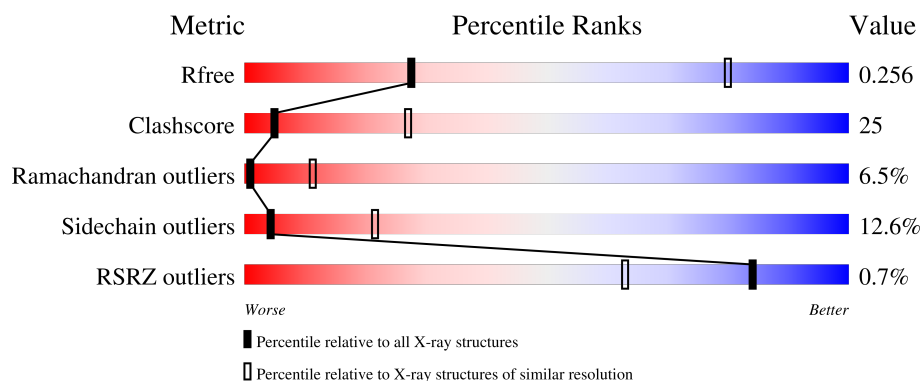
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	
1	B	496	
1	C	496	
1	D	496	
1	E	496	

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Mol	Chain	Length	Quality of chain
1	F	496	53% 33% 9% 5%
1	G	496	% 54% 32% 9% 5%
1	H	496	55% 31% 9% 5%
1	I	496	% 48% 34% 11% 6%
1	J	496	% 54% 32% 9% 6%
1	K	496	% 50% 34% 11% 5%
1	L	496	% 52% 31% 11% 6%

2 Entry composition

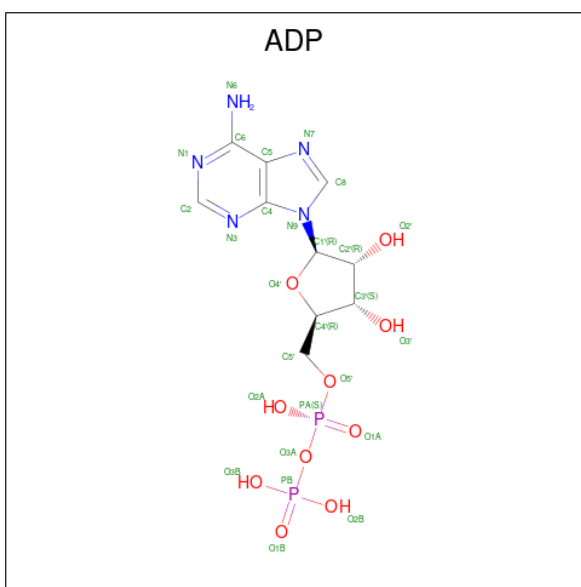
There are 2 unique types of molecules in this entry. The entry contains 46824 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

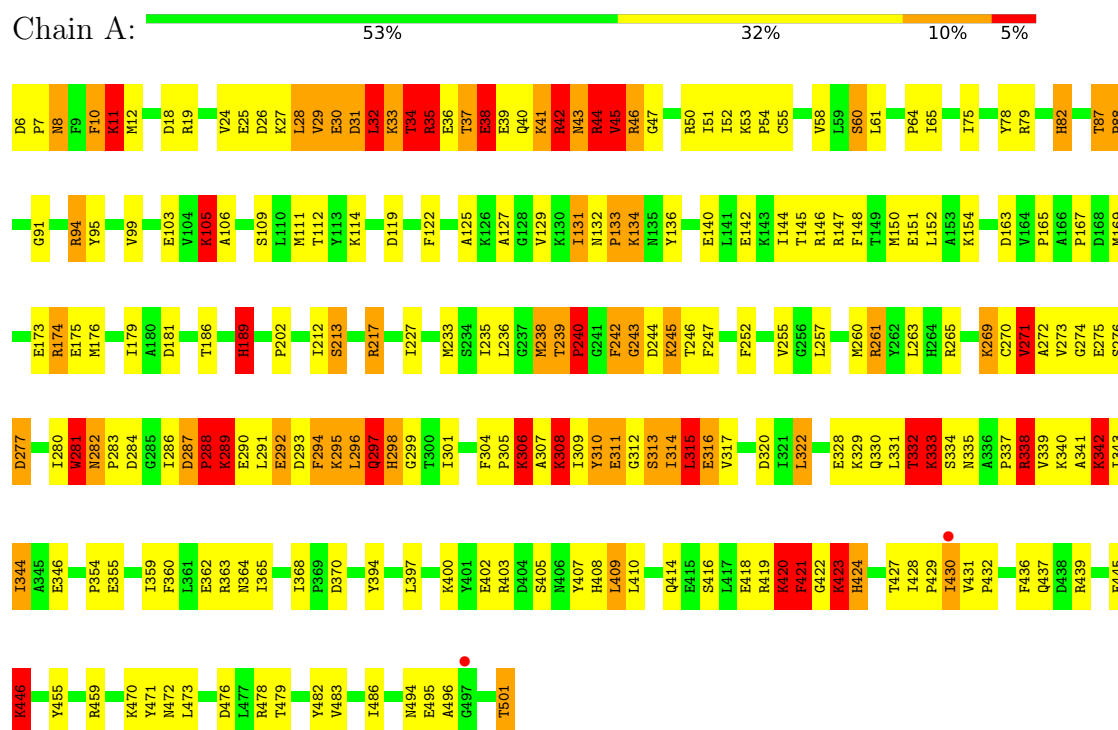


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	G	1	Total 27	C 10	N 5	O 10	P 2	0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

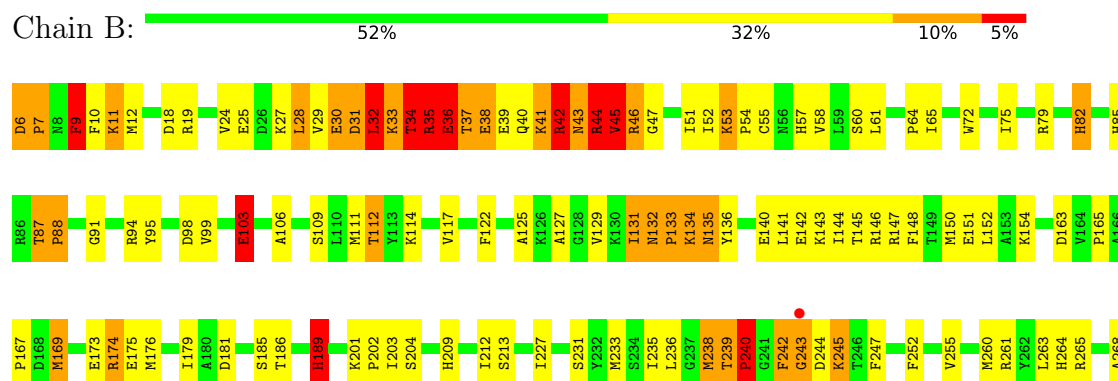
3 Residue-property plots

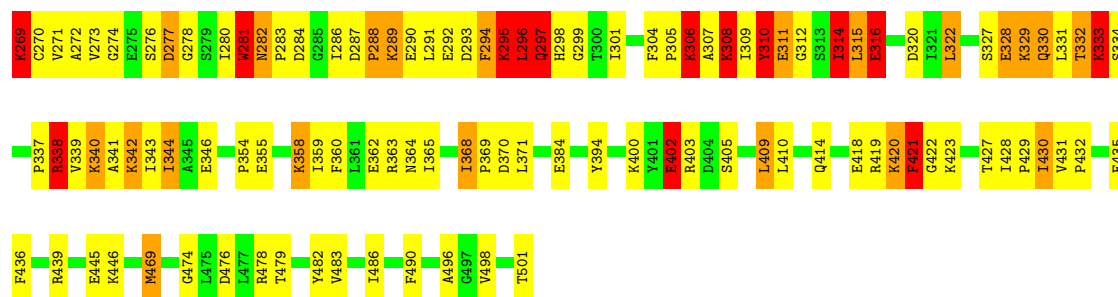
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

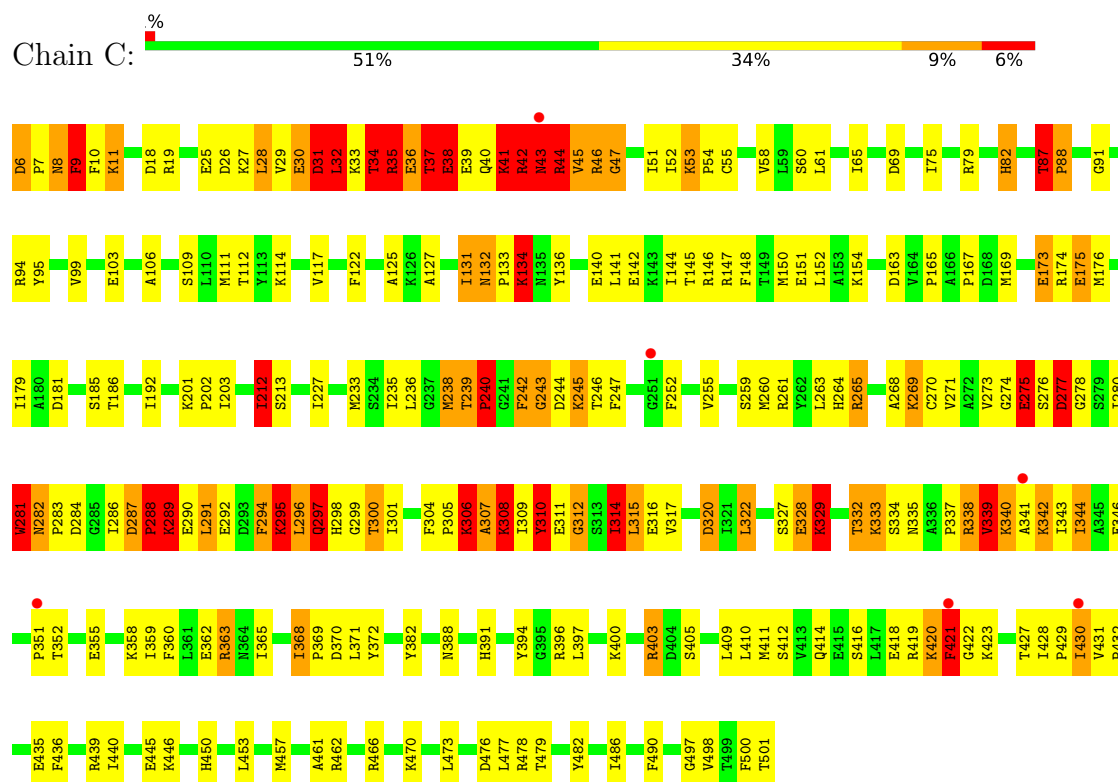


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial

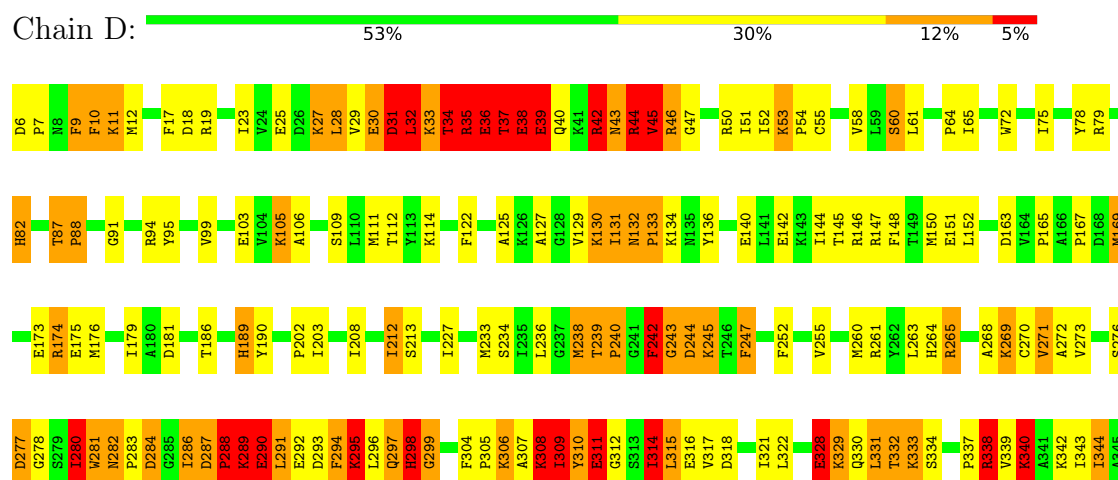


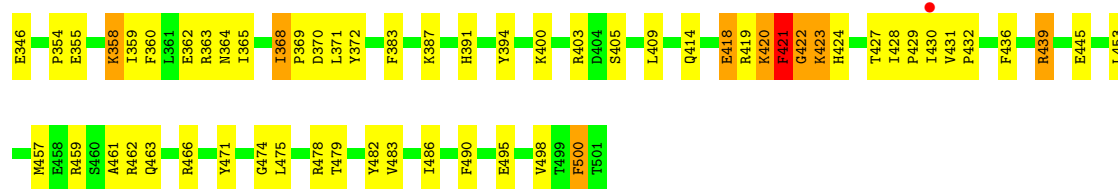


- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



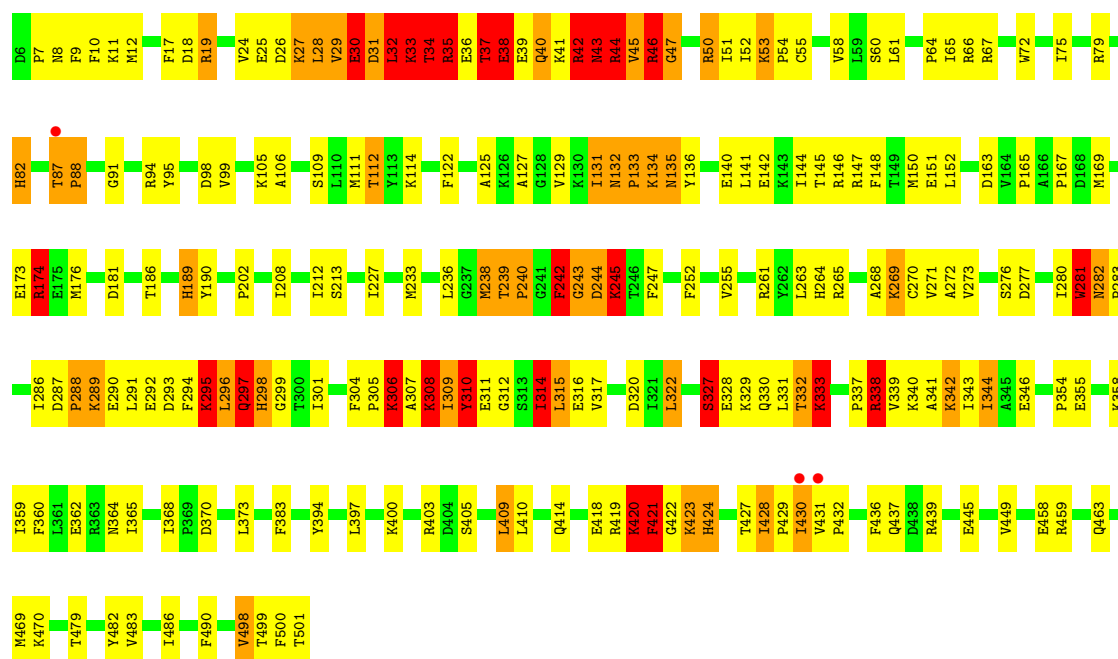
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



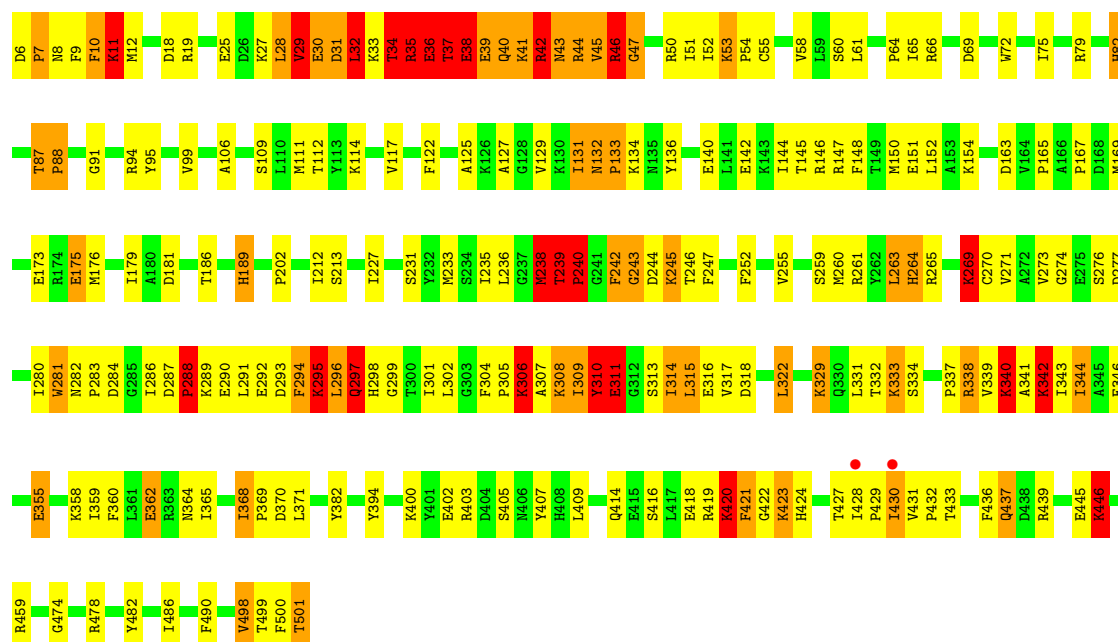




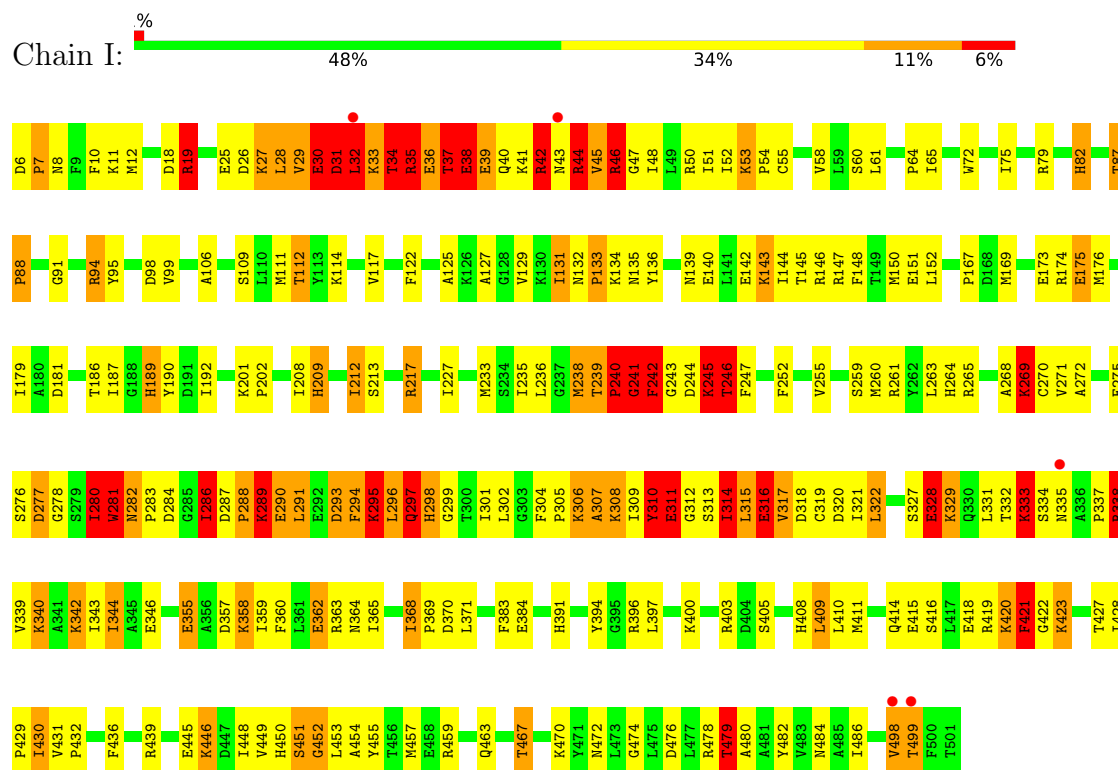
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



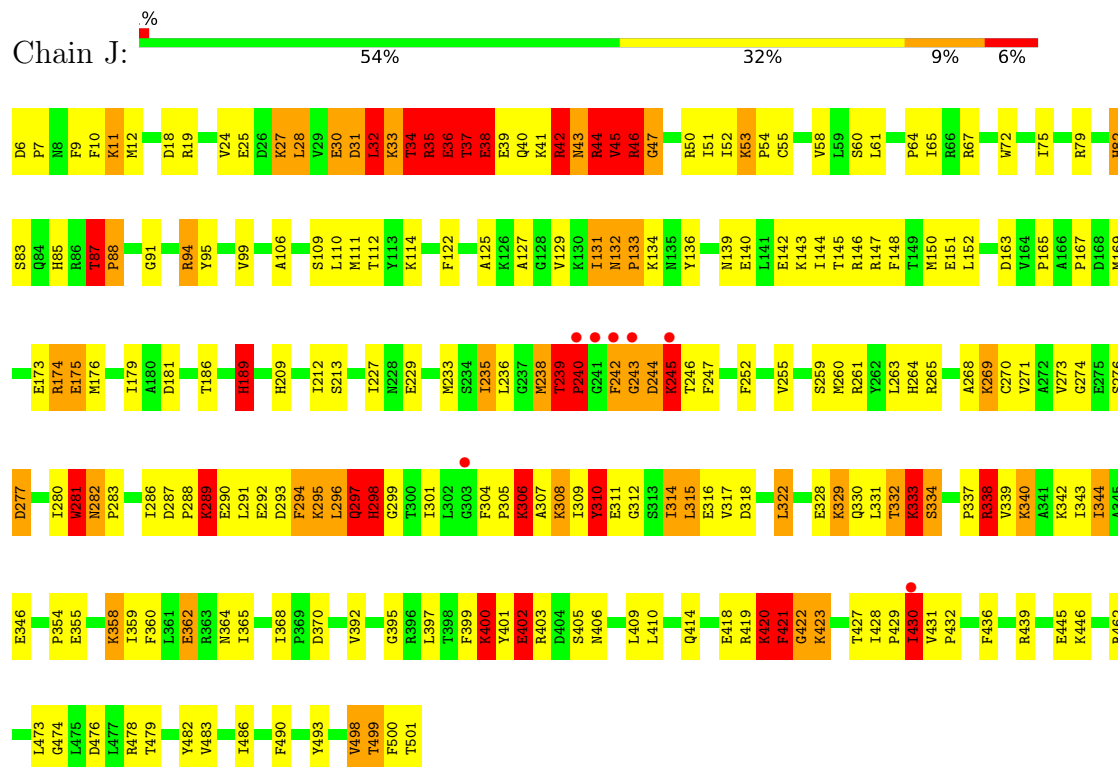
• Molecule 1: Glutamate dehydrogenase 1, mitochondrial



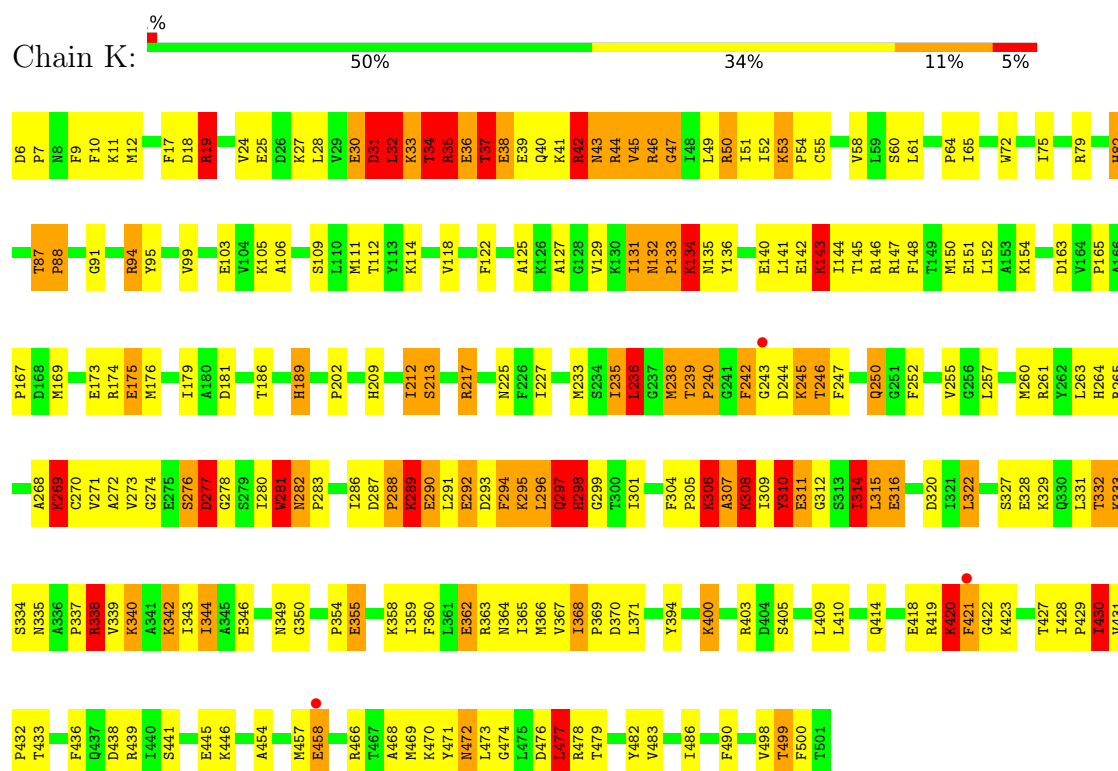
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



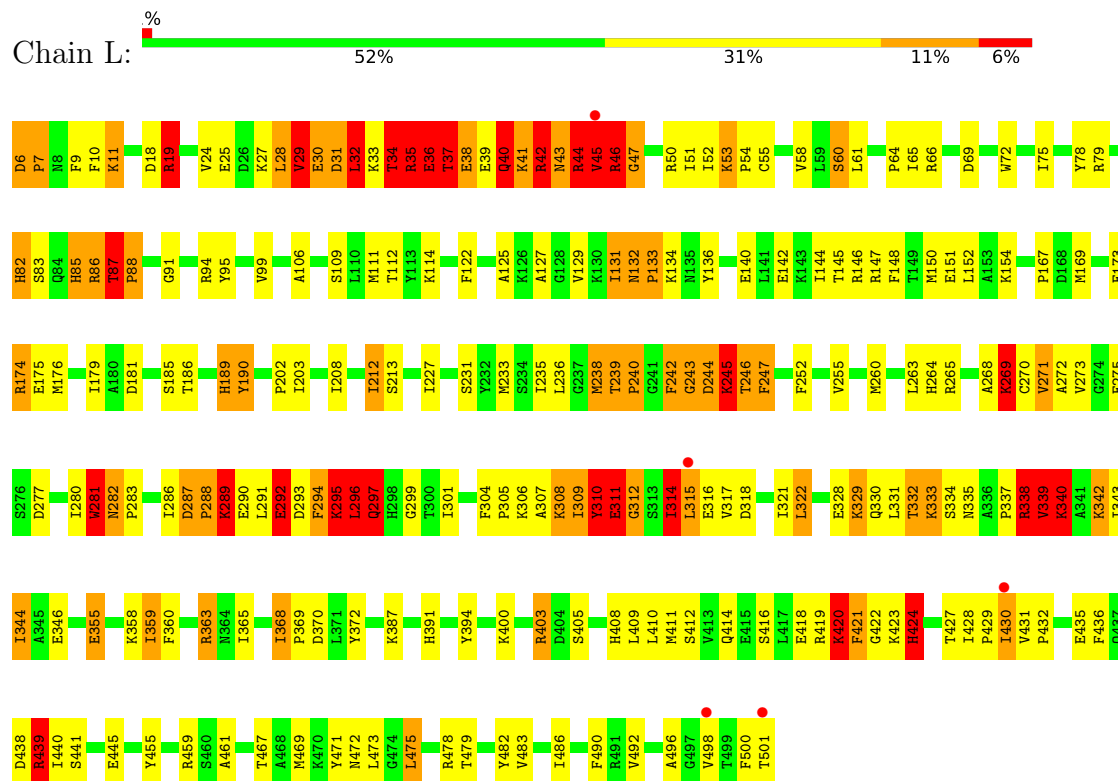
- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



- Molecule 1: Glutamate dehydrogenase 1, mitochondrial



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 29.93 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.93-3.50) 93.8 (29.93-3.50)	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 , 57.9	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	1.21	42/3958 (1.1%)	1.72	100/5341 (1.9%)
1	B	1.17	41/3958 (1.0%)	1.64	111/5341 (2.1%)
1	C	1.17	35/3958 (0.9%)	1.61	102/5341 (1.9%)
1	D	1.31	46/3958 (1.2%)	1.70	104/5341 (1.9%)
1	E	1.19	48/3958 (1.2%)	1.66	102/5341 (1.9%)
1	F	1.11	28/3958 (0.7%)	1.55	89/5341 (1.7%)
1	G	1.21	43/3958 (1.1%)	1.75	120/5341 (2.2%)
1	H	1.26	41/3958 (1.0%)	1.64	100/5341 (1.9%)
1	I	1.28	43/3958 (1.1%)	1.74	125/5341 (2.3%)
1	J	1.11	39/3958 (1.0%)	1.63	95/5341 (1.8%)
1	K	1.19	38/3958 (1.0%)	1.70	118/5341 (2.2%)
1	L	1.23	43/3958 (1.1%)	1.73	101/5341 (1.9%)
All	All	1.21	487/47496 (1.0%)	1.67	1267/64092 (2.0%)

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 (487) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	35	ARG	CD-NE	-21.09	1.16	1.46
1	C	35	ARG	CD-NE	-19.26	1.19	1.46
1	H	298	HIS	CG-ND1	17.90	1.57	1.38
1	A	35	ARG	CZ-NH2	-17.79	1.10	1.33
1	K	35	ARG	CD-NE	-17.74	1.21	1.46
1	E	261	ARG	CZ-NH1	-17.72	1.07	1.32
1	I	35	ARG	CZ-NH2	-17.52	1.10	1.33
1	K	35	ARG	CZ-NH2	-17.38	1.10	1.33
1	G	35	ARG	CD-NE	-17.17	1.22	1.46
1	H	298	HIS	ND1-CE1	-17.04	1.15	1.32
1	F	35	ARG	CZ-NH2	-16.67	1.11	1.33
1	D	280	ILE	CB-CG2	-16.64	0.97	1.52
1	B	35	ARG	CD-NE	-16.56	1.23	1.46
1	L	35	ARG	CD-NE	-16.20	1.23	1.46
1	B	35	ARG	CZ-NH2	-16.16	1.12	1.33
1	D	439	ARG	CZ-NH1	-15.94	1.10	1.32
1	A	35	ARG	CD-NE	-15.20	1.25	1.46
1	H	35	ARG	CD-NE	-14.96	1.25	1.46
1	D	35	ARG	CD-NE	-14.81	1.25	1.46
1	L	363	ARG	CZ-NH1	-14.68	1.12	1.32
1	L	265	ARG	CZ-NH1	-14.65	1.12	1.32
1	H	35	ARG	CZ-NH2	-14.54	1.14	1.33
1	C	35	ARG	NE-CZ	-14.30	1.17	1.33
1	D	35	ARG	CZ-NH2	-14.21	1.15	1.33
1	E	35	ARG	CD-NE	-14.09	1.26	1.46
1	I	35	ARG	CD-NE	-14.03	1.26	1.46
1	K	34	THR	CB-CG2	-13.85	1.06	1.52
1	D	291	LEU	CB-CG	-13.74	1.25	1.53
1	J	35	ARG	CD-NE	-13.57	1.27	1.46
1	A	35	ARG	NE-CZ	-13.44	1.18	1.33
1	L	424	HIS	CB-CG	-13.42	1.31	1.50
1	I	35	ARG	NE-CZ	-13.32	1.18	1.33
1	F	35	ARG	NE-CZ	-13.20	1.18	1.33
1	E	265	ARG	CZ-NH1	-13.12	1.14	1.32
1	J	37	THR	CB-CG2	-13.11	1.09	1.52
1	E	37	THR	CB-CG2	-13.07	1.09	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	298	HIS	CE1-NE2	13.06	1.45	1.32
1	A	34	THR	CB-CG2	-13.04	1.09	1.52
1	H	35	ARG	NE-CZ	-13.00	1.18	1.33
1	A	292	GLU	CD-OE1	-12.66	1.01	1.25
1	H	37	THR	CB-CG2	-12.63	1.10	1.52
1	J	35	ARG	CZ-NH2	-12.49	1.17	1.33
1	B	35	ARG	NE-CZ	-12.36	1.19	1.33
1	C	338	ARG	CG-CD	-12.35	1.15	1.52
1	G	42	ARG	CG-CD	-12.15	1.16	1.52
1	K	35	ARG	NE-CZ	-12.08	1.19	1.33
1	D	35	ARG	CB-CG	-12.08	1.16	1.52
1	G	35	ARG	CZ-NH2	-12.01	1.17	1.33
1	D	296	LEU	CG-CD1	-11.82	1.13	1.52
1	I	34	THR	CB-CG2	-11.79	1.13	1.52
1	L	424	HIS	CG-ND1	11.64	1.51	1.38
1	F	35	ARG	CB-CG	-11.61	1.17	1.52
1	G	42	ARG	CB-CG	-11.61	1.17	1.52
1	B	296	LEU	CG-CD2	-11.60	1.14	1.52
1	L	35	ARG	NE-CZ	-11.34	1.20	1.33
1	B	30	GLU	CD-OE1	-11.34	1.03	1.25
1	G	245	LYS	CB-CG	-11.30	1.18	1.52
1	I	328	GLU	CD-OE1	-11.21	1.04	1.25
1	L	297	GLN	CD-OE1	-11.13	1.02	1.23
1	K	297	GLN	CD-OE1	-11.05	1.02	1.23
1	G	35	ARG	NE-CZ	-11.02	1.21	1.33
1	D	314	ILE	CB-CG2	-11.01	1.16	1.52
1	H	340	LYS	CA-C	-11.01	1.41	1.52
1	L	37	THR	CB-CG2	-11.01	1.16	1.52
1	I	35	ARG	CZ-NH1	-11.01	1.17	1.32
1	D	291	LEU	CA-CB	10.99	1.71	1.53
1	D	35	ARG	NE-CZ	-10.90	1.21	1.33
1	F	245	LYS	CG-CD	-10.78	1.20	1.52
1	C	35	ARG	CZ-NH2	-10.69	1.19	1.33
1	B	316	GLU	CD-OE1	-10.60	1.05	1.25
1	I	35	ARG	CB-CG	-10.46	1.21	1.52
1	A	35	ARG	CB-CG	-10.34	1.21	1.52
1	C	41	LYS	CB-CG	-10.27	1.21	1.52
1	H	264	HIS	CG-ND1	-10.17	1.27	1.38
1	E	35	ARG	NE-CZ	-10.10	1.22	1.33
1	G	424	HIS	ND1-CE1	-9.99	1.22	1.32
1	C	338	ARG	CB-CG	-9.87	1.22	1.52
1	J	35	ARG	NE-CZ	-9.85	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	421	PHE	CD1-CE1	-9.67	1.09	1.38
1	L	44	ARG	CG-CD	-9.62	1.23	1.52
1	D	37	THR	CB-CG2	-9.61	1.20	1.52
1	D	296	LEU	CG-CD2	-9.59	1.21	1.52
1	B	42	ARG	CG-CD	-9.52	1.23	1.52
1	L	338	ARG	CB-CG	-9.50	1.24	1.52
1	G	37	THR	CB-CG2	-9.49	1.21	1.52
1	H	308	LYS	CA-C	-9.48	1.41	1.52
1	G	42	ARG	CA-C	-9.34	1.40	1.52
1	D	9	PHE	CA-C	-9.26	1.40	1.52
1	D	290	GLU	C-O	9.18	1.34	1.24
1	H	42	ARG	CA-C	-9.14	1.41	1.52
1	K	44	ARG	CG-CD	-9.14	1.25	1.52
1	K	37	THR	CB-CG2	-9.10	1.22	1.52
1	K	245	LYS	CA-C	-9.08	1.41	1.52
1	K	42	ARG	CG-CD	-9.07	1.25	1.52
1	A	35	ARG	CZ-NH1	-9.03	1.20	1.32
1	G	306	LYS	CB-CG	-8.95	1.25	1.52
1	D	265	ARG	CZ-NH1	-8.93	1.20	1.32
1	C	35	ARG	CZ-NH1	-8.88	1.20	1.32
1	F	37	THR	CB-CG2	-8.85	1.23	1.52
1	D	291	LEU	CG-CD2	8.80	1.81	1.52
1	C	338	ARG	CA-C	-8.79	1.41	1.52
1	C	297	GLN	CD-OE1	-8.74	1.06	1.23
1	B	37	THR	CB-CG2	-8.72	1.23	1.52
1	A	295	LYS	CB-CG	-8.70	1.26	1.52
1	D	42	ARG	CB-CG	-8.65	1.26	1.52
1	I	42	ARG	CB-CG	-8.58	1.26	1.52
1	E	338	ARG	CB-CG	-8.51	1.26	1.52
1	J	44	ARG	CB-CG	-8.46	1.27	1.52
1	F	34	THR	CB-CG2	-8.43	1.24	1.52
1	I	245	LYS	CD-CE	-8.41	1.27	1.52
1	L	35	ARG	CB-CG	-8.38	1.27	1.52
1	A	37	THR	CB-CG2	-8.37	1.25	1.52
1	D	245	LYS	CB-CG	-8.35	1.27	1.52
1	I	44	ARG	CG-CD	-8.34	1.27	1.52
1	G	295	LYS	CB-CG	-8.33	1.27	1.52
1	J	297	GLN	CD-OE1	-8.33	1.07	1.23
1	C	37	THR	CB-CG2	-8.31	1.25	1.52
1	B	103	GLU	CB-CG	-8.27	1.27	1.52
1	L	295	LYS	CG-CD	-8.24	1.27	1.52
1	B	340	LYS	CA-C	-8.20	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	245	LYS	CG-CD	-8.15	1.28	1.52
1	H	245	LYS	CD-CE	-8.14	1.28	1.52
1	L	289	LYS	CB-CG	-8.13	1.28	1.52
1	J	400	LYS	CB-CG	-7.99	1.28	1.52
1	H	298	HIS	CB-CG	-7.92	1.39	1.50
1	L	42	ARG	CG-CD	-7.87	1.28	1.52
1	I	11	LYS	CA-C	-7.86	1.42	1.52
1	H	338	ARG	CB-CG	-7.84	1.28	1.52
1	G	42	ARG	CD-NE	7.78	1.57	1.46
1	C	340	LYS	CB-CG	-7.76	1.29	1.52
1	B	338	ARG	CB-CG	-7.75	1.29	1.52
1	G	306	LYS	CG-CD	-7.74	1.29	1.52
1	G	134	LYS	CB-CG	-7.74	1.29	1.52
1	I	245	LYS	CB-CG	-7.71	1.29	1.52
1	F	42	ARG	CA-C	-7.67	1.43	1.52
1	B	245	LYS	CG-CD	-7.64	1.29	1.52
1	C	245	LYS	CB-CG	-7.62	1.29	1.52
1	D	306	LYS	CB-CG	-7.61	1.29	1.52
1	L	340	LYS	CB-CG	-7.61	1.29	1.52
1	J	265	ARG	CZ-NH1	-7.60	1.22	1.32
1	B	41	LYS	CG-CD	-7.59	1.29	1.52
1	I	42	ARG	CA-C	-7.59	1.42	1.52
1	K	281	TRP	CA-C	7.58	1.61	1.52
1	G	297	GLN	CD-OE1	-7.57	1.09	1.23
1	I	11	LYS	CB-CG	-7.56	1.29	1.52
1	C	342	LYS	CB-CG	-7.55	1.29	1.52
1	A	34	THR	CB-OG1	-7.54	1.31	1.43
1	D	421	PHE	CB-CG	-7.52	1.33	1.50
1	D	308	LYS	CB-CG	-7.51	1.29	1.52
1	H	44	ARG	CG-CD	-7.47	1.30	1.52
1	A	245	LYS	CG-CD	-7.39	1.30	1.52
1	E	42	ARG	CB-CG	-7.37	1.30	1.52
1	E	42	ARG	CG-CD	-7.37	1.30	1.52
1	I	42	ARG	CG-CD	-7.34	1.30	1.52
1	B	306	LYS	CG-CD	-7.33	1.30	1.52
1	J	42	ARG	CA-C	-7.30	1.43	1.52
1	L	36	GLU	CB-CG	-7.28	1.30	1.52
1	E	11	LYS	CB-CG	-7.26	1.30	1.52
1	K	245	LYS	CB-CG	-7.25	1.30	1.52
1	G	245	LYS	CD-CE	-7.21	1.30	1.52
1	B	316	GLU	CD-OE2	-7.19	1.11	1.25
1	J	330	GLN	CB-CG	-7.18	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	338	ARG	CG-CD	-7.16	1.30	1.52
1	E	245	LYS	CG-CD	-7.13	1.31	1.52
1	H	306	LYS	CB-CG	-7.11	1.31	1.52
1	I	282	ASN	CA-C	7.07	1.60	1.53
1	K	245	LYS	CD-CE	-7.07	1.31	1.52
1	A	245	LYS	CD-CE	-7.06	1.31	1.52
1	F	338	ARG	CG-CD	-7.05	1.31	1.52
1	J	421	PHE	N-CA	-7.05	1.37	1.46
1	K	35	ARG	CZ-NH1	-7.05	1.22	1.32
1	D	314	ILE	CA-C	-7.03	1.43	1.53
1	I	11	LYS	CG-CD	-7.03	1.31	1.52
1	K	308	LYS	CB-CG	-7.01	1.31	1.52
1	H	340	LYS	CG-CD	-7.01	1.31	1.52
1	A	338	ARG	CD-NE	-7.00	1.36	1.46
1	E	45	VAL	N-CA	-6.99	1.37	1.46
1	G	269	LYS	CG-CD	-6.96	1.31	1.52
1	A	265	ARG	CZ-NH1	-6.93	1.23	1.32
1	D	31	ASP	CA-C	6.88	1.61	1.52
1	E	340	LYS	CA-C	-6.87	1.43	1.52
1	A	338	ARG	CB-CG	-6.87	1.31	1.52
1	G	308	LYS	CA-C	-6.86	1.44	1.52
1	J	338	ARG	CB-CG	-6.86	1.31	1.52
1	K	42	ARG	CA-C	-6.86	1.43	1.52
1	G	338	ARG	CB-CG	-6.83	1.31	1.52
1	D	338	ARG	CG-CD	-6.82	1.31	1.52
1	I	307	ALA	CA-C	-6.82	1.44	1.52
1	L	338	ARG	CA-C	-6.80	1.43	1.52
1	D	280	ILE	CA-C	-6.79	1.44	1.52
1	D	35	ARG	CZ-NH1	-6.78	1.23	1.32
1	F	281	TRP	CZ3-CH2	6.76	1.57	1.40
1	L	424	HIS	CE1-NE2	6.76	1.39	1.32
1	H	308	LYS	CB-CG	-6.75	1.32	1.52
1	I	37	THR	CB-CG2	-6.75	1.30	1.52
1	J	174	ARG	CG-CD	-6.75	1.32	1.52
1	E	42	ARG	CA-C	-6.74	1.43	1.52
1	B	340	LYS	CE-NZ	-6.73	1.29	1.49
1	L	289	LYS	CG-CD	-6.71	1.32	1.52
1	H	269	LYS	CG-CD	-6.71	1.32	1.52
1	I	33	LYS	CE-NZ	6.70	1.69	1.49
1	K	306	LYS	CB-CG	-6.69	1.32	1.52
1	A	42	ARG	CA-C	-6.69	1.44	1.52
1	J	421	PHE	CA-CB	-6.65	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	330	GLN	CD-OE1	-6.64	1.10	1.23
1	E	245	LYS	CD-CE	-6.64	1.32	1.52
1	F	35	ARG	CA-CB	-6.64	1.42	1.53
1	D	338	ARG	CB-CG	-6.64	1.32	1.52
1	I	35	ARG	CA-CB	-6.64	1.42	1.53
1	H	265	ARG	CZ-NH1	-6.62	1.23	1.32
1	H	27	LYS	CB-CG	-6.61	1.32	1.52
1	A	34	THR	CA-C	6.60	1.61	1.52
1	J	245	LYS	CD-CE	-6.59	1.32	1.52
1	C	11	LYS	CB-CG	-6.58	1.32	1.52
1	C	269	LYS	CG-CD	-6.58	1.32	1.52
1	K	134	LYS	CB-CG	-6.58	1.32	1.52
1	G	333	LYS	CG-CD	-6.58	1.32	1.52
1	B	330	GLN	CB-CG	-6.57	1.32	1.52
1	E	297	GLN	CD-OE1	-6.57	1.11	1.23
1	E	338	ARG	CG-CD	-6.56	1.32	1.52
1	D	340	LYS	CB-CG	-6.54	1.32	1.52
1	I	281	TRP	CA-C	6.53	1.60	1.52
1	G	424	HIS	CG-ND1	6.53	1.45	1.38
1	B	296	LEU	CG-CD1	-6.53	1.31	1.52
1	I	34	THR	CB-OG1	-6.53	1.33	1.43
1	F	308	LYS	CB-CG	-6.51	1.32	1.52
1	G	245	LYS	CA-C	-6.51	1.44	1.52
1	J	340	LYS	CA-C	-6.50	1.44	1.52
1	H	265	ARG	CZ-NH2	-6.49	1.25	1.33
1	J	36	GLU	CB-CG	-6.48	1.33	1.52
1	K	42	ARG	CD-NE	-6.47	1.37	1.46
1	E	338	ARG	CA-C	-6.46	1.44	1.52
1	E	281	TRP	CA-C	6.46	1.60	1.52
1	I	298	HIS	CG-ND1	6.46	1.45	1.38
1	A	308	LYS	CB-CG	-6.45	1.33	1.52
1	H	265	ARG	CB-CG	-6.45	1.33	1.52
1	F	340	LYS	CA-C	-6.44	1.44	1.52
1	I	289	LYS	CG-CD	-6.39	1.33	1.52
1	J	11	LYS	CG-CD	-6.39	1.33	1.52
1	K	250	GLN	CD-OE1	-6.38	1.11	1.23
1	E	269	LYS	CG-CD	-6.38	1.33	1.52
1	H	264	HIS	ND1-CE1	6.38	1.39	1.32
1	J	340	LYS	CG-CD	-6.36	1.33	1.52
1	E	342	LYS	CG-CD	-6.35	1.33	1.52
1	B	37	THR	CB-OG1	-6.34	1.33	1.43
1	D	245	LYS	CA-C	-6.33	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	340	LYS	CA-C	-6.32	1.44	1.52
1	D	9	PHE	CB-CG	-6.29	1.36	1.50
1	B	289	LYS	CG-CD	-6.26	1.33	1.52
1	G	174	ARG	CZ-NH1	-6.26	1.24	1.32
1	E	134	LYS	CG-CD	-6.26	1.33	1.52
1	I	245	LYS	CG-CD	-6.23	1.33	1.52
1	E	424	HIS	CA-CB	-6.21	1.43	1.53
1	C	42	ARG	CG-CD	-6.20	1.33	1.52
1	H	340	LYS	CD-CE	-6.20	1.33	1.52
1	J	44	ARG	CA-C	-6.20	1.44	1.52
1	H	340	LYS	CB-CG	-6.20	1.33	1.52
1	J	289	LYS	CB-CG	-6.19	1.33	1.52
1	L	42	ARG	CA-C	-6.18	1.44	1.52
1	E	174	ARG	CG-CD	-6.18	1.33	1.52
1	A	281	TRP	CA-C	6.17	1.60	1.52
1	J	308	LYS	CA-C	-6.16	1.45	1.52
1	C	269	LYS	CB-CG	-6.16	1.33	1.52
1	H	245	LYS	CB-CG	-6.15	1.33	1.52
1	G	50	ARG	CB-CG	-6.15	1.33	1.52
1	B	35	ARG	CZ-NH1	-6.15	1.24	1.32
1	G	340	LYS	CA-C	-6.14	1.44	1.52
1	K	338	ARG	CG-CD	-6.14	1.34	1.52
1	L	34	THR	CB-CG2	-6.13	1.32	1.52
1	J	46	ARG	CB-CG	-6.12	1.34	1.52
1	I	308	LYS	CA-C	-6.12	1.45	1.52
1	K	420	LYS	CG-CD	-6.11	1.34	1.52
1	D	295	LYS	CB-CG	-6.11	1.34	1.52
1	B	240	PRO	CG-CD	-6.10	1.30	1.50
1	E	35	ARG	CZ-NH1	-6.10	1.24	1.32
1	J	34	THR	CB-CG2	-6.09	1.32	1.52
1	A	316	GLU	CB-CG	-6.09	1.34	1.52
1	A	42	ARG	CB-CG	-6.08	1.34	1.52
1	B	245	LYS	CB-CG	-6.07	1.34	1.52
1	I	27	LYS	CG-CD	-6.04	1.34	1.52
1	J	297	GLN	CB-CG	-6.04	1.34	1.52
1	D	36	GLU	CB-CG	-6.04	1.34	1.52
1	C	295	LYS	CG-CD	-6.02	1.34	1.52
1	B	308	LYS	CB-CG	-6.02	1.34	1.52
1	C	308	LYS	CB-CG	-6.02	1.34	1.52
1	B	42	ARG	CA-C	-6.01	1.44	1.52
1	B	314	ILE	CG1-CD1	-6.01	1.28	1.51
1	I	265	ARG	CZ-NH1	-6.00	1.24	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	ASN	C-N	6.00	1.38	1.33
1	L	424	HIS	CG-CD2	-5.99	1.29	1.35
1	A	46	ARG	CB-CG	-5.99	1.34	1.52
1	E	424	HIS	N-CA	5.99	1.53	1.46
1	C	281	TRP	CA-C	5.98	1.59	1.52
1	G	328	GLU	CD-OE1	-5.98	1.14	1.25
1	A	340	LYS	CB-CG	-5.98	1.34	1.52
1	F	269	LYS	CB-CG	-5.97	1.34	1.52
1	F	340	LYS	CB-CG	-5.96	1.34	1.52
1	E	11	LYS	CA-C	-5.95	1.45	1.52
1	A	298	HIS	CE1-NE2	-5.94	1.26	1.32
1	D	245	LYS	CG-CD	-5.94	1.34	1.52
1	D	291	LEU	CA-C	5.93	1.61	1.52
1	F	306	LYS	CG-CD	-5.93	1.34	1.52
1	I	44	ARG	N-CA	-5.92	1.38	1.46
1	G	338	ARG	CG-CD	-5.91	1.34	1.52
1	D	340	LYS	CG-CD	-5.91	1.34	1.52
1	A	308	LYS	CA-C	-5.90	1.45	1.52
1	H	245	LYS	CA-C	-5.88	1.45	1.52
1	I	298	HIS	ND1-CE1	-5.88	1.26	1.32
1	E	189	HIS	CE1-NE2	-5.87	1.26	1.32
1	G	308	LYS	CG-CD	-5.82	1.34	1.52
1	L	245	LYS	CD-CE	-5.81	1.35	1.52
1	K	308	LYS	CA-C	-5.79	1.45	1.52
1	K	308	LYS	CG-CD	-5.78	1.35	1.52
1	E	297	GLN	CB-CG	-5.76	1.35	1.52
1	E	269	LYS	CB-CG	-5.76	1.35	1.52
1	J	362	GLU	CA-CB	-5.76	1.44	1.53
1	H	306	LYS	CG-CD	-5.72	1.35	1.52
1	I	340	LYS	CD-CE	-5.72	1.35	1.52
1	K	44	ARG	CB-CG	-5.72	1.35	1.52
1	H	11	LYS	CB-CG	-5.71	1.35	1.52
1	K	245	LYS	CE-NZ	-5.70	1.32	1.49
1	D	291	LEU	N-CA	-5.70	1.39	1.46
1	H	19	ARG	CZ-NH2	5.70	1.40	1.33
1	J	421	PHE	CG-CD1	-5.69	1.26	1.38
1	F	308	LYS	CD-CE	-5.68	1.35	1.52
1	A	363	ARG	CG-CD	-5.68	1.35	1.52
1	C	37	THR	CB-OG1	-5.68	1.34	1.43
1	L	424	HIS	CA-CB	5.68	1.63	1.53
1	K	340	LYS	CB-CG	-5.68	1.35	1.52
1	I	289	LYS	CA-C	-5.67	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	240	PRO	CG-CD	-5.67	1.31	1.50
1	E	298	HIS	CE1-NE2	-5.67	1.26	1.32
1	K	53	LYS	CB-CG	-5.67	1.35	1.52
1	F	37	THR	CA-CB	5.67	1.59	1.52
1	C	37	THR	N-CA	-5.66	1.38	1.46
1	G	269	LYS	CB-CG	-5.66	1.35	1.52
1	B	308	LYS	CA-C	-5.65	1.46	1.52
1	G	281	TRP	CA-C	5.65	1.59	1.52
1	J	245	LYS	CG-CD	-5.64	1.35	1.52
1	G	308	LYS	CB-CG	-5.64	1.35	1.52
1	J	281	TRP	CA-C	5.63	1.59	1.52
1	K	338	ARG	CB-CG	-5.61	1.35	1.52
1	H	42	ARG	CG-CD	-5.60	1.35	1.52
1	A	240	PRO	CG-CD	-5.60	1.31	1.50
1	G	44	ARG	CB-CG	-5.59	1.35	1.52
1	C	42	ARG	CA-C	-5.58	1.45	1.52
1	I	297	GLN	CD-OE1	-5.58	1.12	1.23
1	K	50	ARG	CB-CG	-5.58	1.35	1.52
1	G	327	SER	CB-OG	-5.58	1.30	1.42
1	D	42	ARG	CA-C	-5.57	1.45	1.52
1	A	44	ARG	CB-CG	-5.57	1.35	1.52
1	H	264	HIS	CG-CD2	5.57	1.42	1.35
1	G	340	LYS	CB-CG	-5.56	1.35	1.52
1	G	298	HIS	CG-ND1	-5.56	1.32	1.38
1	J	340	LYS	CB-CG	-5.55	1.35	1.52
1	E	174	ARG	CB-CG	-5.55	1.35	1.52
1	A	306	LYS	CD-CE	-5.54	1.35	1.52
1	H	44	ARG	CD-NE	-5.54	1.38	1.46
1	E	295	LYS	CB-CG	-5.54	1.35	1.52
1	E	308	LYS	CG-CD	-5.54	1.35	1.52
1	G	298	HIS	ND1-CE1	5.54	1.38	1.32
1	E	306	LYS	CB-CG	-5.53	1.35	1.52
1	E	308	LYS	CB-CG	-5.52	1.35	1.52
1	F	281	TRP	CA-C	5.51	1.59	1.52
1	B	269	LYS	CB-CG	-5.51	1.35	1.52
1	E	340	LYS	CB-CG	-5.51	1.35	1.52
1	F	34	THR	CB-OG1	-5.51	1.34	1.43
1	J	333	LYS	CB-CG	-5.51	1.35	1.52
1	D	289	LYS	CB-CG	-5.51	1.35	1.52
1	D	27	LYS	CB-CG	-5.50	1.35	1.52
1	L	308	LYS	CA-C	-5.50	1.45	1.52
1	I	41	LYS	CG-CD	-5.49	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	297	GLN	CD-OE1	-5.49	1.13	1.23
1	C	42	ARG	CB-CG	-5.47	1.36	1.52
1	G	27	LYS	CB-CG	-5.47	1.36	1.52
1	G	37	THR	CB-OG1	-5.47	1.34	1.43
1	J	240	PRO	CG-CD	-5.46	1.32	1.50
1	I	282	ASN	C-N	5.45	1.39	1.33
1	K	34	THR	CB-OG1	-5.45	1.35	1.43
1	D	282	ASN	C-N	5.44	1.38	1.33
1	L	269	LYS	CG-CD	-5.44	1.36	1.52
1	F	265	ARG	CZ-NH1	-5.44	1.25	1.32
1	H	240	PRO	CG-CD	-5.44	1.32	1.50
1	I	291	LEU	CB-CG	-5.44	1.42	1.53
1	L	308	LYS	CB-CG	-5.44	1.36	1.52
1	F	340	LYS	CG-CD	-5.43	1.36	1.52
1	K	35	ARG	CB-CG	-5.43	1.36	1.52
1	B	281	TRP	CA-C	5.43	1.59	1.52
1	F	338	ARG	CB-CG	-5.42	1.36	1.52
1	C	245	LYS	CG-CD	-5.42	1.36	1.52
1	L	245	LYS	CA-C	-5.42	1.45	1.52
1	K	44	ARG	CD-NE	-5.42	1.38	1.46
1	B	265	ARG	CZ-NH1	-5.41	1.25	1.32
1	E	240	PRO	CG-CD	-5.41	1.32	1.50
1	K	295	LYS	CG-CD	-5.41	1.36	1.52
1	C	240	PRO	CG-CD	-5.40	1.32	1.50
1	L	27	LYS	CB-CG	-5.40	1.36	1.52
1	H	298	HIS	N-CA	-5.39	1.39	1.46
1	L	424	HIS	N-CA	5.39	1.53	1.46
1	A	282	ASN	CA-C	5.38	1.58	1.53
1	C	9	PHE	CB-CG	-5.37	1.38	1.50
1	L	281	TRP	CA-C	5.37	1.59	1.52
1	L	189	HIS	N-CA	5.37	1.52	1.46
1	L	44	ARG	CB-CG	-5.36	1.36	1.52
1	L	338	ARG	CG-CD	-5.36	1.36	1.52
1	F	297	GLN	CD-OE1	-5.35	1.13	1.23
1	I	44	ARG	CB-CG	-5.35	1.36	1.52
1	B	306	LYS	CB-CG	-5.34	1.36	1.52
1	J	340	LYS	CD-CE	-5.34	1.36	1.52
1	A	282	ASN	C-N	5.34	1.38	1.33
1	E	35	ARG	CB-CG	-5.34	1.36	1.52
1	L	265	ARG	CZ-NH2	-5.33	1.26	1.33
1	C	46	ARG	CB-CG	-5.32	1.36	1.52
1	A	340	LYS	CA-C	-5.31	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	329	LYS	CB-CG	-5.31	1.36	1.52
1	E	265	ARG	CZ-NH2	-5.30	1.26	1.33
1	A	37	THR	CB-OG1	-5.28	1.35	1.43
1	A	289	LYS	CG-CD	-5.28	1.36	1.52
1	E	340	LYS	CD-CE	-5.28	1.36	1.52
1	A	245	LYS	CB-CG	-5.26	1.36	1.52
1	G	295	LYS	CG-CD	-5.26	1.36	1.52
1	L	44	ARG	CA-C	-5.26	1.45	1.52
1	C	245	LYS	CA-C	-5.26	1.46	1.52
1	J	340	LYS	CE-NZ	-5.26	1.33	1.49
1	D	245	LYS	CD-CE	-5.25	1.36	1.52
1	E	27	LYS	CG-CD	-5.25	1.36	1.52
1	I	37	THR	CB-OG1	-5.25	1.35	1.43
1	A	424	HIS	N-CA	5.25	1.52	1.46
1	G	265	ARG	CZ-NH1	-5.25	1.25	1.32
1	A	308	LYS	CD-CE	-5.24	1.36	1.52
1	D	265	ARG	CB-CG	-5.23	1.36	1.52
1	D	297	GLN	CB-CG	-5.23	1.36	1.52
1	E	36	GLU	CB-CG	-5.22	1.36	1.52
1	B	245	LYS	CA-C	-5.21	1.46	1.52
1	K	289	LYS	CG-CD	-5.21	1.36	1.52
1	B	134	LYS	CG-CD	-5.20	1.36	1.52
1	F	35	ARG	CZ-NH1	-5.20	1.25	1.32
1	F	11	LYS	CG-CD	-5.20	1.36	1.52
1	C	289	LYS	CG-CD	-5.19	1.36	1.52
1	B	44	ARG	CZ-NH1	-5.18	1.25	1.32
1	I	408	HIS	ND1-CE1	-5.18	1.27	1.32
1	B	103	GLU	CD-OE2	-5.18	1.15	1.25
1	L	423	LYS	CA-C	-5.16	1.46	1.53
1	A	235	ILE	CG1-CD1	-5.15	1.31	1.51
1	A	297	GLN	CD-OE1	-5.15	1.13	1.23
1	A	340	LYS	CD-CE	-5.15	1.36	1.52
1	J	338	ARG	CG-CD	-5.15	1.36	1.52
1	D	308	LYS	CD-CE	-5.15	1.37	1.52
1	H	263	LEU	CA-C	5.15	1.59	1.52
1	L	35	ARG	CZ-NH2	-5.15	1.26	1.33
1	K	362	GLU	CA-C	-5.14	1.46	1.52
1	A	333	LYS	CB-CG	-5.14	1.37	1.52
1	B	297	GLN	CG-CD	-5.14	1.39	1.52
1	G	35	ARG	CA-CB	-5.14	1.44	1.53
1	B	245	LYS	CD-CE	-5.14	1.37	1.52
1	E	245	LYS	CB-CG	-5.12	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	342	LYS	CA-C	-5.11	1.46	1.52
1	G	66	ARG	CD-NE	-5.11	1.39	1.46
1	K	265	ARG	CZ-NH1	-5.11	1.25	1.32
1	G	342	LYS	CG-CD	-5.11	1.37	1.52
1	E	308	LYS	CA-C	-5.10	1.46	1.52
1	C	291	LEU	CB-CG	-5.10	1.43	1.53
1	K	37	THR	CB-OG1	-5.10	1.35	1.43
1	C	35	ARG	CA-CB	-5.09	1.44	1.53
1	E	36	GLU	CD-OE1	-5.08	1.15	1.25
1	C	314	ILE	CG1-CD1	-5.08	1.31	1.51
1	E	282	ASN	C-N	5.08	1.38	1.33
1	J	35	ARG	CB-CG	-5.07	1.37	1.52
1	I	329	LYS	CA-CB	-5.06	1.47	1.53
1	C	245	LYS	CD-CE	-5.06	1.37	1.52
1	A	41	LYS	CG-CD	-5.05	1.37	1.52
1	D	342	LYS	CG-CD	-5.05	1.37	1.52
1	E	35	ARG	CZ-NH2	-5.05	1.26	1.33
1	J	308	LYS	CG-CD	-5.05	1.37	1.52
1	L	269	LYS	CB-CG	-5.05	1.37	1.52
1	L	245	LYS	CB-CG	-5.04	1.37	1.52
1	J	342	LYS	CG-CD	-5.04	1.37	1.52
1	F	35	ARG	C-O	-5.04	1.17	1.24
1	B	44	ARG	CB-CG	-5.04	1.37	1.52
1	H	296	LEU	CG-CD1	-5.03	1.35	1.52
1	L	11	LYS	CB-CG	-5.03	1.37	1.52
1	C	308	LYS	CG-CD	-5.02	1.37	1.52
1	B	340	LYS	CD-CE	-5.02	1.37	1.52
1	L	41	LYS	CG-CD	-5.02	1.37	1.52
1	E	333	LYS	CB-CG	-5.01	1.37	1.52
1	L	282	ASN	C-N	5.01	1.38	1.33
1	H	342	LYS	CG-CD	-5.01	1.37	1.52

All (1267) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	239	THR	CA-C-N	26.45	152.90	119.84
1	G	239	THR	C-N-CA	26.45	152.90	119.84
1	E	239	THR	CA-C-N	26.38	152.82	119.84
1	E	239	THR	C-N-CA	26.38	152.82	119.84
1	F	239	THR	CA-C-N	26.06	152.41	119.84
1	F	239	THR	C-N-CA	26.06	152.41	119.84
1	B	239	THR	CA-C-N	25.11	151.22	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	THR	C-N-CA	25.11	151.22	119.84
1	I	239	THR	CA-C-N	24.97	151.05	119.84
1	I	239	THR	C-N-CA	24.97	151.05	119.84
1	H	239	THR	CA-C-N	24.73	150.76	119.84
1	H	239	THR	C-N-CA	24.73	150.76	119.84
1	A	35	ARG	CG-CD-NE	-24.61	57.87	112.00
1	C	239	THR	CA-C-N	24.46	150.42	119.84
1	C	239	THR	C-N-CA	24.46	150.42	119.84
1	K	239	THR	CA-C-N	24.44	150.39	119.84
1	K	239	THR	C-N-CA	24.44	150.39	119.84
1	L	35	ARG	CG-CD-NE	-24.27	58.60	112.00
1	A	239	THR	CA-C-N	24.23	150.12	119.84
1	A	239	THR	C-N-CA	24.23	150.12	119.84
1	L	239	THR	CA-C-N	23.49	149.20	119.84
1	L	239	THR	C-N-CA	23.49	149.20	119.84
1	D	239	THR	CA-C-N	23.15	148.78	119.84
1	D	239	THR	C-N-CA	23.15	148.78	119.84
1	L	363	ARG	NE-CZ-NH2	22.75	139.68	119.20
1	J	239	THR	CA-C-N	22.70	148.22	119.84
1	J	239	THR	C-N-CA	22.70	148.22	119.84
1	E	261	ARG	NE-CZ-NH2	22.02	139.01	119.20
1	D	280	ILE	CG1-CB-CG2	-21.45	46.36	110.70
1	A	338	ARG	NE-CZ-NH2	21.11	138.20	119.20
1	G	35	ARG	CA-CB-CG	20.95	156.01	114.10
1	L	35	ARG	NE-CZ-NH2	-20.38	100.86	119.20
1	D	314	ILE	CG1-CB-CG2	-20.32	49.73	110.70
1	D	35	ARG	CG-CD-NE	-20.21	67.55	112.00
1	L	265	ARG	NE-CZ-NH2	19.49	136.74	119.20
1	I	242	PHE	CA-CB-CG	19.14	132.94	113.80
1	D	439	ARG	NE-CZ-NH2	19.07	136.37	119.20
1	D	296	LEU	CD1-CG-CD2	-18.91	69.21	110.80
1	C	35	ARG	CG-CD-NE	-18.32	71.69	112.00
1	F	35	ARG	CG-CD-NE	-18.01	72.38	112.00
1	A	338	ARG	NE-CZ-NH1	-17.97	103.53	121.50
1	E	265	ARG	NE-CZ-NH2	17.84	135.26	119.20
1	I	34	THR	OG1-CB-CG2	-17.62	74.05	109.30
1	J	421	PHE	CB-CG-CD1	-17.19	91.48	120.70
1	G	314	ILE	CG1-CB-CG2	-16.93	59.92	110.70
1	B	296	LEU	CD1-CG-CD2	-16.42	74.67	110.80
1	I	242	PHE	CB-CG-CD1	-16.26	93.06	120.70
1	J	421	PHE	CA-CB-CG	16.09	129.89	113.80
1	A	34	THR	OG1-CB-CG2	-15.88	77.54	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	GLU	CA-CB-CG	15.50	145.10	114.10
1	J	421	PHE	CB-CG-CD2	15.12	146.41	120.70
1	G	105	LYS	CG-CD-CE	14.66	145.02	111.30
1	H	298	HIS	ND1-CG-CD2	-14.49	91.61	106.10
1	B	35	ARG	NE-CZ-NH2	-14.37	106.27	119.20
1	A	30	GLU	CA-CB-CG	14.34	142.77	114.10
1	H	44	ARG	CA-CB-CG	-14.33	85.44	114.10
1	C	41	LYS	CA-CB-CG	14.28	142.66	114.10
1	L	363	ARG	NE-CZ-NH1	-14.06	107.44	121.50
1	K	245	LYS	CG-CD-CE	-14.05	78.98	111.30
1	G	314	ILE	CA-CB-CG1	14.01	134.22	110.40
1	A	338	ARG	CD-NE-CZ	13.99	143.98	124.40
1	C	35	ARG	NE-CZ-NH2	-13.96	106.63	119.20
1	K	308	LYS	CA-CB-CG	13.95	142.00	114.10
1	D	311	GLU	CA-CB-CG	13.75	141.61	114.10
1	F	35	ARG	NE-CZ-NH2	-13.71	106.86	119.20
1	E	46	ARG	CG-CD-NE	13.69	142.12	112.00
1	E	311	GLU	CA-CB-CG	13.64	141.39	114.10
1	G	35	ARG	CD-NE-CZ	-13.56	105.42	124.40
1	F	35	ARG	N-CA-C	13.34	139.22	110.80
1	J	362	GLU	CB-CG-CD	13.26	135.14	112.60
1	C	30	GLU	CA-CB-CG	13.16	140.42	114.10
1	D	245	LYS	CG-CD-CE	-13.06	81.26	111.30
1	K	217	ARG	NE-CZ-NH2	13.04	130.94	119.20
1	B	306	LYS	CA-CB-CG	12.92	139.94	114.10
1	L	424	HIS	N-CA-CB	12.89	132.28	110.49
1	B	340	LYS	CB-CG-CD	-12.88	81.67	111.30
1	L	363	ARG	CG-CD-NE	12.88	140.34	112.00
1	H	35	ARG	CD-NE-CZ	-12.85	106.41	124.40
1	K	53	LYS	CB-CG-CD	12.83	140.81	111.30
1	L	423	LYS	N-CA-C	12.79	125.09	108.34
1	K	328	GLU	CA-CB-CG	12.77	139.64	114.10
1	G	174	ARG	NE-CZ-NH2	12.70	130.63	119.20
1	L	424	HIS	ND1-CE1-NE2	-12.67	95.73	108.40
1	K	269	LYS	CB-CG-CD	-12.65	82.21	111.30
1	I	35	ARG	N-CA-C	12.51	137.45	110.80
1	J	35	ARG	CG-CD-NE	-12.47	84.56	112.00
1	K	217	ARG	NE-CZ-NH1	-12.47	109.03	121.50
1	H	46	ARG	CG-CD-NE	12.40	139.28	112.00
1	I	44	ARG	CA-CB-CG	-12.40	89.30	114.10
1	A	333	LYS	CA-CB-CG	12.39	138.87	114.10
1	I	32	LEU	CA-CB-CG	12.38	159.61	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	35	ARG	N-CA-CB	-12.37	89.59	110.49
1	H	298	HIS	CG-CD2-NE2	12.35	119.55	107.20
1	H	296	LEU	CA-CB-CG	12.33	159.44	116.30
1	K	53	LYS	CA-CB-CG	12.30	138.70	114.10
1	J	333	LYS	CA-CB-CG	12.23	138.56	114.10
1	D	439	ARG	NE-CZ-NH1	-12.21	109.29	121.50
1	H	245	LYS	N-CA-C	12.15	127.59	109.24
1	I	35	ARG	CG-CD-NE	-12.13	85.32	112.00
1	B	134	LYS	CD-CE-NZ	12.07	150.51	111.90
1	K	296	LEU	CA-CB-CG	12.04	158.46	116.30
1	G	245	LYS	N-CA-C	12.03	126.88	108.96
1	G	358	LYS	CD-CE-NZ	12.00	150.29	111.90
1	G	35	ARG	CG-CD-NE	-11.99	85.63	112.00
1	A	420	LYS	CD-CE-NZ	11.99	150.25	111.90
1	J	362	GLU	CA-CB-CG	11.97	138.03	114.10
1	H	35	ARG	CG-CD-NE	-11.94	85.73	112.00
1	E	261	ARG	NE-CZ-NH1	-11.94	109.56	121.50
1	I	242	PHE	CB-CG-CD2	11.89	140.92	120.70
1	D	30	GLU	CA-CB-CG	11.83	137.76	114.10
1	D	265	ARG	NE-CZ-NH2	11.80	129.82	119.20
1	I	33	LYS	N-CA-C	-11.80	95.86	110.61
1	H	35	ARG	N-CA-CB	-11.74	90.64	110.49
1	E	174	ARG	CA-CB-CG	11.68	137.46	114.10
1	F	329	LYS	CA-CB-CG	11.64	137.37	114.10
1	L	363	ARG	CB-CG-CD	-11.60	84.62	111.30
1	B	6	ASP	CA-C-N	11.58	134.32	119.84
1	B	6	ASP	C-N-CA	11.58	134.32	119.84
1	L	308	LYS	CB-CG-CD	-11.56	84.72	111.30
1	J	265	ARG	NE-CZ-NH2	11.52	129.57	119.20
1	G	30	GLU	CA-CB-CG	11.39	136.88	114.10
1	G	42	ARG	NH1-CZ-NH2	-11.30	104.61	119.30
1	F	50	ARG	NE-CZ-NH1	-11.30	110.20	121.50
1	G	245	LYS	CG-CD-CE	-11.27	85.39	111.30
1	A	35	ARG	CA-CB-CG	11.26	136.61	114.10
1	I	50	ARG	NE-CZ-NH1	-11.25	110.25	121.50
1	G	42	ARG	CA-CB-CG	-11.25	91.61	114.10
1	A	245	LYS	N-CA-C	11.24	126.22	109.24
1	G	35	ARG	CB-CG-CD	11.23	137.12	111.30
1	H	35	ARG	NE-CZ-NH2	-11.21	109.11	119.20
1	I	11	LYS	N-CA-C	11.20	125.06	111.40
1	A	35	ARG	N-CA-CB	-11.14	91.66	110.49
1	A	42	ARG	N-CA-C	-11.11	98.40	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	27	LYS	CB-CG-CD	-11.08	85.81	111.30
1	E	32	LEU	CA-CB-CG	11.07	155.05	116.30
1	J	30	GLU	CA-CB-CG	11.06	136.23	114.10
1	H	42	ARG	N-CA-C	-11.04	98.50	113.18
1	G	66	ARG	NE-CZ-NH1	-11.03	110.47	121.50
1	L	29	VAL	N-CA-C	-11.02	102.41	113.10
1	H	306	LYS	CA-CB-CG	11.02	136.13	114.10
1	K	333	LYS	CA-CB-CG	10.98	136.05	114.10
1	F	50	ARG	NE-CZ-NH2	10.97	129.07	119.20
1	B	35	ARG	N-CA-C	10.96	134.15	110.80
1	I	50	ARG	NE-CZ-NH2	10.96	129.06	119.20
1	A	35	ARG	CD-NE-CZ	-10.93	109.10	124.40
1	A	217	ARG	NE-CZ-NH1	-10.90	110.60	121.50
1	K	245	LYS	CD-CE-NZ	10.89	146.74	111.90
1	B	330	GLN	CA-CB-CG	10.84	135.78	114.10
1	K	27	LYS	CB-CG-CD	-10.83	86.38	111.30
1	G	105	LYS	CB-CG-CD	-10.83	86.39	111.30
1	E	37	THR	OG1-CB-CG2	-10.80	87.71	109.30
1	K	217	ARG	CD-NE-CZ	10.80	139.51	124.40
1	D	314	ILE	CA-CB-CG1	10.77	128.70	110.40
1	C	27	LYS	CB-CG-CD	-10.76	86.55	111.30
1	G	423	LYS	N-CA-C	10.72	122.02	108.19
1	B	245	LYS	N-CA-C	10.71	125.83	109.23
1	B	103	GLU	CB-CA-C	-10.70	90.98	110.56
1	I	289	LYS	CB-CG-CD	10.67	135.84	111.30
1	G	66	ARG	NE-CZ-NH2	10.64	128.78	119.20
1	G	358	LYS	CB-CG-CD	-10.61	86.89	111.30
1	L	37	THR	OG1-CB-CG2	-10.60	88.11	109.30
1	K	269	LYS	N-CA-C	10.59	125.68	108.41
1	C	35	ARG	N-CA-C	10.54	133.26	110.80
1	G	27	LYS	CA-CB-CG	10.54	135.18	114.10
1	B	35	ARG	N-CA-CB	-10.47	92.80	110.49
1	A	287	ASP	CA-C-N	10.46	132.92	119.84
1	A	287	ASP	C-N-CA	10.46	132.92	119.84
1	G	42	ARG	CB-CG-CD	10.46	135.37	111.30
1	K	44	ARG	CA-CB-CG	-10.46	93.17	114.10
1	B	35	ARG	CA-CB-CG	10.40	134.90	114.10
1	K	37	THR	OG1-CB-CG2	-10.33	88.64	109.30
1	C	308	LYS	CA-CB-CG	10.30	134.71	114.10
1	A	292	GLU	CG-CD-OE2	10.28	142.04	118.40
1	I	94	ARG	NE-CZ-NH2	10.28	128.45	119.20
1	H	29	VAL	N-CA-C	-10.27	103.14	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	322	LEU	CB-CG-CD2	-10.27	79.90	110.70
1	J	94	ARG	NE-CZ-NH2	10.25	128.42	119.20
1	K	94	ARG	NE-CZ-NH2	10.24	128.42	119.20
1	A	37	THR	OG1-CB-CG2	-10.23	88.85	109.30
1	A	94	ARG	NE-CZ-NH2	10.20	128.38	119.20
1	L	27	LYS	CA-CB-CG	10.17	134.45	114.10
1	C	423	LYS	N-CA-C	10.16	121.30	108.19
1	A	265	ARG	NE-CZ-NH2	10.16	128.35	119.20
1	A	217	ARG	NE-CZ-NH2	10.11	128.30	119.20
1	G	358	LYS	CG-CD-CE	10.11	134.55	111.30
1	F	243	GLY	N-CA-C	-10.06	99.67	115.67
1	B	36	GLU	CA-CB-CG	10.04	134.19	114.10
1	L	40	GLN	CA-CB-CG	9.97	134.04	114.10
1	H	35	ARG	N-CA-C	9.96	132.02	110.80
1	E	35	ARG	N-CA-C	9.95	131.99	110.80
1	K	420	LYS	CB-CG-CD	9.90	134.06	111.30
1	I	423	LYS	N-CA-C	9.89	120.95	108.19
1	H	35	ARG	CA-CB-CG	9.88	133.87	114.10
1	F	37	THR	OG1-CB-CG2	-9.87	89.56	109.30
1	B	169	MET	CG-SD-CE	9.82	122.50	100.90
1	L	287	ASP	CA-C-N	9.82	132.12	119.84
1	L	287	ASP	C-N-CA	9.82	132.12	119.84
1	F	40	GLN	CA-CB-CG	9.81	133.72	114.10
1	K	35	ARG	CG-CD-NE	-9.81	90.42	112.00
1	G	46	ARG	N-CA-C	-9.80	101.33	113.38
1	H	30	GLU	CA-CB-CG	9.76	133.61	114.10
1	B	35	ARG	CB-CG-CD	9.75	133.73	111.30
1	J	423	LYS	N-CA-C	9.72	121.48	108.07
1	D	130	LYS	CD-CE-NZ	9.70	142.94	111.90
1	K	35	ARG	CD-NE-CZ	-9.70	110.83	124.40
1	F	35	ARG	CD-NE-CZ	-9.69	110.84	124.40
1	J	243	GLY	N-CA-C	-9.68	100.28	115.67
1	B	35	ARG	CG-CD-NE	-9.66	90.75	112.00
1	C	243	GLY	N-CA-C	-9.65	100.33	115.67
1	H	37	THR	OG1-CB-CG2	-9.64	90.01	109.30
1	F	34	THR	CA-CB-OG1	9.63	124.05	109.60
1	D	35	ARG	N-CA-C	9.62	131.28	110.80
1	I	242	PHE	N-CA-C	9.61	131.28	110.80
1	B	243	GLY	N-CA-C	-9.60	100.41	115.67
1	E	30	GLU	CA-CB-CG	9.59	133.29	114.10
1	A	423	LYS	CG-CD-CE	9.57	133.32	111.30
1	I	287	ASP	CA-C-N	9.55	131.78	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	287	ASP	C-N-CA	9.55	131.78	119.84
1	J	400	LYS	N-CA-CB	9.55	124.29	110.16
1	C	46	ARG	N-CA-C	-9.54	101.77	113.50
1	K	333	LYS	N-CA-CB	-9.51	94.42	110.49
1	H	46	ARG	N-CA-C	-9.51	101.81	113.50
1	E	11	LYS	CB-CA-C	-9.49	95.90	110.90
1	E	35	ARG	CD-NE-CZ	-9.47	111.14	124.40
1	B	316	GLU	OE1-CD-OE2	-9.45	100.21	122.90
1	J	46	ARG	CG-CD-NE	9.45	132.79	112.00
1	E	35	ARG	CB-CG-CD	9.45	133.02	111.30
1	J	94	ARG	NE-CZ-NH1	-9.44	112.06	121.50
1	F	239	THR	C-N-CD	-9.44	86.30	125.00
1	K	94	ARG	NE-CZ-NH1	-9.44	112.06	121.50
1	I	322	LEU	CA-CB-CG	9.44	149.32	116.30
1	L	289	LYS	CA-CB-CG	9.43	132.97	114.10
1	H	269	LYS	N-CA-C	9.41	124.65	107.99
1	A	94	ARG	NE-CZ-NH1	-9.41	112.09	121.50
1	I	94	ARG	NE-CZ-NH1	-9.40	112.10	121.50
1	C	269	LYS	N-CA-C	9.38	123.69	108.41
1	K	239	THR	C-N-CD	-9.36	86.62	125.00
1	D	423	LYS	N-CA-C	9.34	120.24	108.19
1	G	420	LYS	CB-CG-CD	9.34	132.78	111.30
1	A	35	ARG	N-CA-C	9.32	130.65	110.80
1	K	50	ARG	CA-CB-CG	9.32	132.74	114.10
1	A	243	GLY	N-CA-C	-9.30	99.82	115.08
1	K	42	ARG	CB-CG-CD	-9.28	89.96	111.30
1	G	328	GLU	CA-CB-CG	9.27	132.63	114.10
1	L	424	HIS	CB-CG-ND1	9.26	136.59	122.70
1	I	338	ARG	CB-CG-CD	-9.25	90.02	111.30
1	J	362	GLU	CB-CA-C	-9.24	95.50	110.84
1	J	500	PHE	N-CA-C	-9.21	100.99	112.88
1	B	296	LEU	CA-CB-CG	9.18	148.44	116.30
1	E	169	MET	CG-SD-CE	9.18	121.10	100.90
1	F	38	GLU	N-CA-C	-9.16	96.45	110.10
1	H	298	HIS	CA-CB-CG	9.13	122.93	113.80
1	B	338	ARG	CG-CD-NE	9.13	132.08	112.00
1	E	243	GLY	N-CA-C	-9.12	101.17	115.67
1	J	333	LYS	CB-CA-C	-9.11	92.30	110.42
1	J	37	THR	OG1-CB-CG2	-9.10	91.09	109.30
1	E	29	VAL	N-CA-C	-9.10	104.28	113.47
1	J	400	LYS	CA-CB-CG	9.07	132.24	114.10
1	C	245	LYS	N-CA-C	9.06	122.92	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	ASP	CA-C-N	9.03	131.13	119.84
1	D	287	ASP	C-N-CA	9.03	131.13	119.84
1	G	245	LYS	CD-CE-NZ	9.03	140.78	111.90
1	I	239	THR	C-N-CD	-9.02	88.02	125.00
1	A	289	LYS	N-CA-C	8.99	129.95	110.80
1	G	314	ILE	CA-CB-CG2	-8.98	95.23	110.50
1	G	314	ILE	N-CA-C	-8.98	104.28	112.90
1	K	35	ARG	CB-CG-CD	8.98	131.94	111.30
1	L	35	ARG	N-CA-C	8.97	129.90	110.80
1	L	35	ARG	NH1-CZ-NH2	8.96	130.95	119.30
1	K	134	LYS	CG-CD-CE	8.96	131.90	111.30
1	H	338	ARG	CD-NE-CZ	-8.95	111.87	124.40
1	J	289	LYS	CA-CB-CG	8.95	132.00	114.10
1	E	358	LYS	CD-CE-NZ	8.92	140.44	111.90
1	K	308	LYS	CD-CE-NZ	8.90	140.39	111.90
1	C	342	LYS	CB-CA-C	8.88	123.83	109.27
1	H	311	GLU	CA-CB-CG	8.88	131.85	114.10
1	D	174	ARG	CB-CG-CD	-8.86	90.92	111.30
1	L	243	GLY	N-CA-C	-8.86	101.58	115.67
1	A	235	ILE	CB-CG1-CD1	8.85	132.39	113.80
1	H	306	LYS	CB-CA-C	-8.85	92.81	110.42
1	K	38	GLU	N-CA-C	-8.85	97.24	110.24
1	B	42	ARG	CG-CD-NE	8.84	131.46	112.00
1	B	239	THR	C-N-CD	-8.84	88.78	125.00
1	F	287	ASP	CA-C-N	8.81	130.85	119.84
1	F	287	ASP	C-N-CA	8.81	130.85	119.84
1	H	36	GLU	CA-CB-CG	8.77	131.64	114.10
1	C	239	THR	C-N-CD	-8.77	89.05	125.00
1	J	338	ARG	CG-CD-NE	8.73	131.21	112.00
1	D	130	LYS	CG-CD-CE	8.71	131.33	111.30
1	L	46	ARG	N-CA-C	-8.71	102.66	113.38
1	C	295	LYS	CA-CB-CG	8.70	131.51	114.10
1	C	46	ARG	CG-CD-NE	8.69	131.12	112.00
1	F	32	LEU	CA-CB-CG	8.69	146.70	116.30
1	H	298	HIS	CE1-NE2-CD2	-8.67	100.33	109.00
1	B	30	GLU	CG-CD-OE2	8.66	138.31	118.40
1	J	245	LYS	N-CA-C	8.65	122.58	108.99
1	J	421	PHE	N-CA-C	8.65	129.23	110.80
1	I	33	LYS	CD-CE-NZ	8.63	139.53	111.90
1	K	42	ARG	CG-CD-NE	8.63	130.98	112.00
1	H	243	GLY	N-CA-C	-8.62	101.96	115.67
1	G	243	GLY	N-CA-C	-8.61	101.98	115.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	35	ARG	N-CA-C	8.59	129.10	110.80
1	I	19	ARG	CG-CD-NE	8.59	130.90	112.00
1	C	287	ASP	CA-C-N	8.58	130.56	119.84
1	C	287	ASP	C-N-CA	8.58	130.56	119.84
1	K	287	ASP	CA-C-N	8.57	130.56	119.84
1	K	287	ASP	C-N-CA	8.57	130.56	119.84
1	D	439	ARG	CG-CD-NE	8.56	130.84	112.00
1	F	27	LYS	N-CA-C	-8.56	99.91	110.61
1	D	174	ARG	CG-CD-NE	8.54	130.79	112.00
1	J	35	ARG	N-CA-C	8.54	128.99	110.80
1	B	265	ARG	NE-CZ-NH2	8.54	126.88	119.20
1	I	242	PHE	N-CA-CB	-8.53	96.07	110.49
1	J	400	LYS	CG-CD-CE	8.53	130.93	111.30
1	L	169	MET	CG-SD-CE	8.53	119.66	100.90
1	F	423	LYS	N-CA-C	8.53	119.19	108.19
1	I	19	ARG	CD-NE-CZ	8.52	136.33	124.40
1	G	35	ARG	N-CA-C	8.51	128.92	110.80
1	G	239	THR	C-N-CD	-8.51	90.12	125.00
1	E	446	LYS	CB-CG-CD	-8.50	91.75	111.30
1	C	87	THR	CA-C-N	-8.49	109.22	119.84
1	C	87	THR	C-N-CA	-8.49	109.22	119.84
1	J	27	LYS	CA-CB-CG	8.49	131.09	114.10
1	F	265	ARG	NE-CZ-NH2	8.48	126.83	119.20
1	H	338	ARG	CG-CD-NE	8.47	130.62	112.00
1	L	269	LYS	CB-CA-C	-8.45	96.13	110.16
1	H	239	THR	C-N-CD	-8.45	90.35	125.00
1	D	35	ARG	CD-NE-CZ	-8.45	112.58	124.40
1	C	27	LYS	CA-CB-CG	8.44	130.98	114.10
1	G	42	ARG	NE-CZ-NH2	8.44	126.79	119.20
1	C	38	GLU	N-CA-C	-8.42	97.55	110.10
1	I	38	GLU	N-CA-C	-8.42	97.55	110.10
1	F	245	LYS	N-CA-C	8.41	122.26	109.23
1	I	358	LYS	N-CA-C	8.41	120.07	111.07
1	E	46	ARG	N-CA-C	-8.38	103.07	113.38
1	B	269	LYS	N-CA-C	8.38	122.18	108.52
1	C	340	LYS	CA-CB-CG	8.37	130.84	114.10
1	A	363	ARG	CB-CG-CD	-8.36	92.08	111.30
1	L	87	THR	CA-C-N	-8.36	109.39	119.84
1	L	87	THR	C-N-CA	-8.36	109.39	119.84
1	A	28	LEU	N-CA-C	-8.36	99.53	112.99
1	I	306	LYS	CB-CG-CD	-8.36	92.08	111.30
1	L	424	HIS	ND1-CG-CD2	-8.35	97.75	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	87	THR	CA-C-N	-8.34	109.41	119.84
1	J	87	THR	C-N-CA	-8.34	109.41	119.84
1	A	217	ARG	CD-NE-CZ	8.33	136.06	124.40
1	B	342	LYS	CD-CE-NZ	8.33	138.55	111.90
1	A	239	THR	C-N-CD	-8.33	90.86	125.00
1	H	169	MET	CG-SD-CE	8.33	119.22	100.90
1	G	306	LYS	CA-CB-CG	8.32	130.74	114.10
1	F	269	LYS	N-CA-C	8.31	121.96	108.41
1	C	44	ARG	NE-CZ-NH2	8.31	126.68	119.20
1	C	332	THR	N-CA-C	-8.31	96.79	110.17
1	A	169	MET	CG-SD-CE	8.30	119.16	100.90
1	L	308	LYS	CA-CB-CG	8.30	130.70	114.10
1	L	289	LYS	CB-CA-C	-8.29	93.92	110.42
1	E	306	LYS	CA-CB-CG	8.28	130.67	114.10
1	G	174	ARG	NE-CZ-NH1	-8.28	113.22	121.50
1	C	297	GLN	CA-CB-CG	8.27	130.64	114.10
1	L	269	LYS	N-CA-C	8.27	121.89	108.41
1	C	41	LYS	CB-CA-C	8.27	125.44	111.22
1	L	19	ARG	CG-CD-NE	8.26	130.18	112.00
1	G	424	HIS	N-CA-CB	-8.26	96.53	110.49
1	E	342	LYS	CB-CG-CD	8.26	130.29	111.30
1	I	44	ARG	CG-CD-NE	8.23	130.12	112.00
1	F	35	ARG	CB-CA-C	-8.23	94.04	110.42
1	B	330	GLN	CB-CA-C	8.23	124.46	110.56
1	E	265	ARG	CG-CD-NE	8.22	130.09	112.00
1	G	330	GLN	N-CA-C	-8.22	103.27	113.38
1	G	424	HIS	CE1-NE2-CD2	-8.22	100.78	109.00
1	C	342	LYS	N-CA-C	-8.20	102.50	114.39
1	D	286	ILE	N-CA-C	-8.20	98.24	109.55
1	B	32	LEU	CA-CB-CG	8.19	144.95	116.30
1	D	35	ARG	N-CA-CB	-8.18	96.67	110.49
1	J	38	GLU	N-CA-C	-8.18	98.37	110.23
1	E	287	ASP	CA-C-N	8.17	130.05	119.84
1	E	287	ASP	C-N-CA	8.17	130.05	119.84
1	L	265	ARG	NE-CZ-NH1	-8.17	113.33	121.50
1	B	310	TYR	N-CA-C	-8.17	97.58	109.18
1	C	269	LYS	CD-CE-NZ	-8.16	85.79	111.90
1	E	306	LYS	CB-CG-CD	-8.14	92.57	111.30
1	I	35	ARG	CD-NE-CZ	-8.14	113.00	124.40
1	G	46	ARG	CG-CD-NE	8.14	129.90	112.00
1	A	33	LYS	N-CA-C	-8.12	100.45	110.61
1	E	423	LYS	CA-CB-CG	8.12	130.34	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	GLU	N-CA-CB	8.12	122.77	110.19
1	E	333	LYS	N-CA-CB	-8.11	96.79	110.49
1	I	245	LYS	N-CA-C	8.11	121.48	109.24
1	L	44	ARG	CA-CB-CG	-8.11	97.89	114.10
1	K	143	LYS	CB-CG-CD	8.10	129.92	111.30
1	H	46	ARG	CB-CG-CD	-8.09	92.69	111.30
1	B	287	ASP	CA-C-N	8.09	129.95	119.84
1	B	287	ASP	C-N-CA	8.09	129.95	119.84
1	E	11	LYS	N-CA-C	8.08	119.87	111.14
1	G	333	LYS	N-CA-CB	-8.07	96.85	110.49
1	A	420	LYS	CG-CD-CE	8.07	129.85	111.30
1	E	134	LYS	CB-CG-CD	8.07	129.85	111.30
1	F	310	TYR	N-CA-C	-8.06	97.74	109.18
1	F	269	LYS	CD-CE-NZ	-8.05	86.14	111.90
1	E	42	ARG	CB-CG-CD	8.04	129.80	111.30
1	C	358	LYS	N-CA-C	8.03	120.81	111.02
1	K	143	LYS	CG-CD-CE	8.02	129.75	111.30
1	A	423	LYS	N-CA-C	8.02	119.29	108.23
1	A	292	GLU	CG-CD-OE1	-8.01	99.97	118.40
1	D	169	MET	CG-SD-CE	8.00	118.51	100.90
1	I	235	ILE	CB-CG1-CD1	8.00	130.60	113.80
1	F	308	LYS	CA-CB-CG	8.00	130.09	114.10
1	K	169	MET	CG-SD-CE	7.99	118.48	100.90
1	A	340	LYS	CB-CG-CD	-7.99	92.92	111.30
1	G	327	SER	CA-CB-OG	7.97	127.05	111.10
1	J	306	LYS	CB-CG-CD	-7.97	92.97	111.30
1	K	328	GLU	CB-CG-CD	7.97	126.15	112.60
1	H	340	LYS	CA-CB-CG	7.97	130.03	114.10
1	D	245	LYS	N-CA-C	7.96	121.57	109.23
1	E	134	LYS	CA-CB-CG	-7.96	98.19	114.10
1	E	245	LYS	N-CA-C	7.95	121.48	108.99
1	K	306	LYS	CB-CA-C	-7.95	94.61	110.42
1	F	329	LYS	N-CA-CB	-7.92	100.26	112.30
1	F	42	ARG	N-CA-C	-7.91	105.61	114.62
1	D	174	ARG	CD-NE-CZ	-7.90	113.34	124.40
1	F	42	ARG	CB-CG-CD	-7.88	93.18	111.30
1	I	340	LYS	CB-CG-CD	-7.85	93.24	111.30
1	G	424	HIS	CB-CG-CD2	7.83	141.38	131.20
1	G	287	ASP	CA-C-N	7.82	129.62	119.84
1	G	287	ASP	C-N-CA	7.82	129.62	119.84
1	A	29	VAL	N-CA-C	-7.82	105.40	112.90
1	L	340	LYS	CA-CB-CG	7.81	129.71	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	ARG	N-CA-C	-7.79	102.82	113.18
1	G	105	LYS	CD-CE-NZ	7.79	136.84	111.90
1	B	333	LYS	N-CA-CB	-7.79	97.33	110.49
1	J	46	ARG	N-CA-C	-7.79	103.57	113.23
1	C	295	LYS	CD-CE-NZ	7.78	136.81	111.90
1	E	174	ARG	CB-CG-CD	7.78	129.19	111.30
1	D	297	GLN	CA-CB-CG	-7.78	98.55	114.10
1	A	38	GLU	N-CA-C	-7.76	98.53	110.10
1	I	30	GLU	CB-CG-CD	7.75	125.77	112.60
1	K	27	LYS	CG-CD-CE	7.74	129.10	111.30
1	H	46	ARG	CA-CB-CG	7.73	129.56	114.10
1	B	38	GLU	N-CA-C	-7.72	98.59	110.10
1	G	174	ARG	CG-CD-NE	7.72	128.99	112.00
1	A	42	ARG	NE-CZ-NH2	7.72	126.15	119.20
1	A	46	ARG	N-CA-C	-7.70	103.71	113.72
1	E	329	LYS	CB-CG-CD	-7.69	93.61	111.30
1	D	38	GLU	N-CA-C	-7.68	98.51	109.96
1	H	38	GLU	N-CA-C	-7.68	98.65	110.10
1	L	363	ARG	NH1-CZ-NH2	-7.68	109.31	119.30
1	D	296	LEU	CA-CB-CG	7.68	143.17	116.30
1	B	338	ARG	CD-NE-CZ	-7.67	113.66	124.40
1	K	53	LYS	CA-C-N	-7.67	112.80	120.31
1	K	53	LYS	C-N-CA	-7.67	112.80	120.31
1	K	32	LEU	CA-CB-CG	7.67	143.13	116.30
1	B	37	THR	OG1-CB-CG2	-7.66	93.98	109.30
1	J	329	LYS	CD-CE-NZ	7.66	136.40	111.90
1	D	306	LYS	CA-CB-CG	7.64	129.39	114.10
1	K	290	GLU	N-CA-C	-7.64	101.39	111.24
1	J	27	LYS	CB-CG-CD	-7.62	93.76	111.30
1	J	32	LEU	CA-CB-CG	7.62	142.96	116.30
1	D	36	GLU	CA-CB-CG	7.62	129.33	114.10
1	G	35	ARG	NE-CZ-NH2	-7.61	112.35	119.20
1	G	310	TYR	N-CA-C	-7.61	98.38	109.18
1	A	269	LYS	N-CA-C	7.60	121.32	108.02
1	H	35	ARG	NH1-CZ-NH2	7.60	129.18	119.30
1	H	32	LEU	CA-CB-CG	7.59	142.88	116.30
1	D	314	ILE	CA-CB-CG2	-7.59	97.60	110.50
1	L	239	THR	C-N-CD	-7.58	93.92	125.00
1	J	287	ASP	CA-C-N	7.58	129.31	119.84
1	J	287	ASP	C-N-CA	7.58	129.31	119.84
1	A	42	ARG	NE-CZ-NH1	-7.55	113.95	121.50
1	C	169	MET	CG-SD-CE	7.54	117.49	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	87	THR	CA-C-N	-7.54	110.42	119.84
1	F	87	THR	C-N-CA	-7.54	110.42	119.84
1	G	269	LYS	N-CA-C	7.53	121.20	108.02
1	H	87	THR	CA-C-N	-7.53	110.43	119.84
1	H	87	THR	C-N-CA	-7.53	110.43	119.84
1	K	87	THR	CA-C-N	-7.51	110.45	119.84
1	K	87	THR	C-N-CA	-7.51	110.45	119.84
1	E	239	THR	C-N-CD	-7.50	94.23	125.00
1	D	87	THR	CA-C-N	-7.49	110.48	119.84
1	D	87	THR	C-N-CA	-7.49	110.48	119.84
1	B	295	LYS	CD-CE-NZ	7.48	135.85	111.90
1	I	94	ARG	CD-NE-CZ	7.48	134.88	124.40
1	E	342	LYS	N-CA-C	-7.48	104.69	113.88
1	A	94	ARG	CD-NE-CZ	7.47	134.86	124.40
1	A	292	GLU	CB-CA-C	-7.47	95.56	110.42
1	J	34	THR	OG1-CB-CG2	-7.47	94.37	109.30
1	J	400	LYS	CB-CA-C	-7.44	98.20	110.85
1	J	94	ARG	CD-NE-CZ	7.44	134.81	124.40
1	F	306	LYS	CA-CB-CG	7.43	128.96	114.10
1	J	306	LYS	CD-CE-NZ	7.43	135.67	111.90
1	I	50	ARG	CD-NE-CZ	7.42	134.79	124.40
1	K	94	ARG	CD-NE-CZ	7.42	134.79	124.40
1	G	333	LYS	N-CA-C	7.42	126.60	110.80
1	D	342	LYS	N-CA-C	-7.41	104.49	113.97
1	C	27	LYS	CG-CD-CE	7.40	128.32	111.30
1	J	239	THR	C-N-CD	-7.40	94.67	125.00
1	L	32	LEU	CA-CB-CG	7.39	142.18	116.30
1	D	9	PHE	CB-CA-C	-7.39	98.99	110.81
1	A	87	THR	CA-C-N	-7.38	110.61	119.84
1	A	87	THR	C-N-CA	-7.38	110.61	119.84
1	D	239	THR	C-N-CD	-7.38	94.76	125.00
1	I	286	ILE	N-CA-C	-7.38	97.47	109.12
1	G	295	LYS	CB-CA-C	-7.37	98.51	110.08
1	E	265	ARG	NE-CZ-NH1	-7.36	114.14	121.50
1	L	296	LEU	CD1-CG-CD2	-7.36	94.60	110.80
1	F	50	ARG	CD-NE-CZ	7.36	134.71	124.40
1	I	328	GLU	CG-CD-OE2	7.36	135.33	118.40
1	G	342	LYS	N-CA-C	-7.35	104.56	113.97
1	L	269	LYS	CB-CG-CD	7.35	128.20	111.30
1	E	87	THR	CA-C-N	-7.34	110.66	119.84
1	E	87	THR	C-N-CA	-7.34	110.66	119.84
1	K	329	LYS	CD-CE-NZ	7.34	135.38	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	245	LYS	N-CA-C	7.34	121.29	108.75
1	J	340	LYS	CA-CB-CG	7.33	128.77	114.10
1	G	87	THR	CA-C-N	-7.32	110.69	119.84
1	G	87	THR	C-N-CA	-7.32	110.69	119.84
1	K	245	LYS	N-CA-C	7.30	120.55	109.23
1	B	103	GLU	CA-CB-CG	7.29	128.68	114.10
1	B	296	LEU	CB-CA-C	-7.28	98.76	110.84
1	G	29	VAL	N-CA-C	-7.28	105.92	112.90
1	J	289	LYS	N-CA-C	7.28	126.30	110.80
1	K	308	LYS	CB-CA-C	7.27	122.16	109.80
1	C	338	ARG	CG-CD-NE	-7.27	96.00	112.00
1	F	169	MET	CG-SD-CE	7.27	116.89	100.90
1	A	284	ASP	N-CA-C	-7.26	104.55	113.41
1	J	35	ARG	CD-NE-CZ	-7.25	114.25	124.40
1	A	363	ARG	CA-CB-CG	7.25	128.59	114.10
1	B	42	ARG	CB-CG-CD	-7.24	94.65	111.30
1	B	289	LYS	N-CA-C	7.23	126.21	110.80
1	D	306	LYS	CB-CA-C	-7.22	96.05	110.42
1	G	38	GLU	N-CA-C	-7.22	99.63	110.24
1	B	44	ARG	NE-CZ-NH2	7.21	125.69	119.20
1	L	265	ARG	NH1-CZ-NH2	-7.21	109.92	119.30
1	B	342	LYS	N-CA-C	-7.20	104.75	113.97
1	K	35	ARG	NE-CZ-NH2	-7.18	112.74	119.20
1	B	282	ASN	CA-C-N	-7.17	113.51	120.83
1	B	282	ASN	C-N-CA	-7.17	113.51	120.83
1	F	30	GLU	CA-CB-CG	7.17	128.44	114.10
1	L	275	GLU	CB-CA-C	-7.16	97.61	112.44
1	E	358	LYS	CG-CD-CE	7.16	127.77	111.30
1	F	342	LYS	N-CA-C	-7.15	104.82	113.97
1	I	308	LYS	CA-CB-CG	7.15	128.39	114.10
1	E	27	LYS	CA-CB-CG	7.14	128.38	114.10
1	D	329	LYS	CB-CG-CD	-7.13	94.89	111.30
1	L	289	LYS	N-CA-C	7.13	125.98	110.80
1	I	321	ILE	CA-C-N	-7.12	112.60	122.93
1	I	321	ILE	C-N-CA	-7.12	112.60	122.93
1	D	280	ILE	N-CA-C	7.10	119.45	108.44
1	D	423	LYS	CA-CB-CG	7.10	128.30	114.10
1	I	338	ARG	CG-CD-NE	7.10	127.61	112.00
1	G	34	THR	OG1-CB-CG2	-7.08	95.13	109.30
1	A	261	ARG	N-CA-CB	7.07	120.74	110.20
1	D	174	ARG	N-CA-C	7.07	118.99	111.28
1	I	296	LEU	CA-CB-CG	7.07	141.03	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	LYS	CB-CA-C	-7.06	96.37	110.42
1	L	342	LYS	N-CA-C	-7.06	104.93	113.97
1	K	46	ARG	N-CA-C	-7.06	104.70	113.38
1	J	174	ARG	CG-CD-NE	7.06	127.52	112.00
1	E	174	ARG	N-CA-CB	-7.05	98.57	110.49
1	I	143	LYS	CB-CG-CD	7.04	127.50	111.30
1	G	306	LYS	CB-CA-C	-7.04	96.41	110.42
1	E	261	ARG	CG-CD-NE	7.04	127.49	112.00
1	D	311	GLU	CB-CG-CD	7.04	124.56	112.60
1	H	310	TYR	N-CA-C	-7.04	98.72	109.41
1	D	46	ARG	N-CA-C	-7.03	104.58	113.72
1	F	46	ARG	N-CA-C	-7.03	104.73	113.38
1	K	265	ARG	NE-CZ-NH2	7.03	125.53	119.20
1	G	174	ARG	CB-CG-CD	-7.02	95.15	111.30
1	K	236	LEU	N-CA-C	-7.01	104.73	113.28
1	G	28	LEU	N-CA-C	-7.01	101.71	112.99
1	B	134	LYS	CG-CD-CE	7.00	127.41	111.30
1	H	44	ARG	CB-CG-CD	7.00	127.41	111.30
1	E	296	LEU	CD1-CG-CD2	-7.00	95.40	110.80
1	C	310	TYR	N-CA-C	-6.99	98.78	109.41
1	A	329	LYS	CD-CE-NZ	6.99	134.25	111.90
1	K	34	THR	N-CA-CB	-6.97	98.72	110.49
1	A	105	LYS	CG-CD-CE	-6.95	95.31	111.30
1	H	44	ARG	CG-CD-NE	6.94	127.26	112.00
1	I	32	LEU	CB-CA-C	-6.94	96.62	110.42
1	B	41	LYS	CG-CD-CE	6.93	127.25	111.30
1	I	269	LYS	N-CA-C	6.91	120.22	107.99
1	J	342	LYS	N-CA-C	-6.91	105.13	113.97
1	F	245	LYS	CD-CE-NZ	-6.90	89.82	111.90
1	G	37	THR	CB-CA-C	6.88	124.12	110.42
1	C	306	LYS	CA-CB-CG	6.88	127.86	114.10
1	K	34	THR	OG1-CB-CG2	-6.87	95.57	109.30
1	I	35	ARG	CB-CA-C	-6.86	96.76	110.42
1	J	329	LYS	CA-C-N	-6.86	111.69	122.73
1	J	329	LYS	C-N-CA	-6.86	111.69	122.73
1	D	50	ARG	CD-NE-CZ	6.85	134.00	124.40
1	L	363	ARG	CD-NE-CZ	-6.84	114.82	124.40
1	G	333	LYS	CA-CB-CG	6.84	127.78	114.10
1	L	27	LYS	CB-CG-CD	-6.84	95.57	111.30
1	L	40	GLN	CB-CA-C	6.83	124.01	110.42
1	D	36	GLU	CB-CA-C	-6.80	96.90	110.42
1	G	134	LYS	CG-CD-CE	6.80	126.93	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	287	ASP	CA-C-N	6.80	128.33	119.84
1	H	287	ASP	C-N-CA	6.80	128.33	119.84
1	G	265	ARG	NE-CZ-NH2	6.79	125.31	119.20
1	B	46	ARG	N-CA-C	-6.79	104.89	113.72
1	G	174	ARG	N-CA-C	6.79	118.68	111.28
1	H	35	ARG	CA-C-N	6.79	133.61	120.99
1	H	35	ARG	C-N-CA	6.79	133.61	120.99
1	D	174	ARG	NE-CZ-NH1	-6.78	114.72	121.50
1	H	329	LYS	CB-CG-CD	-6.78	95.71	111.30
1	E	306	LYS	CB-CA-C	-6.78	96.93	110.42
1	F	333	LYS	N-CA-C	6.78	125.23	110.80
1	K	34	THR	CA-CB-CG2	6.77	122.01	110.50
1	G	269	LYS	CA-CB-CG	-6.76	100.58	114.10
1	H	306	LYS	CG-CD-CE	-6.76	95.75	111.30
1	E	11	LYS	CA-CB-CG	6.75	127.61	114.10
1	B	41	LYS	CD-CE-NZ	6.75	133.50	111.90
1	I	310	TYR	N-CA-C	-6.75	99.59	109.18
1	H	311	GLU	N-CA-CB	-6.75	99.08	110.49
1	B	36	GLU	N-CA-CB	-6.73	98.57	110.42
1	E	265	ARG	NH1-CZ-NH2	-6.73	110.55	119.30
1	K	35	ARG	CA-CB-CG	-6.73	100.64	114.10
1	E	27	LYS	N-CA-C	-6.73	102.28	111.56
1	A	289	LYS	CB-CA-C	-6.73	97.03	110.42
1	G	30	GLU	CB-CA-C	-6.72	97.05	110.42
1	G	424	HIS	CG-CD2-NE2	6.72	113.92	107.20
1	K	420	LYS	CD-CE-NZ	6.71	133.39	111.90
1	G	338	ARG	CD-NE-CZ	-6.71	115.01	124.40
1	G	132	ASN	CA-C-N	6.71	128.22	119.84
1	G	132	ASN	C-N-CA	6.71	128.22	119.84
1	H	44	ARG	CD-NE-CZ	-6.70	115.01	124.40
1	G	297	GLN	CB-CG-CD	6.70	123.98	112.60
1	C	296	LEU	CA-CB-CG	6.69	139.71	116.30
1	A	42	ARG	CD-NE-CZ	-6.68	115.05	124.40
1	E	269	LYS	N-CA-C	6.68	119.91	108.02
1	I	169	MET	CG-SD-CE	6.68	115.59	100.90
1	G	245	LYS	CB-CA-C	-6.68	95.94	111.09
1	E	32	LEU	CB-CG-CD2	-6.67	90.67	110.70
1	G	169	MET	CG-SD-CE	6.67	115.58	100.90
1	E	245	LYS	CD-CE-NZ	-6.67	90.56	111.90
1	D	333	LYS	N-CA-C	6.67	125.00	110.80
1	F	27	LYS	CA-CB-CG	6.67	127.43	114.10
1	B	402	GLU	CA-CB-CG	6.66	127.43	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	34	THR	OG1-CB-CG2	-6.66	95.99	109.30
1	I	143	LYS	CG-CD-CE	6.65	126.60	111.30
1	H	36	GLU	N-CA-CB	-6.65	98.22	110.32
1	B	289	LYS	CB-CA-C	-6.65	97.19	110.42
1	I	11	LYS	CB-CG-CD	6.64	126.58	111.30
1	H	338	ARG	NE-CZ-NH1	-6.64	114.86	121.50
1	K	306	LYS	CA-CB-CG	6.64	127.38	114.10
1	C	41	LYS	CB-CG-CD	-6.62	96.07	111.30
1	L	30	GLU	CA-CB-CG	6.62	127.34	114.10
1	L	338	ARG	CA-CB-CG	-6.62	100.87	114.10
1	K	27	LYS	CA-CB-CG	6.61	127.31	114.10
1	E	311	GLU	CB-CG-CD	6.60	123.82	112.60
1	B	87	THR	CA-C-N	-6.60	111.60	119.84
1	B	87	THR	C-N-CA	-6.60	111.60	119.84
1	I	112	THR	N-CA-C	-6.58	104.19	111.36
1	L	424	HIS	CE1-NE2-CD2	6.58	115.58	109.00
1	G	328	GLU	CB-CG-CD	6.57	123.76	112.60
1	H	340	LYS	CB-CA-C	-6.56	99.61	110.37
1	I	293	ASP	N-CA-C	-6.55	104.07	111.14
1	G	295	LYS	CD-CE-NZ	6.54	132.82	111.90
1	B	112	THR	N-CA-C	-6.53	104.24	111.36
1	I	11	LYS	CA-CB-CG	-6.53	101.05	114.10
1	L	282	ASN	CA-C-N	-6.53	114.17	120.83
1	L	282	ASN	C-N-CA	-6.53	114.17	120.83
1	B	329	LYS	CD-CE-NZ	6.52	132.78	111.90
1	K	308	LYS	N-CA-CB	-6.52	99.88	110.71
1	J	169	MET	CG-SD-CE	6.52	115.24	100.90
1	K	53	LYS	CB-CA-C	-6.52	97.33	110.17
1	C	9	PHE	N-CA-C	6.52	124.68	110.80
1	J	310	TYR	N-CA-C	-6.52	99.51	109.41
1	C	363	ARG	N-CA-C	-6.51	105.32	113.20
1	B	269	LYS	CB-CA-C	-6.51	99.52	110.19
1	K	33	LYS	N-CA-C	-6.48	102.51	110.61
1	E	342	LYS	CG-CD-CE	-6.47	96.41	111.30
1	C	300	THR	N-CA-C	6.46	117.97	108.86
1	F	42	ARG	CD-NE-CZ	-6.45	115.36	124.40
1	G	44	ARG	CB-CG-CD	6.45	126.13	111.30
1	H	340	LYS	CG-CD-CE	-6.45	96.47	111.30
1	G	67	ARG	CD-NE-CZ	-6.44	115.38	124.40
1	A	281	TRP	CB-CG-CD2	6.44	135.81	126.80
1	A	44	ARG	CB-CG-CD	6.44	126.11	111.30
1	G	295	LYS	CA-CB-CG	6.44	126.98	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	330	GLN	CB-CG-CD	6.44	123.54	112.60
1	B	27	LYS	CA-CB-CG	6.44	126.97	114.10
1	C	28	LEU	N-CA-C	-6.44	102.63	112.99
1	I	11	LYS	CB-CA-C	-6.44	99.98	110.79
1	C	339	VAL	N-CA-C	-6.41	96.01	109.34
1	C	284	ASP	N-CA-C	6.40	120.83	112.89
1	K	340	LYS	CG-CD-CE	6.39	126.01	111.30
1	C	246	THR	OG1-CB-CG2	6.39	122.08	109.30
1	F	34	THR	N-CA-CB	-6.38	99.70	110.49
1	I	290	GLU	CB-CA-C	-6.38	101.06	110.95
1	A	235	ILE	CG1-CB-CG2	-6.37	91.58	110.70
1	A	342	LYS	N-CA-C	-6.37	105.81	113.97
1	J	28	LEU	N-CA-C	-6.37	102.74	112.99
1	D	265	ARG	NE-CZ-NH1	-6.37	115.14	121.50
1	K	132	ASN	CA-C-N	6.37	127.80	119.84
1	K	132	ASN	C-N-CA	6.37	127.80	119.84
1	C	132	ASN	CA-C-N	6.36	127.79	119.84
1	C	132	ASN	C-N-CA	6.36	127.79	119.84
1	G	308	LYS	CA-CB-CG	6.36	126.82	114.10
1	F	42	ARG	CA-CB-CG	6.36	126.82	114.10
1	B	306	LYS	CD-CE-NZ	6.36	132.24	111.90
1	C	295	LYS	CB-CA-C	-6.35	100.11	110.08
1	I	245	LYS	CB-CA-C	-6.34	96.11	110.07
1	K	44	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	G	424	HIS	ND1-CE1-NE2	6.34	114.74	108.40
1	G	296	LEU	CA-CB-CG	6.34	138.48	116.30
1	A	292	GLU	N-CA-CB	6.34	121.20	110.49
1	A	245	LYS	CA-CB-CG	-6.33	101.43	114.10
1	B	329	LYS	CB-CA-C	-6.33	100.68	111.26
1	D	28	LEU	N-CA-C	-6.32	102.81	112.99
1	F	296	LEU	CA-CB-CG	6.32	138.43	116.30
1	B	30	GLU	CG-CD-OE1	-6.32	103.86	118.40
1	G	338	ARG	CA-CB-CG	-6.31	101.47	114.10
1	E	333	LYS	CA-CB-CG	6.31	126.73	114.10
1	I	342	LYS	N-CA-C	-6.31	105.90	113.97
1	D	282	ASN	CA-C-N	-6.30	114.40	120.83
1	D	282	ASN	C-N-CA	-6.30	114.40	120.83
1	G	112	THR	N-CA-C	-6.30	104.49	111.36
1	K	430	ILE	N-CA-C	6.30	122.45	109.34
1	E	310	TYR	N-CA-C	-6.30	100.23	109.18
1	D	328	GLU	CA-CB-CG	6.30	126.70	114.10
1	L	329	LYS	CB-CG-CD	-6.30	96.82	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	35	ARG	CB-CG-CD	-6.29	96.82	111.30
1	L	312	GLY	N-CA-C	-6.29	98.26	113.18
1	J	30	GLU	CB-CA-C	-6.29	97.90	110.42
1	C	212	ILE	N-CA-C	6.28	117.06	110.72
1	D	9	PHE	O-C-N	6.27	128.62	122.09
1	G	174	ARG	CD-NE-CZ	-6.27	115.62	124.40
1	I	87	THR	CA-C-N	-6.27	112.01	119.84
1	I	87	THR	C-N-CA	-6.27	112.01	119.84
1	L	308	LYS	N-CA-C	6.27	119.72	109.06
1	L	424	HIS	CG-ND1-CE1	6.25	119.93	109.30
1	K	310	TYR	N-CA-C	-6.24	99.92	109.41
1	B	330	GLN	N-CA-C	-6.24	105.25	112.92
1	H	44	ARG	NE-CZ-NH1	-6.24	115.26	121.50
1	B	333	LYS	CA-CB-CG	6.24	126.57	114.10
1	C	30	GLU	CB-CG-CD	6.23	123.20	112.60
1	K	174	ARG	CB-CG-CD	-6.23	96.96	111.30
1	F	340	LYS	CA-CB-CG	6.22	126.55	114.10
1	L	310	TYR	N-CA-C	-6.22	99.96	109.41
1	H	423	LYS	CA-CB-CG	6.22	126.53	114.10
1	E	311	GLU	N-CA-CB	-6.21	99.99	110.49
1	H	437	GLN	CA-CB-CG	-6.21	101.69	114.10
1	J	423	LYS	CB-CA-C	-6.20	100.16	114.41
1	G	329	LYS	CA-CB-CG	6.20	126.49	114.10
1	C	421	PHE	N-CA-CB	-6.19	100.02	110.49
1	L	329	LYS	CD-CE-NZ	6.19	131.72	111.90
1	K	446	LYS	CB-CG-CD	-6.19	97.06	111.30
1	E	282	ASN	CA-C-N	-6.19	113.58	120.45
1	E	282	ASN	C-N-CA	-6.19	113.58	120.45
1	K	312	GLY	N-CA-C	-6.17	101.48	112.22
1	F	44	ARG	CD-NE-CZ	6.17	133.04	124.40
1	C	275	GLU	CA-CB-CG	6.17	126.44	114.10
1	E	423	LYS	CB-CA-C	-6.17	98.15	110.42
1	C	42	ARG	CA-CB-CG	6.16	126.43	114.10
1	I	28	LEU	N-CA-C	-6.16	103.07	112.99
1	E	38	GLU	N-CA-C	-6.16	101.18	110.24
1	A	296	LEU	CA-CB-CG	6.16	137.86	116.30
1	A	329	LYS	CB-CA-C	-6.16	101.19	111.23
1	C	333	LYS	N-CA-C	6.16	123.91	110.80
1	F	358	LYS	CB-CG-CD	-6.15	97.14	111.30
1	L	36	GLU	CB-CA-C	-6.15	96.73	110.21
1	L	86	ARG	N-CA-CB	6.15	120.24	110.65
1	G	50	ARG	CG-CD-NE	-6.14	98.49	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	LYS	N-CA-C	-6.13	101.29	110.06
1	H	333	LYS	CB-CG-CD	-6.13	97.20	111.30
1	D	245	LYS	CB-CA-C	-6.12	95.96	109.56
1	E	30	GLU	CB-CA-C	-6.10	98.29	110.42
1	H	298	HIS	CB-CG-CD2	6.10	139.13	131.20
1	J	329	LYS	CB-CA-C	-6.10	101.29	111.23
1	J	265	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	I	35	ARG	CA-CB-CG	6.09	126.27	114.10
1	B	284	ASP	N-CA-C	-6.08	104.93	112.90
1	K	28	LEU	N-CA-C	-6.08	103.19	112.99
1	B	9	PHE	N-CA-C	6.08	123.76	110.80
1	J	132	ASN	CA-C-N	6.08	127.44	119.84
1	J	132	ASN	C-N-CA	6.08	127.44	119.84
1	L	333	LYS	N-CA-C	6.08	123.74	110.80
1	F	42	ARG	NE-CZ-NH2	6.07	124.67	119.20
1	E	261	ARG	NH1-CZ-NH2	-6.07	111.41	119.30
1	I	44	ARG	NE-CZ-NH1	-6.06	115.44	121.50
1	I	306	LYS	CD-CE-NZ	6.06	131.29	111.90
1	L	423	LYS	CB-CA-C	-6.05	98.86	113.19
1	C	289	LYS	N-CA-C	6.04	123.67	110.80
1	F	189	HIS	CB-CA-C	-6.04	101.39	110.88
1	F	329	LYS	CB-CA-C	6.04	121.06	111.51
1	J	297	GLN	CB-CG-CD	6.04	122.86	112.60
1	H	46	ARG	CD-NE-CZ	6.02	132.83	124.40
1	J	174	ARG	CA-CB-CG	6.02	126.14	114.10
1	J	296	LEU	CA-CB-CG	6.02	137.37	116.30
1	H	44	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	D	329	LYS	CD-CE-NZ	6.01	131.14	111.90
1	J	308	LYS	CB-CA-C	-6.00	98.38	109.37
1	C	37	THR	OG1-CB-CG2	-6.00	97.29	109.30
1	F	44	ARG	CB-CG-CD	6.00	125.10	111.30
1	K	289	LYS	N-CA-C	6.00	123.58	110.80
1	E	297	GLN	CA-CB-CG	-5.99	102.11	114.10
1	B	368	ILE	CA-C-N	5.99	125.95	119.78
1	B	368	ILE	C-N-CA	5.99	125.95	119.78
1	F	295	LYS	CD-CE-NZ	5.99	131.07	111.90
1	K	329	LYS	CB-CA-C	-5.99	101.60	111.36
1	L	424	HIS	CB-CA-C	-5.99	98.51	110.42
1	I	317	VAL	N-CA-C	-5.98	101.84	109.80
1	E	38	GLU	CA-CB-CG	5.98	126.06	114.10
1	C	35	ARG	NH1-CZ-NH2	5.98	127.07	119.30
1	K	245	LYS	CB-CA-C	-5.97	96.30	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	GLU	N-CA-C	5.97	120.30	112.89
1	F	312	GLY	N-CA-C	-5.97	101.83	112.22
1	A	282	ASN	CA-C-N	-5.97	114.74	120.83
1	A	282	ASN	C-N-CA	-5.97	114.74	120.83
1	D	174	ARG	NE-CZ-NH2	5.97	124.57	119.20
1	I	132	ASN	CA-C-N	5.97	127.30	119.84
1	I	132	ASN	C-N-CA	5.97	127.30	119.84
1	J	265	ARG	CB-CG-CD	-5.97	97.57	111.30
1	E	28	LEU	N-CA-C	-5.97	104.21	112.03
1	F	282	ASN	CA-C-N	-5.97	113.83	120.45
1	F	282	ASN	C-N-CA	-5.97	113.83	120.45
1	F	338	ARG	CG-CD-NE	5.97	125.13	112.00
1	G	368	ILE	CA-C-N	5.97	125.93	119.78
1	G	368	ILE	C-N-CA	5.97	125.93	119.78
1	C	32	LEU	CB-CG-CD1	5.96	128.59	110.70
1	I	308	LYS	CB-CA-C	-5.96	98.46	109.37
1	L	338	ARG	CB-CG-CD	5.96	125.00	111.30
1	H	423	LYS	CB-CA-C	-5.95	98.57	110.42
1	I	246	THR	OG1-CB-CG2	5.95	121.20	109.30
1	C	312	GLY	N-CA-C	-5.95	101.87	112.22
1	K	19	ARG	CD-NE-CZ	-5.95	116.08	124.40
1	E	29	VAL	CG1-CB-CG2	5.94	123.87	110.80
1	J	400	LYS	CD-CE-NZ	5.94	130.91	111.90
1	B	46	ARG	CB-CA-C	5.94	119.52	109.55
1	I	35	ARG	N-CA-CB	-5.93	100.46	110.49
1	E	35	ARG	CG-CD-NE	-5.93	98.96	112.00
1	E	296	LEU	CA-CB-CG	5.92	137.02	116.30
1	J	329	LYS	CB-CG-CD	-5.92	97.68	111.30
1	E	368	ILE	CA-C-N	5.92	125.88	119.78
1	E	368	ILE	C-N-CA	5.92	125.88	119.78
1	I	316	GLU	CB-CG-CD	5.92	122.66	112.60
1	J	35	ARG	NE-CZ-NH2	-5.92	113.87	119.20
1	F	281	TRP	CB-CG-CD2	5.91	135.08	126.80
1	F	368	ILE	CA-C-N	5.91	125.87	119.78
1	F	368	ILE	C-N-CA	5.91	125.87	119.78
1	H	28	LEU	N-CA-C	-5.91	103.47	112.99
1	I	333	LYS	CD-CE-NZ	5.91	130.82	111.90
1	D	298	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	B	174	ARG	CG-CD-NE	5.91	125.00	112.00
1	C	11	LYS	CB-CG-CD	5.91	124.89	111.30
1	A	132	ASN	CA-C-N	5.90	127.22	119.84
1	A	132	ASN	C-N-CA	5.90	127.22	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	368	ILE	CA-C-N	5.90	125.86	119.78
1	D	368	ILE	C-N-CA	5.90	125.86	119.78
1	B	9	PHE	CA-C-N	5.89	130.12	120.63
1	B	9	PHE	C-N-CA	5.89	130.12	120.63
1	E	35	ARG	CA-CB-CG	-5.89	102.31	114.10
1	L	368	ILE	CA-C-N	5.89	125.85	119.78
1	L	368	ILE	C-N-CA	5.89	125.85	119.78
1	B	338	ARG	CA-CB-CG	-5.89	102.32	114.10
1	I	472	ASN	N-CA-CB	-5.89	102.83	112.25
1	A	368	ILE	CA-C-N	5.88	125.84	119.78
1	A	368	ILE	C-N-CA	5.88	125.84	119.78
1	G	40	GLN	CB-CG-CD	-5.88	102.60	112.60
1	D	189	HIS	CB-CA-C	-5.88	101.04	110.79
1	H	245	LYS	CA-CB-CG	-5.88	102.35	114.10
1	H	500	PHE	N-CA-C	-5.88	105.95	114.12
1	J	269	LYS	N-CA-C	5.88	118.30	108.02
1	I	289	LYS	CB-CA-C	-5.87	98.73	110.42
1	B	28	LEU	N-CA-C	-5.87	103.81	113.50
1	F	329	LYS	CG-CD-CE	-5.87	97.80	111.30
1	J	245	LYS	CA-CB-CG	-5.87	102.36	114.10
1	H	329	LYS	CB-CA-C	-5.86	101.80	111.36
1	J	368	ILE	CA-C-N	5.86	125.82	119.78
1	J	368	ILE	C-N-CA	5.86	125.82	119.78
1	L	27	LYS	CD-CE-NZ	5.86	130.66	111.90
1	D	421	PHE	N-CA-CB	-5.86	100.58	110.49
1	H	265	ARG	N-CA-C	5.86	123.28	110.80
1	K	368	ILE	CA-C-N	5.86	125.82	119.78
1	K	368	ILE	C-N-CA	5.86	125.82	119.78
1	F	340	LYS	CB-CA-C	-5.86	98.77	110.42
1	I	209	HIS	CG-CD2-NE2	-5.86	101.34	107.20
1	G	66	ARG	CD-NE-CZ	5.85	132.59	124.40
1	I	333	LYS	CB-CG-CD	-5.84	97.86	111.30
1	H	368	ILE	CA-C-N	5.84	125.80	119.78
1	H	368	ILE	C-N-CA	5.84	125.80	119.78
1	E	423	LYS	N-CA-C	5.84	123.24	110.80
1	L	28	LEU	N-CA-C	-5.84	103.59	112.99
1	H	245	LYS	CG-CD-CE	-5.84	97.87	111.30
1	L	19	ARG	CD-NE-CZ	5.83	132.57	124.40
1	B	132	ASN	CA-C-N	5.83	127.13	119.84
1	B	132	ASN	C-N-CA	5.83	127.13	119.84
1	D	291	LEU	N-CA-CB	5.83	119.63	109.72
1	B	423	LYS	N-CA-C	5.83	123.22	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ARG	NE-CZ-NH1	-5.82	115.68	121.50
1	G	312	GLY	N-CA-C	-5.82	102.09	112.22
1	I	280	ILE	CG1-CB-CG2	-5.82	93.24	110.70
1	E	132	ASN	CA-C-N	5.82	127.11	119.84
1	E	132	ASN	C-N-CA	5.82	127.11	119.84
1	H	132	ASN	CA-C-N	5.82	127.11	119.84
1	H	132	ASN	C-N-CA	5.82	127.11	119.84
1	J	306	LYS	CA-CB-CG	5.82	125.74	114.10
1	G	47	GLY	N-CA-C	-5.82	105.73	112.83
1	F	297	GLN	CB-CG-CD	5.81	122.48	112.60
1	I	368	ILE	CA-C-N	5.80	125.75	119.78
1	I	368	ILE	C-N-CA	5.80	125.75	119.78
1	F	34	THR	N-CA-C	5.80	123.15	110.80
1	E	33	LYS	N-CA-C	-5.79	103.49	110.44
1	I	235	ILE	CG1-CB-CG2	-5.79	93.33	110.70
1	C	368	ILE	CA-C-N	5.79	125.74	119.78
1	C	368	ILE	C-N-CA	5.79	125.74	119.78
1	G	333	LYS	CG-CD-CE	-5.79	97.99	111.30
1	K	27	LYS	CB-CA-C	-5.79	103.93	111.40
1	G	340	LYS	CB-CG-CD	-5.79	98.00	111.30
1	C	291	LEU	N-CA-CB	5.78	119.21	109.78
1	K	298	HIS	ND1-CE1-NE2	-5.77	102.63	108.40
1	H	47	GLY	N-CA-C	-5.77	105.79	112.83
1	I	242	PHE	CG-CD1-CE1	5.77	130.51	120.70
1	F	132	ASN	CA-C-N	5.76	127.04	119.84
1	F	132	ASN	C-N-CA	5.76	127.04	119.84
1	A	245	LYS	CG-CD-CE	-5.76	98.05	111.30
1	L	174	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	D	132	ASN	CA-C-N	5.75	127.03	119.84
1	D	132	ASN	C-N-CA	5.75	127.03	119.84
1	J	312	GLY	N-CA-C	-5.74	102.23	112.22
1	G	308	LYS	CB-CA-C	-5.74	99.05	109.38
1	K	174	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	I	298	HIS	CA-CB-CG	5.73	119.53	113.80
1	D	363	ARG	N-CA-C	-5.73	106.27	113.20
1	F	297	GLN	CA-CB-CG	5.73	125.56	114.10
1	D	289	LYS	N-CA-C	5.72	122.99	110.80
1	B	311	GLU	CA-CB-CG	5.72	125.54	114.10
1	H	265	ARG	CB-CA-C	-5.72	99.04	110.42
1	F	174	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	B	295	LYS	CB-CA-C	-5.71	101.11	110.08
1	L	132	ASN	CA-C-N	5.71	126.98	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	132	ASN	C-N-CA	5.71	126.98	119.84
1	D	423	LYS	CB-CA-C	-5.71	102.05	114.10
1	E	143	LYS	CG-CD-CE	5.71	124.43	111.30
1	I	37	THR	CB-CA-C	5.71	121.78	110.42
1	K	297	GLN	CG-CD-NE2	5.71	124.96	116.40
1	J	282	ASN	CA-C-N	-5.70	114.12	120.45
1	J	282	ASN	C-N-CA	-5.70	114.12	120.45
1	D	329	LYS	CB-CA-C	-5.70	102.08	111.36
1	F	306	LYS	N-CA-CB	-5.70	100.87	110.49
1	C	295	LYS	N-CA-CB	5.69	120.25	110.34
1	J	47	GLY	N-CA-C	-5.69	105.88	112.83
1	J	297	GLN	CG-CD-NE2	5.69	124.94	116.40
1	G	282	ASN	CA-C-N	-5.69	114.13	120.45
1	G	282	ASN	C-N-CA	-5.69	114.13	120.45
1	I	269	LYS	CB-CA-C	-5.69	101.52	110.79
1	L	6	ASP	CA-C-N	5.69	126.95	119.84
1	L	6	ASP	C-N-CA	5.69	126.95	119.84
1	C	47	GLY	N-CA-C	-5.69	105.89	112.83
1	H	264	HIS	CB-CG-ND1	-5.69	114.17	122.70
1	I	37	THR	OG1-CB-CG2	-5.68	97.94	109.30
1	B	35	ARG	NH1-CZ-NH2	5.68	126.68	119.30
1	E	36	GLU	CG-CD-OE1	-5.68	105.34	118.40
1	K	174	ARG	CD-NE-CZ	-5.68	116.45	124.40
1	D	265	ARG	NH1-CZ-NH2	-5.67	111.93	119.30
1	D	311	GLU	N-CA-CB	-5.67	100.91	110.49
1	H	42	ARG	CB-CA-C	-5.67	100.25	110.23
1	C	338	ARG	CB-CG-CD	5.66	124.32	111.30
1	E	47	GLY	N-CA-C	-5.66	105.93	112.83
1	C	282	ASN	CA-C-N	-5.65	114.18	120.45
1	C	282	ASN	C-N-CA	-5.65	114.18	120.45
1	L	47	GLY	N-CA-C	-5.65	105.94	112.83
1	K	282	ASN	CA-C-N	-5.65	114.18	120.45
1	K	282	ASN	C-N-CA	-5.65	114.18	120.45
1	F	330	GLN	N-CA-C	-5.64	106.06	113.17
1	D	42	ARG	N-CA-C	-5.64	98.79	110.80
1	H	46	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	L	53	LYS	CA-C-N	-5.64	114.78	120.31
1	L	53	LYS	C-N-CA	-5.64	114.78	120.31
1	L	311	GLU	CG-CD-OE1	-5.63	105.44	118.40
1	B	11	LYS	CB-CG-CD	-5.63	98.35	111.30
1	B	338	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	C	11	LYS	CB-CA-C	-5.63	100.26	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	50	ARG	CA-CB-CG	5.63	125.35	114.10
1	L	295	LYS	CA-CB-CG	5.63	125.35	114.10
1	D	243	GLY	N-CA-C	-5.62	99.85	113.18
1	B	289	LYS	CG-CD-CE	5.62	124.23	111.30
1	E	329	LYS	CB-CA-C	-5.62	102.20	111.36
1	C	306	LYS	CD-CE-NZ	5.62	129.87	111.90
1	D	245	LYS	CB-CG-CD	5.61	124.21	111.30
1	F	174	ARG	CB-CG-CD	-5.61	98.40	111.30
1	K	289	LYS	CB-CA-C	-5.61	99.26	110.42
1	G	329	LYS	N-CA-C	5.61	119.16	111.54
1	H	269	LYS	CB-CA-C	-5.61	101.65	110.79
1	H	269	LYS	CB-CG-CD	5.61	124.19	111.30
1	L	295	LYS	N-CA-CB	-5.61	101.02	110.49
1	E	29	VAL	CA-C-O	5.60	124.02	118.98
1	I	284	ASP	N-CA-C	5.60	119.83	112.89
1	E	269	LYS	CA-CB-CG	-5.59	102.92	114.10
1	A	10	PHE	CA-C-N	5.59	130.05	120.71
1	A	10	PHE	C-N-CA	5.59	130.05	120.71
1	E	312	GLY	N-CA-C	-5.59	102.50	112.22
1	L	314	ILE	N-CA-C	-5.59	106.35	113.22
1	A	338	ARG	CG-CD-NE	-5.58	99.72	112.00
1	G	189	HIS	CB-CA-C	-5.58	101.52	110.79
1	H	41	LYS	CB-CG-CD	5.58	124.14	111.30
1	I	286	ILE	CA-C-N	-5.58	115.08	122.56
1	I	286	ILE	C-N-CA	-5.58	115.08	122.56
1	J	53	LYS	CA-C-N	-5.58	114.84	120.31
1	J	53	LYS	C-N-CA	-5.58	114.84	120.31
1	D	290	GLU	CA-C-N	-5.57	112.33	121.19
1	D	290	GLU	C-N-CA	-5.57	112.33	121.19
1	B	37	THR	CB-CA-C	5.57	121.51	110.42
1	E	134	LYS	CG-CD-CE	5.57	124.11	111.30
1	L	329	LYS	CB-CA-C	-5.57	102.15	111.23
1	G	421	PHE	N-CA-CB	-5.57	101.08	110.49
1	J	46	ARG	CB-CG-CD	5.57	124.11	111.30
1	H	311	GLU	CB-CG-CD	5.57	122.06	112.60
1	C	342	LYS	N-CA-CB	-5.56	103.64	110.98
1	I	53	LYS	CA-C-N	-5.56	114.86	120.31
1	I	53	LYS	C-N-CA	-5.56	114.86	120.31
1	L	11	LYS	CG-CD-CE	5.56	124.08	111.30
1	E	42	ARG	CA-CB-CG	-5.55	103.00	114.10
1	A	11	LYS	N-CA-C	5.55	118.17	111.40
1	I	479	THR	CA-CB-CG2	-5.54	101.08	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	27	LYS	N-CA-CB	-5.54	103.89	111.65
1	I	189	HIS	CB-CA-C	-5.54	101.59	110.79
1	D	37	THR	OG1-CB-CG2	-5.54	98.22	109.30
1	I	363	ARG	N-CA-C	-5.54	106.50	113.20
1	I	312	GLY	N-CA-C	-5.54	102.59	112.22
1	I	446	LYS	CG-CD-CE	5.53	124.03	111.30
1	B	358	LYS	CB-CG-CD	-5.53	98.58	111.30
1	K	358	LYS	CG-CD-CE	5.53	124.02	111.30
1	A	275	GLU	CB-CG-CD	5.53	122.00	112.60
1	I	340	LYS	CA-CB-CG	5.53	125.16	114.10
1	C	265	ARG	CB-CG-CD	-5.53	98.59	111.30
1	A	261	ARG	CA-CB-CG	5.52	125.15	114.10
1	F	53	LYS	CA-C-N	-5.52	114.90	120.31
1	F	53	LYS	C-N-CA	-5.52	114.90	120.31
1	K	174	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	B	333	LYS	N-CA-C	5.52	122.55	110.80
1	G	340	LYS	CA-CB-CG	5.52	125.13	114.10
1	H	53	LYS	CA-C-N	-5.52	114.90	120.31
1	H	53	LYS	C-N-CA	-5.52	114.90	120.31
1	C	53	LYS	CA-C-N	-5.50	114.92	120.31
1	C	53	LYS	C-N-CA	-5.50	114.92	120.31
1	E	472	ASN	N-CA-CB	-5.50	103.82	112.13
1	H	338	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	J	175	GLU	N-CA-C	-5.50	105.44	111.82
1	L	308	LYS	CG-CD-CE	5.49	123.93	111.30
1	G	42	ARG	NE-CZ-NH1	5.49	126.99	121.50
1	I	30	GLU	CG-CD-OE1	-5.49	105.77	118.40
1	C	338	ARG	CB-CA-C	-5.49	99.50	110.42
1	E	32	LEU	CB-CA-C	-5.48	99.51	110.42
1	I	175	GLU	N-CA-C	-5.48	105.46	111.82
1	B	134	LYS	CB-CG-CD	-5.48	98.69	111.30
1	K	423	LYS	N-CA-C	5.48	122.47	110.80
1	B	143	LYS	CB-CG-CD	5.48	123.90	111.30
1	K	446	LYS	CD-CE-NZ	5.47	129.41	111.90
1	G	53	LYS	CA-C-N	-5.47	114.95	120.31
1	G	53	LYS	C-N-CA	-5.47	114.95	120.31
1	C	37	THR	CB-CA-C	5.47	121.30	110.42
1	I	265	ARG	CB-CG-CD	-5.47	98.72	111.30
1	C	265	ARG	CB-CA-C	-5.46	99.55	110.42
1	C	245	LYS	CB-CA-C	-5.46	98.06	110.07
1	K	340	LYS	CA-CB-CG	5.46	125.02	114.10
1	B	169	MET	CB-CG-SD	5.46	129.07	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	296	LEU	CB-CA-C	-5.45	101.79	110.84
1	I	265	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	L	46	ARG	CG-CD-NE	5.45	123.98	112.00
1	E	112	THR	N-CA-C	-5.44	105.35	111.28
1	C	338	ARG	CA-CB-CG	5.44	124.98	114.10
1	I	297	GLN	CA-CB-CG	5.44	124.98	114.10
1	B	44	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	D	333	LYS	CB-CG-CD	-5.43	98.80	111.30
1	L	174	ARG	CG-CD-NE	5.43	123.95	112.00
1	D	53	LYS	CA-C-N	-5.43	114.99	120.31
1	D	53	LYS	C-N-CA	-5.43	114.99	120.31
1	D	130	LYS	CB-CG-CD	-5.43	98.80	111.30
1	J	338	ARG	CD-NE-CZ	-5.43	116.80	124.40
1	A	265	ARG	CB-CG-CD	-5.43	98.81	111.30
1	C	8	ASN	N-CA-C	5.43	117.32	109.07
1	C	41	LYS	N-CA-CB	-5.42	101.30	110.46
1	H	264	HIS	CG-CD2-NE2	-5.42	101.78	107.20
1	C	329	LYS	CB-CA-C	-5.42	102.53	111.36
1	H	35	ARG	CB-CG-CD	5.42	123.77	111.30
1	K	298	HIS	ND1-CG-CD2	-5.42	100.68	106.10
1	A	46	ARG	CB-CA-C	5.42	118.65	109.55
1	H	333	LYS	N-CA-C	5.42	122.34	110.80
1	I	30	GLU	CG-CD-OE2	5.42	130.86	118.40
1	D	297	GLN	CB-CG-CD	5.41	121.80	112.60
1	A	245	LYS	CD-CE-NZ	5.41	129.21	111.90
1	A	311	GLU	CA-CB-CG	5.41	124.92	114.10
1	K	295	LYS	CG-CD-CE	5.41	123.74	111.30
1	H	340	LYS	CB-CG-CD	5.41	123.73	111.30
1	E	53	LYS	CA-C-N	-5.40	115.01	120.31
1	E	53	LYS	C-N-CA	-5.40	115.01	120.31
1	K	212	ILE	N-CA-C	5.40	116.18	110.72
1	D	46	ARG	CB-CA-C	5.40	118.62	109.55
1	H	295	LYS	CD-CE-NZ	5.40	129.17	111.90
1	I	314	ILE	CG1-CB-CG2	-5.39	94.53	110.70
1	B	53	LYS	CA-C-N	-5.39	115.03	120.31
1	B	53	LYS	C-N-CA	-5.39	115.03	120.31
1	C	245	LYS	CG-CD-CE	-5.39	98.91	111.30
1	I	34	THR	N-CA-C	5.38	122.26	110.80
1	D	306	LYS	CB-CG-CD	-5.38	98.93	111.30
1	F	287	ASP	CB-CA-C	5.38	119.48	110.55
1	D	312	GLY	N-CA-C	-5.38	102.86	112.22
1	K	269	LYS	CB-CA-C	-5.38	101.24	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	309	ILE	CB-CG1-CD1	5.37	125.08	113.80
1	I	275	GLU	N-CA-C	5.37	118.03	109.81
1	F	11	LYS	CD-CE-NZ	5.37	129.08	111.90
1	D	289	LYS	CB-CG-CD	-5.37	98.95	111.30
1	F	11	LYS	CB-CG-CD	-5.37	98.95	111.30
1	G	314	ILE	CB-CG1-CD1	-5.36	102.54	113.80
1	I	295	LYS	CD-CE-NZ	5.36	129.06	111.90
1	F	296	LEU	CD1-CG-CD2	-5.36	99.00	110.80
1	F	38	GLU	CA-CB-CG	5.36	124.82	114.10
1	I	37	THR	N-CA-CB	-5.36	101.44	110.49
1	K	311	GLU	N-CA-C	5.36	116.66	108.52
1	I	241	GLY	O-C-N	5.35	129.66	122.70
1	B	38	GLU	CA-CB-CG	5.35	124.80	114.10
1	D	30	GLU	CB-CG-CD	5.35	121.69	112.60
1	L	340	LYS	CB-CG-CD	-5.35	99.00	111.30
1	A	281	TRP	CG-CD1-NE1	5.34	117.14	110.20
1	H	245	LYS	CB-CA-C	-5.34	98.33	110.07
1	B	33	LYS	N-CA-C	-5.33	103.94	110.61
1	A	42	ARG	CB-CA-C	-5.33	100.84	110.23
1	I	44	ARG	CB-CG-CD	5.33	123.57	111.30
1	D	439	ARG	N-CA-C	-5.33	104.90	111.40
1	I	415	GLU	CA-CB-CG	5.33	124.76	114.10
1	K	38	GLU	CA-CB-CG	5.33	124.75	114.10
1	C	296	LEU	CD1-CG-CD2	-5.32	99.09	110.80
1	F	245	LYS	CB-CA-C	-5.32	97.74	109.56
1	J	330	GLN	CG-CD-NE2	5.32	124.39	116.40
1	B	340	LYS	CA-CB-CG	5.32	124.74	114.10
1	K	49	LEU	CA-C-N	-5.32	113.06	122.26
1	K	49	LEU	C-N-CA	-5.32	113.06	122.26
1	G	338	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	E	35	ARG	N-CA-CB	-5.30	101.53	110.49
1	B	27	LYS	CB-CG-CD	-5.29	99.12	111.30
1	J	338	ARG	NE-CZ-NH2	5.29	123.97	119.20
1	L	359	ILE	N-CA-C	-5.29	105.55	110.53
1	D	37	THR	CB-CA-C	5.29	120.95	110.42
1	I	42	ARG	CG-CD-NE	-5.29	100.36	112.00
1	G	327	SER	CB-CA-C	-5.29	99.90	110.42
1	G	469	MET	N-CA-C	-5.28	107.85	114.56
1	H	308	LYS	N-CA-C	5.28	118.01	109.40
1	K	472	ASN	N-CA-C	5.28	122.06	110.80
1	L	295	LYS	CB-CG-CD	5.28	123.45	111.30
1	L	296	LEU	CA-CB-CG	5.28	134.79	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	314	ILE	N-CA-C	-5.28	105.29	113.16
1	B	35	ARG	CD-NE-CZ	-5.28	117.01	124.40
1	C	42	ARG	CB-CA-C	-5.28	100.95	110.23
1	A	312	GLY	N-CA-C	-5.27	103.04	112.22
1	C	269	LYS	CB-CA-C	-5.27	101.41	110.16
1	D	280	ILE	CA-CB-CG1	5.27	119.36	110.40
1	E	169	MET	CA-CB-CG	-5.26	103.58	114.10
1	J	42	ARG	CA-CB-CG	5.26	124.62	114.10
1	A	446	LYS	CD-CE-NZ	5.26	128.73	111.90
1	H	175	GLU	N-CA-C	-5.26	105.72	111.82
1	K	41	LYS	CA-CB-CG	5.26	124.62	114.10
1	F	446	LYS	CG-CD-CE	5.26	123.39	111.30
1	I	46	ARG	N-CA-C	-5.25	106.92	113.38
1	I	311	GLU	N-CA-C	5.25	116.50	108.52
1	B	409	LEU	CA-CB-CG	5.24	134.66	116.30
1	K	477	LEU	N-CA-C	5.24	121.97	110.80
1	A	494	ASN	CB-CA-C	-5.24	102.89	110.96
1	A	174	ARG	CG-CD-NE	5.23	123.51	112.00
1	G	314	ILE	CB-CA-C	5.23	117.69	111.20
1	H	446	LYS	CD-CE-NZ	5.23	128.63	111.90
1	L	275	GLU	CG-CD-OE1	-5.23	106.37	118.40
1	C	35	ARG	N-CA-CB	-5.23	101.66	110.49
1	H	306	LYS	CD-CE-NZ	5.23	128.63	111.90
1	K	269	LYS	CA-C-O	5.23	125.89	120.30
1	L	439	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	F	40	GLN	CB-CA-C	5.22	119.97	111.26
1	C	308	LYS	N-CA-CB	-5.21	102.05	110.81
1	G	340	LYS	CB-CA-C	-5.21	100.05	110.42
1	B	312	GLY	N-CA-C	-5.21	103.16	112.22
1	I	289	LYS	N-CA-C	5.21	121.89	110.80
1	G	297	GLN	CA-CB-CG	5.20	124.50	114.10
1	C	175	GLU	N-CA-C	-5.19	105.70	111.36
1	J	402	GLU	CA-CB-CG	5.19	124.48	114.10
1	B	421	PHE	N-CA-C	5.19	121.85	110.80
1	H	30	GLU	CB-CG-CD	5.19	121.42	112.60
1	L	85	HIS	CA-C-O	5.19	125.64	119.10
1	B	34	THR	N-CA-CB	-5.18	101.73	110.49
1	F	44	ARG	NE-CZ-NH1	-5.18	116.32	121.50
1	J	430	ILE	N-CA-C	5.18	120.11	109.34
1	G	30	GLU	CB-CG-CD	-5.17	103.81	112.60
1	H	342	LYS	CD-CE-NZ	5.17	128.45	111.90
1	B	314	ILE	CG1-CB-CG2	-5.17	95.19	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	289	LYS	N-CA-CB	-5.17	101.76	110.49
1	H	311	GLU	CB-CA-C	5.16	120.70	110.42
1	I	329	LYS	CB-CA-C	-5.16	100.58	110.65
1	I	342	LYS	CA-CB-CG	-5.16	103.77	114.10
1	D	284	ASP	N-CA-C	-5.16	106.14	112.90
1	H	423	LYS	N-CA-C	5.16	121.79	110.80
1	A	333	LYS	N-CA-C	5.16	121.78	110.80
1	D	286	ILE	CG1-CB-CG2	-5.15	95.24	110.70
1	J	33	LYS	N-CA-C	-5.15	102.69	110.06
1	K	420	LYS	CA-CB-CG	-5.15	103.80	114.10
1	A	329	LYS	CB-CG-CD	-5.14	99.47	111.30
1	G	37	THR	OG1-CB-CG2	-5.14	99.02	109.30
1	B	314	ILE	N-CA-C	-5.14	105.50	113.16
1	K	314	ILE	CG1-CB-CG2	-5.14	95.29	110.70
1	F	34	THR	CA-CB-CG2	5.14	119.23	110.50
1	C	338	ARG	CD-NE-CZ	-5.13	117.22	124.40
1	A	363	ARG	CG-CD-NE	5.12	123.25	112.00
1	F	423	LYS	CB-CA-C	-5.12	103.31	114.10
1	A	30	GLU	CB-CG-CD	-5.11	103.91	112.60
1	A	32	LEU	CB-CG-CD2	5.11	126.02	110.70
1	A	174	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	E	314	ILE	CA-CB-CG2	5.11	119.18	110.50
1	G	37	THR	CA-CB-CG2	5.11	119.18	110.50
1	D	358	LYS	CB-CG-CD	-5.11	99.56	111.30
1	K	246	THR	OG1-CB-CG2	-5.11	99.09	109.30
1	B	245	LYS	CA-CB-CG	-5.10	103.90	114.10
1	C	9	PHE	CA-CB-CG	-5.10	108.70	113.80
1	I	30	GLU	CA-CB-CG	-5.09	103.92	114.10
1	L	265	ARG	CG-CD-NE	5.09	123.20	112.00
1	L	42	ARG	N-CA-C	-5.08	99.98	110.80
1	B	338	ARG	CB-CG-CD	5.08	122.98	111.30
1	E	329	LYS	CD-CE-NZ	5.08	128.15	111.90
1	J	298	HIS	N-CA-CB	5.08	119.07	110.49
1	L	42	ARG	CA-CB-CG	5.08	124.25	114.10
1	A	271	VAL	N-CA-C	5.08	115.85	110.72
1	D	309	ILE	CG1-CB-CG2	5.07	125.92	110.70
1	E	289	LYS	CA-CB-CG	5.07	124.24	114.10
1	I	328	GLU	CG-CD-OE1	-5.07	106.74	118.40
1	C	44	ARG	CG-CD-NE	-5.07	100.85	112.00
1	D	31	ASP	N-CA-CB	-5.06	101.93	110.49
1	F	175	GLU	N-CA-C	-5.06	105.95	111.82
1	L	41	LYS	CD-CE-NZ	5.06	128.11	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	289	LYS	CG-CD-CE	-5.06	99.66	111.30
1	F	269	LYS	CB-CA-C	-5.06	101.76	110.16
1	B	329	LYS	CA-C-N	-5.06	114.56	122.65
1	B	329	LYS	C-N-CA	-5.06	114.56	122.65
1	A	11	LYS	CB-CA-C	-5.06	102.29	110.79
1	C	38	GLU	CA-CB-CG	5.06	124.22	114.10
1	I	36	GLU	CA-C-N	5.06	131.20	121.54
1	I	36	GLU	C-N-CA	5.06	131.20	121.54
1	F	173	GLU	CA-C-N	5.06	129.23	121.19
1	F	173	GLU	C-N-CA	5.06	129.23	121.19
1	K	296	LEU	CB-CA-C	-5.05	102.45	110.84
1	K	333	LYS	N-CA-C	5.05	121.56	110.80
1	K	47	GLY	N-CA-C	-5.05	106.67	112.73
1	C	342	LYS	CA-CB-CG	5.05	124.19	114.10
1	K	175	GLU	N-CA-C	-5.05	105.97	111.82
1	D	31	ASP	CB-CA-C	5.04	120.46	110.42
1	D	44	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	D	421	PHE	CB-CG-CD2	-5.04	112.13	120.70
1	I	287	ASP	CB-CA-C	5.04	118.54	110.62
1	K	50	ARG	CB-CA-C	5.04	118.42	109.65
1	A	27	LYS	CA-CB-CG	5.04	124.18	114.10
1	E	36	GLU	CA-C-N	5.04	131.16	121.54
1	E	36	GLU	C-N-CA	5.04	131.16	121.54
1	G	33	LYS	N-CA-C	-5.03	100.30	109.56
1	K	468	ALA	CA-C-N	5.03	127.29	120.65
1	K	468	ALA	C-N-CA	5.03	127.29	120.65
1	H	264	HIS	ND1-CE1-NE2	-5.03	103.37	108.40
1	D	333	LYS	N-CA-CB	-5.03	101.99	110.49
1	E	357	ASP	CA-C-N	5.03	126.98	120.44
1	E	357	ASP	C-N-CA	5.03	126.98	120.44
1	K	329	LYS	CB-CG-CD	-5.02	99.75	111.30
1	C	306	LYS	N-CA-CB	-5.02	102.01	110.49
1	J	358	LYS	CB-CG-CD	-5.02	99.75	111.30
1	J	36	GLU	CB-CA-C	-5.02	100.44	110.42
1	J	340	LYS	CB-CA-C	-5.02	100.44	110.42
1	C	173	GLU	CA-C-N	5.02	128.34	120.82
1	C	173	GLU	C-N-CA	5.02	128.34	120.82
1	C	134	LYS	N-CA-C	5.01	117.52	111.40
1	A	423	LYS	N-CA-CB	-5.01	103.39	110.51
1	D	242	PHE	N-CA-C	5.01	121.47	110.80
1	C	329	LYS	N-CA-C	5.01	118.97	112.86
1	A	174	ARG	NE-CZ-NH2	5.00	123.70	119.20

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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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	233	0
1	B	3875	0	3845	200	0
1	C	3875	0	3845	202	2
1	D	3875	0	3845	212	0
1	E	3875	0	3845	209	2
1	F	3875	0	3845	204	0
1	G	3875	0	3845	200	0
1	H	3875	0	3845	193	0
1	I	3875	0	3844	213	0
1	J	3875	0	3845	195	0
1	K	3875	0	3845	201	0
1	L	3875	0	3845	219	0
2	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2340	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 25.

All (2340) 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
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:D:240:PRO:HG3	1:D:245:LYS:HZ3	1.04	1.08
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: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:J:419:ARG:C	1:J:421:PHE:H	1.61	1.02
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: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:F:18:ASP:OD1	1:F:53:LYS:NZ	1.97	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:42:ARG:C	1:E:44:ARG:H	1.72	0.94
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:I:42:ARG:C	1:I:44:ARG:H	1.77	0.92
1:D:291:LEU:CD2	1:D:291:LEU:CB	2.46	0.92
1:A:423:LYS:HZ2	1:H:437:GLN:HE21	0.99	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:A:281:TRP:C	1:A:281:TRP:HD1	1.79	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
1:J:240:PRO:HG3	1:J:245:LYS:HZ2	1.35	0.89
1:J:42:ARG:C	1:J:44:ARG:H	1.78	0.89
1:E:240:PRO:HG3	1:E:245:LYS:NZ	1.88	0.89
1:A:423:LYS:HZ2	1:H:437:GLN:NE2	1.71	0.89
1:L:240:PRO:HG3	1:L:245:LYS:HZ2	1.36	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:K:225:ASN:HD21	1:K:458:GLU:CD	1.81	0.88
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:H:281:TRP:C	1:H:281:TRP:HD1	1.82	0.87
1:G:30:GLU:O	1:G:32:LEU:N	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:L:281:TRP:HD1	1:L:281:TRP:C	1.83	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:I:281:TRP:C	1:I:281:TRP:HD1	1.85	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: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:H:42:ARG:C	1:H:44:ARG:N	2.35	0.84
1:H:281:TRP:C	1:H:281:TRP:CD1	2.55	0.84
1:C:281:TRP:C	1:C:281:TRP:HD1	1.86	0.84
1:F:240:PRO:HG2	1:F:245:LYS:NZ	1.92	0.84
1:G:281:TRP:HD1	1:G:281:TRP:C	1.85	0.84
1:H:42:ARG:C	1:H:44:ARG:H	1.86	0.84
1:J:233:MET:HB3	1:J:239:THR:H	1.43	0.83
1:B:469:MET:HE3	1:G:308:LYS:HE2	1.60	0.83
1:D:281:TRP:HD1	1:D:281:TRP:C	1.86	0.83
1:I:42:ARG:C	1:I:44:ARG:N	2.34	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:K:261:ARG:NH2	1:K:292:GLU:OE2	2.10	0.83
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:C:240:PRO:HG2	1:C:245:LYS:HZ1	1.43	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:K:281:TRP:C	1:K:281:TRP:HD1	1.87	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:34:THR:O	1:L:35:ARG:HB3	1.78	0.82
1:E:42:ARG:C	1:E:44:ARG:N	2.33	0.82
1:C:396:ARG:NH1	1:E:119:ASP:O	2.11	0.82
1:F:281:TRP:CD1	1:F:281:TRP:C	2.57	0.81
1:A:42:ARG:C	1:A:44:ARG:N	2.37	0.81
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:J:35:ARG:C	1:J:37:THR:H	1.85	0.81
1:A:281:TRP:C	1:A:281:TRP:CD1	2.57	0.81
1:H:439:ARG:NH2	1:L:405:SER:OG	2.14	0.81
1:K:42:ARG:C	1:K:44:ARG:H	1.88	0.81
1:D:44:ARG:C	1:D:46:ARG:H	1.89	0.81
1:D:281:TRP:HE1	1:D:283:PRO:HD3	1.44	0.81
1:G:42:ARG:C	1:G:44:ARG:H	1.89	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:D:42:ARG:C	1:D:44:ARG:H	1.89	0.81
1:A:42:ARG:C	1:A:44:ARG:H	1.88	0.80
1:A:281:TRP:HE1	1:A:283:PRO:CD	1.94	0.80
1:C:281:TRP:C	1:C:281:TRP:CD1	2.59	0.80
1:A:44:ARG:C	1:A:46:ARG:H	1.88	0.80
1:E:44:ARG:C	1:E:46:ARG:H	1.88	0.80
1:I:35:ARG:C	1:I:37:THR:H	1.89	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:K:44:ARG:C	1:K:46:ARG:H	1.89	0.80
1:L:42:ARG:C	1:L:44:ARG:H	1.89	0.80
1:J:240:PRO:HG3	1:J:245:LYS:NZ	1.95	0.80
1:L:42:ARG:C	1:L:44:ARG:N	2.39	0.80
1:B:44:ARG:C	1:B:46:ARG:H	1.90	0.80
1:J:281:TRP:HD1	1:J:281:TRP:C	1.89	0.80
1:D:281:TRP:C	1:D:281:TRP:CD1	2.59	0.79
1:G:42:ARG:C	1:G:44:ARG:N	2.40	0.79
1:D:42:ARG:C	1:D:44:ARG:N	2.39	0.79
1:B:42:ARG:C	1:B:44:ARG:N	2.40	0.79
1:I:35:ARG:HG2	1:I:35:ARG:NH1	1.91	0.79
1:J:281:TRP:C	1:J:281:TRP:CD1	2.60	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:281:TRP:HE1	1:K:283:PRO:CD	1.94	0.79
1:L:42:ARG:O	1:L:44:ARG:N	2.15	0.79
1:E:281:TRP:CD1	1:E:281:TRP:C	2.61	0.79
1:K:30:GLU:O	1:K:34:THR:N	2.15	0.79
1:K:281:TRP:C	1:K:281:TRP:CD1	2.57	0.79
1:D:19:ARG:HE	1:D:479:THR:HG21	1.48	0.79
1:E:281:TRP:C	1:E:281:TRP:HD1	1.91	0.79
1:I:32:LEU:CD1	1:I:33:LYS:HD2	2.12	0.78
1:K:42:ARG:C	1:K:44:ARG:N	2.39	0.78
1:B:42:ARG:C	1:B:44:ARG:H	1.90	0.78
1:B:281:TRP:HE1	1:B:283:PRO:CD	1.96	0.78
1:G:405:SER:OG	1:L:439:ARG:NH2	2.17	0.78
1:G:44:ARG:C	1:G:46:ARG:H	1.91	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:J:44:ARG:C	1:J:46:ARG:H	1.89	0.78
1:I:30:GLU:O	1:I:32:LEU:N	2.17	0.78
1:J:42:ARG:C	1:J:44:ARG:N	2.39	0.78
1:A:34:THR:HB	1:A:35:ARG:CB	2.14	0.78
1:D:419:ARG:O	1:D:421:PHE:N	2.18	0.77
1:E:35:ARG:C	1:E:37:THR:H	1.91	0.77
1:A:423:LYS:NZ	1:H:437:GLN:NE2	2.28	0.77
1:I:44:ARG:C	1:I:46:ARG:H	1.92	0.77
1:F:240:PRO:HG2	1:F:245:LYS:HZ2	1.47	0.77
1:C:44:ARG:C	1:C:46:ARG:H	1.93	0.76
1:L:44:ARG:C	1:L:46:ARG:H	1.93	0.76
1:C:42:ARG:C	1:C:44:ARG:N	2.41	0.76
1:J:189:HIS:HD2	1:L:154:LYS:HE2	1.49	0.76
1:B:281:TRP:CD1	1:B:281:TRP:C	2.63	0.76
1:J:281:TRP:HE1	1:J:283:PRO:CD	1.97	0.76
1:D:281:TRP:HE1	1:D:283:PRO:CD	1.99	0.76
1:H:44:ARG:C	1:H:46:ARG:H	1.93	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:42:ARG:C	1:F:44:ARG:N	2.44	0.75
1:F:281:TRP:C	1:F:281:TRP:HD1	1.95	0.75
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: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:D:30:GLU:O	1:D:32:LEU:N	2.20	0.74
1:G:281:TRP:C	1:G:281:TRP:CD1	2.59	0.74
1:F:44:ARG:C	1:F:46:ARG:H	1.94	0.74
1:H:281:TRP:HE1	1:H:283:PRO:CD	2.00	0.74
1:C:294:PHE:HA	1:C:297:GLN:HG3	1.69	0.74
1:L:281:TRP:C	1:L:281:TRP:CD1	2.59	0.74
1:B:186:THR:HG23	1:E:186:THR:HG23	1.67	0.74
1:B:240:PRO:HG2	1:B:245:LYS:HZ2	1.50	0.74
1:G:33:LYS:O	1:G:35:ARG:N	2.21	0.74
1:L:33:LYS:C	1:L:35:ARG:H	1.94	0.74
1:E:419:ARG:O	1:E:421:PHE:N	2.21	0.73
1:A:30:GLU:O	1:A:34:THR:N	2.21	0.73
1:E:240:PRO:HG3	1:E:245:LYS:HZ1	1.49	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:240:PRO:HG2	1:C:245:LYS:HZ2	1.53	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:B:281:TRP:C	1:B:281:TRP:HD1	1.95	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:A:423:LYS:HZ3	1:H:437:GLN:HE21	1.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:243:GLY:O	1:L:245:LYS:N	2.22	0.73
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:D:42:ARG:O	1:D:44:ARG:N	2.18	0.72
1:C:35:ARG:C	1:C:37:THR:H	1.94	0.72
1:F:35:ARG:C	1:F:37:THR:H	1.97	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: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: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:C:335:ASN:HA	1:C:338:ARG:HG3	1.70	0.71
1:H:35:ARG:C	1:H:37:THR:H	1.96	0.71
1:I:419:ARG:O	1:I:421:PHE:N	2.23	0.71
1:E:281:TRP:HE1	1:E:283:PRO:HD3	1.54	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:H:39:GLU:HB3	1:H:41:LYS:HG2	1.73	0.71
1:J:243:GLY:O	1:J:245:LYS:N	2.24	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: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
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:D:35:ARG:C	1:D:37:THR:H	1.95	0.70
1:F:281:TRP:CD1	1:F:282:ASN:N	2.59	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:281:TRP:C	1:I:281:TRP:CD1	2.63	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:I:476:ASP:CG	1:I:479:THR:HG21	2.17	0.70
1:J:419:ARG:C	1:J:421:PHE:N	2.38	0.70
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:D:37:THR:OG1	1:D:40:GLN:HA	1.91	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: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:F:42:ARG:C	1:F:44:ARG:H	2.01	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:C:42:ARG:C	1:C:44:ARG:H	2.01	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:K:35:ARG:C	1:K:37:THR:H	2.00	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
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:L:35:ARG:C	1:L:37:THR:H	2.02	0.67
1:G:419:ARG:O	1:G:421:PHE:N	2.27	0.66
1:G:439:ARG:HH21	1:H:405:SER:HG	1.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:42:ARG:O	1:F:44:ARG:N	2.24	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
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: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:J:406:ASN:ND2	1:J:436:PHE:HZ	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:33:LYS:C	1:F:35:ARG:HB2	2.23	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:44:ARG:C	1:E:46:ARG:N	2.54	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:G:28:LEU:C	1:G:32:LEU:HD22	2.22	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
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:D:419:ARG:C	1:D:421:PHE:N	2.56	0.64
1:E:42:ARG:HA	1:E:45:VAL:HG22	1.80	0.64
1:G:35:ARG:C	1:G:37:THR:H	2.04	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:35:ARG:C	1:B:37:THR:H	2.06	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:I:42:ARG:O	1:I:44:ARG:N	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:189:HIS:C	1:A:189:HIS:HD1	2.07	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:I:33:LYS:C	1:I:35:ARG:HB2	2.24	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:D:233:MET:HE1	1:D:343:ILE:HD11	1.82	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:G:44:ARG:C	1:G:46:ARG:N	2.58	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:A:314:ILE:C	1:A:316:GLU:H	2.09	0.61
1:B:469:MET:HB3	1:G:308:LYS:HZ3	1.66	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:233:MET:HE1	1:F:343:ILE:HD11	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:35:ARG:C	1:A:37:THR:H	2.05	0.60
1:A:272:ALA:HB1	1:A:314:ILE:CD1	2.31	0.60
1:C:233:MET:HE1	1:C:343:ILE:HD11	1.82	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:189:HIS:HD1	1:J:189:HIS:C	2.09	0.60
1:J:314:ILE:O	1:J:316:GLU:N	2.34	0.60
1:L:233:MET:HE1	1:L:343:ILE:HD11	1.82	0.60
1:D:9:PHE:O	1:D:11:LYS:N	2.34	0.60
1:J:233:MET:HE1	1:J:343:ILE:HD11	1.82	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:189:HIS:HD1	1:B:189:HIS:C	2.08	0.60
1:B:281:TRP:CD1	1:B:282:ASN:N	2.69	0.60
1:L:142:GLU:OE2	1:L:146:ARG:NH1	2.33	0.60
1:A:233:MET:HE1	1:A:343:ILE:HD11	1.82	0.60
1:A:281:TRP:CD1	1:A:282:ASN:N	2.69	0.60
1:E:28:LEU:C	1:E:32:LEU:HD11	2.27	0.60
1:F:30:GLU:O	1:F:32:LEU:N	2.34	0.60
1:G:132:ASN:C	1:G:134:LYS:H	2.10	0.60
1:G:419:ARG:C	1:G:421:PHE:N	2.59	0.60
1:H:245:LYS:O	1:H:269:LYS:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:308:LYS:HZ3	1:L:469:MET:HB3	1.65	0.60
1:G:233:MET:HE1	1:G:343:ILE:HD11	1.83	0.60
1:L:290:GLU:CD	1:L:306:LYS:HZ3	2.10	0.60
1:A:261:ARG:NH2	1:A:292:GLU:OE2	2.34	0.60
1:B:233:MET:HE1	1:B:343:ILE:HD11	1.83	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:H:9:PHE:C	1:H:11:LYS:H	2.09	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:K:233:MET:HE1	1:K:343:ILE:HD11	1.83	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:H:233:MET:HE1	1:H:343:ILE:HD11	1.83	0.60
1:F:281:TRP:CD1	1:F:282:ASN:HA	2.37	0.60
1:A:44:ARG:C	1:A:46:ARG:N	2.58	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:D:44:ARG:C	1:D:46:ARG:N	2.57	0.59
1:G:17:PHE:CD2	1:G:53:LYS:HD2	2.37	0.59
1:I:233:MET:HE1	1:I:343:ILE:HD11	1.83	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: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: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:D:9:PHE:C	1:D:11:LYS:N	2.54	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:33:LYS:C	1:J:35:ARG:N	2.61	0.59
1:K:419:ARG:C	1:K:421:PHE:N	2.59	0.59
1:A:236:LEU:HB2	1:A:238:MET:HG3	1.84	0.59
1:C:238:MET:HE1	1:C:320:ASP:HB3	1.85	0.59
1:D:9:PHE:C	1:D:11:LYS:H	2.09	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:E:238:MET:O	1:E:239:THR:C	2.46	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:E:233:MET:HE1	1:E:343:ILE:HD11	1.83	0.58
1:F:419:ARG:C	1:F:421:PHE:N	2.60	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:C:419:ARG:C	1:C:421:PHE:N	2.59	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:A:142:GLU:CD	1:F:499:THR:HB	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:419:ARG:C	1:E:421:PHE:N	2.60	0.58
1:L:44:ARG:C	1:L:46:ARG:N	2.58	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
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:35:ARG:C	1:J:37:THR:N	2.60	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: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: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: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:B:42:ARG:O	1:B:44:ARG:N	2.20	0.57
1:C:38:GLU:O	1:C:39:GLU:HB2	2.02	0.57
1:E:238:MET:C	1:E:240:PRO:N	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:419:ARG:C	1:L:421:PHE:N	2.62	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
1:F:6:ASP:OD1	1:F:332:THR:HB	2.04	0.57
1:H:419:ARG:C	1:H:421:PHE:N	2.61	0.57
1:L:252:PHE:HD2	1:L:295:LYS:HZ1	1.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:293:ASP:O	1:K:297:GLN:HB2	2.04	0.56
1:A:419:ARG:C	1:A:421:PHE:N	2.63	0.56
1:B:314:ILE:C	1:B:316:GLU:H	2.12	0.56
1:F:44:ARG:C	1:F:46:ARG:N	2.59	0.56
1:F:293:ASP:O	1:F:297:GLN:HB2	2.05	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:K:33:LYS:C	1:K:35:ARG:N	2.63	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
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:33:LYS:C	1:L:35:ARG:N	2.53	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:K:44:ARG:C	1:K:46:ARG:N	2.56	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:315:LEU:O	1:L:339:VAL:HG12	2.05	0.56
1:H:150:MET:O	1:H:154:LYS:HG3	2.06	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: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:J:238:MET:C	1:J:240:PRO:N	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:405:SER:HG	1:F:439:ARG:HH21	1.52	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: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: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:A:28:LEU:C	1:A:32:LEU:HD22	2.31	0.55
1:G:33:LYS:C	1:G:35:ARG:HB3	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:44:ARG:C	1:J:46:ARG:N	2.57	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: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: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: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: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:K:132:ASN:C	1:K:134:LYS:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ILE:O	1:C:391:HIS:NE2	2.39	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:I:419:ARG:C	1:I:421:PHE:N	2.65	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:B:419:ARG:C	1:B:421:PHE:N	2.66	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:229:GLU:CD	1:J:462:ARG:HH22	2.16	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:33:LYS:C	1:C:35:ARG:N	2.66	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:E:33:LYS:C	1:E:35:ARG:N	2.66	0.54
1:L:328:GLU:HB3	1:L:329:LYS:HG3	1.89	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:428:ILE:CD1	1:G:239:THR:HG21	2.37	0.54
1:D:28:LEU:C	1:D:32:LEU:HD22	2.32	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:I:36:GLU:HG3	1:I:42:ARG:HH21	1.73	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:I:44:ARG:C	1:I:46:ARG:N	2.60	0.53
1:K:147:ARG:NH1	1:K:151:GLU:OE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:44:ARG:C	1:C:46:ARG:N	2.60	0.53
1:D:23:ILE:HG22	1:D:471:TYR:CE2	2.43	0.53
1:E:30:GLU:C	1:E:32:LEU:N	2.67	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:D:33:LYS:C	1:D:35:ARG:N	2.66	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: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:J:238:MET:O	1:J:239:THR:C	2.52	0.53
1:K:39:GLU:O	1:K:40:GLN:HB3	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:30:GLU:H	1:H:32:LEU:HD12	1.72	0.53
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:L:37:THR:CG2	1:L:40:GLN:HA	2.38	0.52
1:B:240:PRO:HG2	1:B:245:LYS:HZ1	1.74	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: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:240:PRO:HG2	1:H:245:LYS:HZ3	1.71	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:A:305:PRO:C	1:A:306:LYS:HG3	2.34	0.52
1:C:281:TRP:HD1	1:C:282:ASN:CA	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:238:MET:C	1:K:240:PRO:N	2.64	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
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:C:482:TYR:O	1:C:486:ILE:HG12	2.09	0.52
1:D:495:GLU:O	1:E:177:SER:OG	2.20	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: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:I:134:LYS:C	1:I:136:TYR:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:TRP:HD1	1:B:282:ASN:CA	2.23	0.51
1:B:294:PHE:C	1:B:297:GLN:HB3	2.35	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
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: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:C:134:LYS:C	1:C:136:TYR:H	2.17	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:K:35:ARG:C	1:K:37:THR:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HG	1:A:33:LYS:HG3	1.92	0.51
1:C:305:PRO:C	1:C:307:ALA:H	2.18	0.51
1:J:87:THR:HG22	1:J:88:PRO:HD3	1.92	0.51
1:J:189:HIS:C	1:J:189:HIS:ND1	2.68	0.51
1:A:134:LYS:C	1:A:136:TYR:H	2.18	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
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:J:134:LYS:C	1:J:136:TYR:H	2.19	0.51
1:L:87:THR:HG22	1:L:88:PRO:HD3	1.93	0.51
1:L:134:LYS:C	1:L:136:TYR:H	2.19	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:E:293:ASP:C	1:E:295:LYS:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:GLU:C	1:E:27:LYS:H	2.18	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:H:34:THR:CA	1:H:35:ARG:HB3	2.16	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: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:E:281:TRP:HD1	1:E:282:ASN:N	2.05	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:B:134:LYS:C	1:B:136:TYR:H	2.20	0.50
1:F:134:LYS:C	1:F:136:TYR:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:305:PRO:C	1:D:307:ALA:H	2.20	0.49
1:E:28:LEU:HD21	1:E:490:PHE:CG	2.47	0.49
1:E:305:PRO:C	1:E:307:ALA:H	2.20	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: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:30:GLU:C	1:I:32:LEU:N	2.71	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:367:VAL:O	1:K:477:LEU:HD23	2.12	0.49
1:L:293:ASP:C	1:L:295:LYS:H	2.20	0.49
1:A:439:ARG:HH21	1:B:405:SER:HG	1.58	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:294:PHE:C	1:H:297:GLN:HB3	2.37	0.49
1:K:44:ARG:O	1:K:44:ARG:HG3	1.97	0.49
1:L:35:ARG:C	1:L:37:THR:N	2.70	0.49
1:L:60:SER:HB3	1:L:78:TYR:CD1	2.46	0.49
1:L:314:ILE:C	1:L:316:GLU:H	2.20	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
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:E:134:LYS:C	1:E:136:TYR:H	2.21	0.49
1:G:42:ARG:O	1:G:44:ARG:N	2.23	0.49
1:I:201:LYS:HG2	1:I:384:GLU:OE1	2.12	0.49
1:L:335:ASN:C	1:L:338:ARG:HB2	2.37	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:H:134:LYS:C	1:H:136:TYR:H	2.19	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:F:305:PRO:C	1:F:307:ALA:H	2.19	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:305:PRO:O	1:C:307:ALA:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:499:THR:HG1	1:L:142:GLU:CD	2.19	0.49
1:I:362:GLU:C	1:I:364:ASN:H	2.20	0.49
1:A:239:THR:HA	1:A:240:PRO:HD3	1.45	0.48
1:D:35:ARG:C	1:D:37:THR:N	2.69	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:I:44:ARG:O	1:I:44:ARG:HG2	1.91	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
1:K:305:PRO:C	1:K:307:ALA:H	2.21	0.48
1:L:247:PHE:CE1	1:L:269:LYS:C	2.91	0.48
1:B:281:TRP:HD1	1:B:282:ASN:N	2.10	0.48
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:D:134:LYS:C	1:D:136:TYR:H	2.20	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:238:MET:C	1:L:240:PRO:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:240:PRO:HG2	1:F:245:LYS:HZ1	1.77	0.48
1:H:293:ASP:C	1:H:295:LYS:H	2.22	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:J:362:GLU:C	1:J:364:ASN:H	2.21	0.48
1:K:238:MET:O	1:K:239:THR:C	2.55	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:247:PHE:CE1	1:B:269:LYS:C	2.91	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:C:239:THR:O	1:C:239:THR:HG23	2.12	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
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: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:189:HIS:C	1:A:189:HIS:ND1	2.68	0.48
1:A:315:LEU:O	1:A:339:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:260:MET:HE2	1:A:260:MET:HB3	1.70	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:F:467:THR:C	1:F:469:MET:H	2.20	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:L:240:PRO:CG	1:L:245:LYS:HZ2	2.19	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:F:25:GLU:C	1:F:27:LYS:H	2.21	0.48
1:H:238:MET:O	1:H:239:THR:C	2.56	0.48
1:H:239:THR:HA	1:H:240:PRO:HD3	1.39	0.48
1:J:39:GLU:O	1:J:40:GLN:HB3	2.13	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
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:189:HIS:C	1:B:189:HIS:ND1	2.68	0.47
1:B:315:LEU:O	1:B:339:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:293:ASP:C	1:A:295:LYS:H	2.23	0.47
1:A:437:GLN:HG2	1:H:423:LYS:HZ2	1.77	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:260:MET:HE2	1:K:260:MET:HB3	1.68	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
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:B:305:PRO:C	1:B:307:ALA:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ARG:O	1:C:37:THR:HG22	2.15	0.47
1:D:9:PHE:O	1:D:10:PHE:C	2.57	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:H:9:PHE:C	1:H:11:LYS:N	2.70	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:L:305:PRO:C	1:L:307:ALA:H	2.23	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:D:252:PHE:CZ	1:D:260:MET:HE1	2.50	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:H:240:PRO:HG2	1:H:245:LYS:HZ1	1.73	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: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:E:150:MET:HE1	1:E:186:THR:HG21	1.97	0.47
1:F:167:PRO:HG3	1:F:176:MET:HG3	1.96	0.47
1:I:6:ASP:N	1:I:7:PRO:HD3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:238:MET:O	1:L:239:THR:C	2.58	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: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:A:294:PHE:C	1:A:297:GLN:HB3	2.41	0.46
1:C:35:ARG:C	1:C:37:THR:N	2.67	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:GLU:C	1:D:364:ASN:H	2.24	0.46
1:E:95:TYR:HB3	1:E:133:PRO:HG3	1.97	0.46
1:G:9:PHE:C	1:G:11:LYS:H	2.23	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:J:34:THR:C	1:J:35:ARG:HG2	2.40	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:F:414:GLN:O	1:F:418:GLU:HG3	2.15	0.46
1:H:44:ARG:C	1:H:46:ARG:N	2.60	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:305:PRO:C	1:H:307:ALA:H	2.23	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:I:310:TYR:CG	1:I:311:GLU:N	2.83	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:277:ASP:HB2	1:C:278:GLY:H	1.59	0.46
1:D:238:MET:C	1:D:240:PRO:N	2.67	0.46
1:E:29:VAL:HG22	1:E:42:ARG:HB2	1.98	0.46
1:E:362:GLU:C	1:E:364:ASN:H	2.23	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:F:150:MET:HE1	1:F:186:THR:HG21	1.97	0.46
1:F:247:PHE:CE1	1:F:269:LYS:C	2.94	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:L:150:MET:HE1	1:L:186:THR:HG21	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:55:CYS:HA	1:K:82:HIS:HA	1.96	0.46
1:K:150:MET:HE1	1:K:186:THR:HG21	1.98	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:B:150:MET:HE1	1:B:186:THR:HG21	1.98	0.46
1:B:469:MET:C	1:G:308:LYS:HZ1	2.23	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:F:293:ASP:C	1:F:295:LYS:H	2.24	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:J:150:MET:HE1	1:J:186:THR:HG21	1.97	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: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:132:ASN:C	1:J:134:LYS:H	2.23	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: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:G:252:PHE:CD1	1:G:273:VAL:HG11	2.51	0.46
1:H:150:MET:HE1	1:H:186:THR:HG21	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:305:PRO:C	1:A:307:ALA:H	2.24	0.45
1:A:414:GLN:O	1:A:418:GLU:HG3	2.16	0.45
1:F:88:PRO:HG2	1:F:122:PHE:CE1	2.51	0.45
1:I:150:MET:HE1	1:I:186:THR:HG21	1.97	0.45
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:55:CYS:HA	1:H:82:HIS:HA	1.99	0.45
1:I:247:PHE:CE1	1:I:269:LYS:C	2.95	0.45
1:I:305:PRO:C	1:I:307:ALA:H	2.25	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: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:K:314:ILE:C	1:K:316:GLU:H	2.25	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:C:150:MET:HE1	1:C:186:THR:HG21	1.97	0.45
1:C:405:SER:HG	1:E:439:ARG:HH21	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ASP:C	1:D:295:LYS:H	2.24	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:209:HIS:HD2	1:J:445:GLU:HB3	1.81	0.45
1:J:260:MET:HE2	1:J:260:MET:HB3	1.70	0.45
1:A:35:ARG:C	1:A:37:THR:N	2.74	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
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:134:LYS:C	1:I:136:TYR:N	2.75	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:J:362:GLU:C	1:J:364:ASN:N	2.75	0.45
1:K:94:ARG:HD2	1:K:99:VAL:HG12	1.96	0.45
1:K:134:LYS:C	1:K:136:TYR:H	2.24	0.45
1:K:466:ARG:C	1:K:469:MET:HB2	2.42	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:238:MET:C	1:F:240:PRO:N	2.75	0.45
1:F:469:MET:HA	1:F:472:ASN:ND2	2.31	0.45
1:G:41:LYS:C	1:G:44:ARG:HB2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:346:GLU:CD	1:J:478:ARG:HH22	2.22	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:D:150:MET:HE1	1:D:186:THR:HG21	1.98	0.45
1:D:238:MET:O	1:D:239:THR:C	2.57	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: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:B:362:GLU:C	1:B:364:ASN:H	2.24	0.45
1:C:414:GLN:O	1:C:418:GLU:HG3	2.16	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
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:G:150:MET:HE1	1:G:186:THR:HG21	1.98	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:314:ILE:C	1:C:316:GLU:H	2.25	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: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:I:470:LYS:HD2	1:I:470:LYS:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:260:MET:HB3	1:C:260:MET:HE2	1.70	0.45
1:C:439:ARG:NH2	1:D:405:SER:OG	2.46	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:260:MET:HE2	1:H:260:MET:HB3	1.72	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:I:238:MET:C	1:I:240:PRO:N	2.74	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: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:C:28:LEU:C	1:C:32:LEU:HD22	2.42	0.44
1:C:238:MET:C	1:C:240:PRO:N	2.75	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:G:362:GLU:C	1:G:364:ASN:H	2.25	0.44
1:H:362:GLU:C	1:H:364:ASN:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:414:GLN:OE1	1:J:428:ILE:HA	2.17	0.44
1:K:247:PHE:CE1	1:K:269:LYS:C	2.95	0.44
1:L:467:THR:C	1:L:469:MET:H	2.26	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:D:103:GLU:C	1:D:105:LYS:N	2.75	0.44
1:D:314:ILE:C	1:D:316:GLU:H	2.25	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: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: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: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: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:L:9:PHE:C	1:L:11:LYS:H	2.23	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: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:G:30:GLU:C	1:G:32:LEU:N	2.68	0.44
1:H:259:SER:O	1:H:263:LEU:HB2	2.17	0.44
1:H:294:PHE:O	1:H:294:PHE:CG	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:PHE:CE2	1:C:152:LEU:HD11	2.51	0.44
1:D:260:MET:HE3	1:D:288:PRO:HA	1.98	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:F:499:THR:HG1	1:F:500:PHE:HD2	1.64	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:33:LYS:C	1:B:35:ARG:HB3	2.42	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:J:41:LYS:C	1:J:44:ARG:HB2	2.42	0.44
1:J:314:ILE:C	1:J:316:GLU:H	2.25	0.44
1:A:8:ASN:C	1:A:8:ASN:OD1	2.60	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
1:B:238:MET:C	1:B:240:PRO:N	2.75	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:414:GLN:OE1	1:A:428:ILE:HA	2.18	0.44
1:C:247:PHE:CE1	1:C:269:LYS:C	2.96	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: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:134:LYS:C	1:C:136:TYR:N	2.76	0.44
1:C:497:GLY:HA3	1:C:501:THR:HB	2.00	0.44
1:F:362:GLU:C	1:F:364:ASN:H	2.25	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
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:293:ASP:C	1:I:295:LYS:H	2.26	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:410:LEU:HB3	1:L:430:ILE:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLU:C	1:A:105:LYS:N	2.76	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:134:LYS:C	1:F:136:TYR:N	2.77	0.43
1:H:282:ASN:OD1	1:H:283:PRO:HD2	2.18	0.43
1:H:293:ASP:O	1:H:295:LYS:N	2.50	0.43
1:I:28:LEU:C	1:I:32:LEU:HD11	2.43	0.43
1:J:24:VAL:HG22	1:J:483:VAL:HG13	2.00	0.43
1:J:247:PHE:CE1	1:J:269:LYS:C	2.97	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:238:MET:C	1:A:240:PRO:N	2.76	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: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:38:GLU:C	1:I:40:GLN:H	2.26	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:A:314:ILE:C	1:A:316:GLU:N	2.74	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
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:A:362:GLU:C	1:A:364:ASN:H	2.25	0.43
1:B:41:LYS:C	1:B:42:ARG:HG2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:338:ARG:C	1:C:339:VAL:O	2.58	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:H:189:HIS:ND1	1:H:189:HIS:C	2.77	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: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: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:247:PHE:CE1	1:A:269:LYS:C	2.97	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
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:G:247:PHE:CE1	1:G:269:LYS:C	2.97	0.43
1:I:238:MET:O	1:I:239:THR:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:33:LYS:C	1:A:35:ARG:N	2.75	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: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:41:LYS:C	1:B:44:ARG:HB3	2.44	0.43
1:D:12:MET:SD	1:D:354:PRO:HD3	2.58	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:H:247:PHE:CE1	1:H:269:LYS:C	2.97	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:134:LYS:C	1:L:136:TYR:N	2.77	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: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:35:ARG:C	1:I:35:ARG:CD	2.91	0.42
1:I:173:GLU:O	1:I:202:PRO:HD3	2.19	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:239:THR:HA	1:D:240:PRO:HD2	1.66	0.42
1:E:362:GLU:C	1:E:364:ASN:N	2.77	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
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:K:247:PHE:CD1	1:K:269:LYS:C	2.97	0.42
1:L:38:GLU:H	1:L:38:GLU:CD	2.26	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:9:PHE:CZ	1:B:328:GLU:CD	2.97	0.42
1:B:65:ILE:HD13	1:B:144:ILE:HG12	2.01	0.42
1:B:362:GLU:C	1:B:364:ASN:N	2.77	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:E:247:PHE:CE1	1:E:269:LYS:C	2.97	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:G:498:VAL:HG22	1:H:142:GLU:CD	2.44	0.42
1:H:134:LYS:C	1:H:136:TYR:N	2.77	0.42
1:I:357:ASP:OD2	1:I:478:ARG:NE	2.52	0.42
1:L:363:ARG:HH11	1:L:363:ARG:HD3	1.23	0.42
1:A:134:LYS:C	1:A:136:TYR:N	2.77	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:C:290:GLU:O	1:C:291:LEU:C	2.62	0.42
1:D:290:GLU:O	1:D:291:LEU:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:305:PRO:C	1:G:307:ALA:H	2.26	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
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:L:260:MET:HB3	1:L:260:MET:HE2	1.70	0.42
1:B:140:GLU:O	1:B:144:ILE:HG13	2.19	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:L:289:LYS:C	1:L:292:GLU:HB3	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ASN:O	1:B:134:LYS:N	2.53	0.42
1:B:231:SER:HG	1:G:281:TRP:HH2	1.67	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
1:E:132:ASN:C	1:E:134:LYS:H	2.28	0.42
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:G:134:LYS:C	1:G:136:TYR:H	2.25	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:E:168:ASP:CG	1:E:169:MET:H	2.27	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:G:294:PHE:C	1:G:297:GLN:HB3	2.45	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:28:LEU:O	1:F:32:LEU:HD11	2.20	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:J:134:LYS:C	1:J:136:TYR:N	2.78	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:J:30:GLU:N	1:J:32:LEU:HD12	2.35	0.41
1:J:305:PRO:C	1:J:307:ALA:H	2.27	0.41
1:J:315:LEU:C	1:J:316:GLU:HG3	2.45	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:D:134:LYS:C	1:D:136:TYR:N	2.78	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:F:362:GLU:C	1:F:364:ASN:N	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ILE:HG21	1:C:314:ILE:HD13	1.74	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
1:K:189:HIS:ND1	1:K:189:HIS:C	2.77	0.41
1:K:273:VAL:C	1:K:314:ILE:HD13	2.46	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:260:MET:HE2	1:D:260:MET:HB3	1.68	0.41
1:D:314:ILE:C	1:D:316:GLU:N	2.77	0.41
1:D:362:GLU:C	1:D:364:ASN:N	2.78	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: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:L:314:ILE:C	1:L:316:GLU:N	2.78	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:B:238:MET:O	1:B:239:THR:C	2.62	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:B:44:ARG:C	1:B:46:ARG:N	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:134:LYS:C	1:E:136:TYR:N	2.78	0.41
1:E:282:ASN:OD1	1:E:283:PRO:HD2	2.21	0.41
1:G:8:ASN:O	1:G:12:MET:HG3	2.21	0.41
1:K:263:LEU:HD12	1:K:263:LEU:HA	1.84	0.41
1:K:362:GLU:C	1:K:364:ASN:H	2.26	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:362:GLU:C	1:A:364:ASN:N	2.78	0.41
1:A:501:THR:HG22	1:E:147:ARG:CZ	2.51	0.41
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:238:MET:O	1:F:239:THR:C	2.63	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:G:314:ILE:C	1:G:316:GLU:H	2.28	0.41
1:H:42:ARG:O	1:H:44:ARG:N	2.20	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:OD1	1:I:135:ASN:N	2.54	0.41
1:I:259:SER:O	1:I:263:LEU:HB2	2.21	0.41
1:I:362:GLU:C	1:I:364:ASN:N	2.78	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:35:ARG:O	1:K:35:ARG:HG2	1.97	0.41
1:K:103:GLU:C	1:K:105:LYS:N	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:260:MET:HB3	1:E:260:MET:HE2	1.70	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:65:ILE:HG21	1:G:144:ILE:HG12	2.03	0.41
1:G:362:GLU:C	1:G:364:ASN:N	2.78	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:L:263:LEU:HD12	1:L:263:LEU:HA	1.88	0.41
1:A:129:VAL:HG12	1:A:131:ILE:HB	2.03	0.40
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: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:132:ASN:C	1:D:134:LYS:H	2.29	0.40
1:D:247:PHE:CE1	1:D:269:LYS:C	2.99	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:E:314:ILE:C	1:E:316:GLU:H	2.29	0.40
1:F:40:GLN:O	1:F:40:GLN:CD	2.63	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:I:260:MET:HE2	1:I:260:MET:HB3	1.64	0.40
1:J:360:PHE:CG	1:J:365:ILE:HD11	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:260:MET:HE2	1:B:260:MET:HB3	1.70	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: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:259:SER:O	1:F:263:LEU:HB2	2.22	0.40
1:F:260:MET:HE2	1:F:260:MET:HB3	1.70	0.40
1:F:308:LYS:NZ	1:L:469:MET:HB3	2.33	0.40
1:G:238:MET:O	1:G:239:THR:C	2.62	0.40
1:G:322:LEU:HB2	1:G:341:ALA:CB	2.52	0.40
1:J:47:GLY:O	1:J:51:ILE:HG13	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:A:238:MET:O	1:A:239:THR:C	2.61	0.40
1:B:65:ILE:HG21	1:B:144:ILE:HG12	2.03	0.40
1:B:132:ASN:C	1:B:134:LYS:H	2.29	0.40
1:C:31:ASP:OD2	1:C:470:LYS:NZ	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:247:PHE:CD1	1:B:269:LYS:C	3.00	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:E:111:MET:HE2	1:E:378:VAL:HG22	2.04	0.40
1:F:186:THR:HB	1:F:187:ILE:H	1.61	0.40
1:F:314:ILE:C	1:F:316:GLU:H	2.30	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:G:238:MET:C	1:G:240:PRO:N	2.79	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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/496 (100%)	404 (82%)	59 (12%)	31 (6%)	1	12
1	B	494/496 (100%)	404 (82%)	60 (12%)	30 (6%)	1	12
1	C	494/496 (100%)	410 (83%)	54 (11%)	30 (6%)	1	12
1	D	494/496 (100%)	404 (82%)	58 (12%)	32 (6%)	1	11
1	E	494/496 (100%)	410 (83%)	50 (10%)	34 (7%)	1	10
1	F	494/496 (100%)	407 (82%)	56 (11%)	31 (6%)	1	12
1	G	494/496 (100%)	407 (82%)	57 (12%)	30 (6%)	1	12
1	H	494/496 (100%)	407 (82%)	53 (11%)	34 (7%)	1	10
1	I	494/496 (100%)	400 (81%)	61 (12%)	33 (7%)	1	11
1	J	494/496 (100%)	407 (82%)	52 (10%)	35 (7%)	1	10
1	K	494/496 (100%)	403 (82%)	57 (12%)	34 (7%)	1	10
1	L	494/496 (100%)	408 (83%)	54 (11%)	32 (6%)	1	11
All	All	5928/5952 (100%)	4871 (82%)	671 (11%)	386 (6%)	1	11

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	362 (88%)	51 (12%)	4	22
1	B	413/413 (100%)	361 (87%)	52 (13%)	4	21
1	C	413/413 (100%)	363 (88%)	50 (12%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	413/413 (100%)	359 (87%)	54 (13%)	4	20
1	E	413/413 (100%)	358 (87%)	55 (13%)	4	20
1	F	413/413 (100%)	369 (89%)	44 (11%)	6	27
1	G	413/413 (100%)	362 (88%)	51 (12%)	4	22
1	H	413/413 (100%)	360 (87%)	53 (13%)	4	21
1	I	413/413 (100%)	356 (86%)	57 (14%)	3	19
1	J	413/413 (100%)	367 (89%)	46 (11%)	6	25
1	K	413/413 (100%)	357 (86%)	56 (14%)	3	19
1	L	413/413 (100%)	359 (87%)	54 (13%)	4	20
All	All	4956/4956 (100%)	4333 (87%)	623 (13%)	4	21

All (623) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	8	ASN
1	A	11	LYS
1	A	32	LEU
1	A	35	ARG
1	A	38	GLU
1	A	42	ARG
1	A	44	ARG
1	A	45	VAL
1	A	50	ARG
1	A	58	VAL
1	A	60	SER
1	A	61	LEU
1	A	105	LYS
1	A	112	THR
1	A	131	ILE
1	A	134	LYS
1	A	145	THR
1	A	189	HIS
1	A	212	ILE
1	A	213	SER
1	A	227	ILE
1	A	242	PHE
1	A	255	VAL
1	A	271	VAL

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Mol	Chain	Res	Type
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	314	ILE
1	A	315	LEU
1	A	317	VAL
1	A	320	ASP
1	A	322	LEU
1	A	332	THR
1	A	333	LYS
1	A	334	SER
1	A	342	LYS
1	A	344	ILE
1	A	355	GLU
1	A	359	ILE
1	A	409	LEU
1	A	420	LYS
1	A	421	PHE
1	A	423	LYS
1	A	430	ILE
1	A	431	VAL
1	A	446	LYS
1	A	501	THR
1	B	11	LYS
1	B	29	VAL
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	58	VAL
1	B	60	SER
1	B	61	LEU
1	B	98	ASP
1	B	103	GLU
1	B	112	THR

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Mol	Chain	Res	Type
1	B	131	ILE
1	B	135	ASN
1	B	145	THR
1	B	169	MET
1	B	174	ARG
1	B	189	HIS
1	B	212	ILE
1	B	213	SER
1	B	227	ILE
1	B	235	ILE
1	B	242	PHE
1	B	255	VAL
1	B	269	LYS
1	B	271	VAL
1	B	281	TRP
1	B	295	LYS
1	B	306	LYS
1	B	308	LYS
1	B	314	ILE
1	B	322	LEU
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	344	ILE
1	B	402	GLU
1	B	409	LEU
1	B	421	PHE
1	B	430	ILE
1	B	431	VAL
1	B	435	GLU
1	B	446	LYS
1	B	469	MET
1	C	6	ASP
1	C	34	THR
1	C	38	GLU
1	C	41	LYS
1	C	42	ARG
1	C	45	VAL

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Mol	Chain	Res	Type
1	C	58	VAL
1	C	60	SER
1	C	61	LEU
1	C	69	ASP
1	C	87	THR
1	C	112	THR
1	C	131	ILE
1	C	134	LYS
1	C	145	THR
1	C	212	ILE
1	C	213	SER
1	C	227	ILE
1	C	235	ILE
1	C	242	PHE
1	C	255	VAL
1	C	265	ARG
1	C	271	VAL
1	C	275	GLU
1	C	277	ASP
1	C	281	TRP
1	C	289	LYS
1	C	295	LYS
1	C	300	THR
1	C	306	LYS
1	C	308	LYS
1	C	314	ILE
1	C	317	VAL
1	C	320	ASP
1	C	322	LEU
1	C	327	SER
1	C	328	GLU
1	C	329	LYS
1	C	334	SER
1	C	339	VAL
1	C	344	ILE
1	C	352	THR
1	C	362	GLU
1	C	403	ARG
1	C	421	PHE
1	C	430	ILE
1	C	431	VAL
1	C	435	GLU

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Mol	Chain	Res	Type
1	C	477	LEU
1	C	498	VAL
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	45	VAL
1	D	58	VAL
1	D	60	SER
1	D	61	LEU
1	D	105	LYS
1	D	112	THR
1	D	130	LYS
1	D	131	ILE
1	D	145	THR
1	D	169	MET
1	D	174	ARG
1	D	212	ILE
1	D	213	SER
1	D	227	ILE
1	D	234	SER
1	D	242	PHE
1	D	247	PHE
1	D	255	VAL
1	D	265	ARG
1	D	269	LYS
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	314	ILE
1	D	317	VAL

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Mol	Chain	Res	Type
1	D	328	GLU
1	D	331	LEU
1	D	332	THR
1	D	334	SER
1	D	338	ARG
1	D	340	LYS
1	D	344	ILE
1	D	409	LEU
1	D	418	GLU
1	D	421	PHE
1	D	430	ILE
1	D	431	VAL
1	D	439	ARG
1	D	498	VAL
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	58	VAL
1	E	60	SER
1	E	61	LEU
1	E	112	THR
1	E	131	ILE
1	E	145	THR
1	E	169	MET
1	E	174	ARG
1	E	212	ILE
1	E	213	SER
1	E	227	ILE
1	E	235	ILE
1	E	242	PHE
1	E	245	LYS
1	E	255	VAL
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	317	VAL
1	E	320	ASP
1	E	322	LEU
1	E	332	THR
1	E	333	LYS
1	E	334	SER
1	E	340	LYS
1	E	342	LYS
1	E	344	ILE
1	E	358	LYS
1	E	378	VAL
1	E	400	LYS
1	E	420	LYS
1	E	423	LYS
1	E	430	ILE
1	E	431	VAL
1	E	435	GLU
1	E	446	LYS
1	E	472	ASN
1	F	6	ASP
1	F	11	LYS
1	F	29	VAL
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	58	VAL
1	F	60	SER
1	F	61	LEU
1	F	112	THR
1	F	131	ILE

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Mol	Chain	Res	Type
1	F	145	THR
1	F	212	ILE
1	F	227	ILE
1	F	235	ILE
1	F	242	PHE
1	F	255	VAL
1	F	269	LYS
1	F	271	VAL
1	F	277	ASP
1	F	281	TRP
1	F	289	LYS
1	F	295	LYS
1	F	306	LYS
1	F	309	ILE
1	F	314	ILE
1	F	316	GLU
1	F	317	VAL
1	F	322	LEU
1	F	329	LYS
1	F	332	THR
1	F	333	LYS
1	F	344	ILE
1	F	400	LYS
1	F	420	LYS
1	F	421	PHE
1	F	423	LYS
1	F	430	ILE
1	F	431	VAL
1	F	446	LYS
1	G	19	ARG
1	G	27	LYS
1	G	30	GLU
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

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Mol	Chain	Res	Type
1	G	58	VAL
1	G	60	SER
1	G	61	LEU
1	G	98	ASP
1	G	112	THR
1	G	131	ILE
1	G	135	ASN
1	G	145	THR
1	G	174	ARG
1	G	212	ILE
1	G	213	SER
1	G	227	ILE
1	G	242	PHE
1	G	245	LYS
1	G	255	VAL
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	317	VAL
1	G	322	LEU
1	G	327	SER
1	G	332	THR
1	G	333	LYS
1	G	344	ILE
1	G	409	LEU
1	G	420	LYS
1	G	421	PHE
1	G	423	LYS
1	G	424	HIS
1	G	428	ILE
1	G	430	ILE
1	G	431	VAL
1	G	458	GLU
1	G	470	LYS
1	H	6	ASP
1	H	11	LYS
1	H	32	LEU
1	H	34	THR

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Mol	Chain	Res	Type
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	58	VAL
1	H	60	SER
1	H	61	LEU
1	H	69	ASP
1	H	112	THR
1	H	131	ILE
1	H	145	THR
1	H	189	HIS
1	H	212	ILE
1	H	213	SER
1	H	227	ILE
1	H	231	SER
1	H	235	ILE
1	H	238	MET
1	H	239	THR
1	H	242	PHE
1	H	246	THR
1	H	255	VAL
1	H	269	LYS
1	H	271	VAL
1	H	281	TRP
1	H	295	LYS
1	H	302	LEU
1	H	306	LYS
1	H	309	ILE
1	H	311	GLU
1	H	313	SER
1	H	314	ILE
1	H	317	VAL
1	H	322	LEU
1	H	332	THR
1	H	334	SER
1	H	340	LYS
1	H	342	LYS
1	H	344	ILE
1	H	355	GLU

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Mol	Chain	Res	Type
1	H	362	GLU
1	H	420	LYS
1	H	430	ILE
1	H	431	VAL
1	H	446	LYS
1	H	498	VAL
1	H	501	THR
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	44	ARG
1	I	45	VAL
1	I	46	ARG
1	I	58	VAL
1	I	60	SER
1	I	61	LEU
1	I	98	ASP
1	I	112	THR
1	I	131	ILE
1	I	145	THR
1	I	212	ILE
1	I	213	SER
1	I	217	ARG
1	I	227	ILE
1	I	242	PHE
1	I	245	LYS
1	I	246	THR
1	I	255	VAL
1	I	261	ARG
1	I	269	LYS
1	I	271	VAL
1	I	280	ILE
1	I	281	TRP
1	I	286	ILE
1	I	289	LYS
1	I	291	LEU
1	I	295	LYS
1	I	302	LEU
1	I	311	GLU

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Mol	Chain	Res	Type
1	I	313	SER
1	I	314	ILE
1	I	316	GLU
1	I	317	VAL
1	I	322	LEU
1	I	327	SER
1	I	328	GLU
1	I	332	THR
1	I	333	LYS
1	I	334	SER
1	I	344	ILE
1	I	355	GLU
1	I	359	ILE
1	I	362	GLU
1	I	409	LEU
1	I	421	PHE
1	I	423	LYS
1	I	430	ILE
1	I	431	VAL
1	I	451	SER
1	I	479	THR
1	I	498	VAL
1	J	11	LYS
1	J	27	LYS
1	J	32	LEU
1	J	38	GLU
1	J	44	ARG
1	J	45	VAL
1	J	46	ARG
1	J	50	ARG
1	J	58	VAL
1	J	60	SER
1	J	61	LEU
1	J	87	THR
1	J	112	THR
1	J	131	ILE
1	J	145	THR
1	J	189	HIS
1	J	212	ILE
1	J	213	SER
1	J	227	ILE
1	J	235	ILE

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Mol	Chain	Res	Type
1	J	242	PHE
1	J	245	LYS
1	J	255	VAL
1	J	271	VAL
1	J	277	ASP
1	J	281	TRP
1	J	289	LYS
1	J	295	LYS
1	J	297	GLN
1	J	298	HIS
1	J	308	LYS
1	J	314	ILE
1	J	317	VAL
1	J	322	LEU
1	J	332	THR
1	J	333	LYS
1	J	334	SER
1	J	338	ARG
1	J	344	ILE
1	J	400	LYS
1	J	402	GLU
1	J	420	LYS
1	J	421	PHE
1	J	430	ILE
1	J	431	VAL
1	J	501	THR
1	K	6	ASP
1	K	11	LYS
1	K	19	ARG
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	50	ARG
1	K	58	VAL
1	K	60	SER
1	K	61	LEU
1	K	112	THR
1	K	131	ILE
1	K	134	LYS

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Mol	Chain	Res	Type
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	227	ILE
1	K	235	ILE
1	K	236	LEU
1	K	242	PHE
1	K	246	THR
1	K	250	GLN
1	K	255	VAL
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	306	LYS
1	K	308	LYS
1	K	314	ILE
1	K	316	GLU
1	K	322	LEU
1	K	327	SER
1	K	332	THR
1	K	334	SER
1	K	338	ARG
1	K	340	LYS
1	K	344	ILE
1	K	349	ASN
1	K	355	GLU
1	K	363	ARG
1	K	400	LYS
1	K	430	ILE
1	K	431	VAL
1	K	458	GLU
1	K	477	LEU
1	L	19	ARG
1	L	32	LEU

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Mol	Chain	Res	Type
1	L	36	GLU
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	58	VAL
1	L	60	SER
1	L	61	LEU
1	L	69	ASP
1	L	87	THR
1	L	112	THR
1	L	131	ILE
1	L	145	THR
1	L	190	TYR
1	L	212	ILE
1	L	213	SER
1	L	227	ILE
1	L	231	SER
1	L	235	ILE
1	L	242	PHE
1	L	245	LYS
1	L	246	THR
1	L	247	PHE
1	L	255	VAL
1	L	269	LYS
1	L	271	VAL
1	L	281	TRP
1	L	292	GLU
1	L	295	LYS
1	L	296	LEU
1	L	311	GLU
1	L	314	ILE
1	L	317	VAL
1	L	322	LEU
1	L	332	THR
1	L	334	SER
1	L	338	ARG
1	L	344	ILE
1	L	355	GLU

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Mol	Chain	Res	Type
1	L	403	ARG
1	L	420	LYS
1	L	424	HIS
1	L	430	ILE
1	L	431	VAL
1	L	435	GLU
1	L	439	ARG
1	L	475	LEU
1	L	498	VAL
1	L	501	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	254	ASN
1	A	297	GLN
1	A	298	HIS
1	A	437	GLN
1	A	494	ASN
1	B	43	ASN
1	B	209	HIS
1	B	254	ASN
1	B	484	ASN
1	B	494	ASN
1	C	43	ASN
1	C	132	ASN
1	C	254	ASN
1	C	264	HIS
1	C	450	HIS
1	C	484	ASN
1	D	43	ASN
1	D	254	ASN
1	D	297	GLN
1	E	43	ASN
1	E	254	ASN
1	E	298	HIS
1	E	388	ASN
1	E	391	HIS
1	E	472	ASN
1	F	43	ASN
1	F	254	ASN

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Mol	Chain	Res	Type
1	F	408	HIS
1	F	472	ASN
1	F	484	ASN
1	G	43	ASN
1	G	254	ASN
1	G	450	HIS
1	G	484	ASN
1	H	43	ASN
1	H	221	HIS
1	H	254	ASN
1	H	437	GLN
1	H	450	HIS
1	H	494	ASN
1	I	43	ASN
1	I	209	HIS
1	I	254	ASN
1	J	43	ASN
1	J	225	ASN
1	J	254	ASN
1	J	406	ASN
1	J	408	HIS
1	J	494	ASN
1	K	43	ASN
1	K	209	HIS
1	K	254	ASN
1	L	43	ASN
1	L	254	ASN
1	L	408	HIS
1	L	424	HIS
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	602	-	28,29,29	1.42	4 (14%)	43,45,45	1.82	9 (20%)
2	ADP	I	601	-	28,29,29	1.44	5 (17%)	43,45,45	1.78	8 (18%)
2	ADP	H	601	-	28,29,29	1.43	5 (17%)	43,45,45	1.81	9 (20%)
2	ADP	L	601	-	28,29,29	1.44	5 (17%)	43,45,45	1.82	8 (18%)
2	ADP	C	601	-	28,29,29	1.43	4 (14%)	43,45,45	1.82	9 (20%)
2	ADP	J	601	-	28,29,29	1.45	5 (17%)	43,45,45	1.79	9 (20%)
2	ADP	D	601	-	28,29,29	1.42	4 (14%)	43,45,45	1.81	10 (23%)
2	ADP	G	601	-	28,29,29	1.43	5 (17%)	43,45,45	1.81	8 (18%)
2	ADP	A	601	-	28,29,29	1.43	5 (17%)	43,45,45	1.80	10 (23%)
2	ADP	K	601	-	28,29,29	1.42	4 (14%)	43,45,45	1.82	9 (20%)
2	ADP	B	601	-	28,29,29	1.44	5 (17%)	43,45,45	1.79	9 (20%)
2	ADP	F	601	-	28,29,29	1.44	5 (17%)	43,45,45	1.83	10 (23%)

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	C	602	-	-	2/16/32/32	0/3/3/3
2	ADP	I	601	-	-	1/16/32/32	0/3/3/3
2	ADP	H	601	-	-	3/16/32/32	0/3/3/3
2	ADP	L	601	-	-	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	C	601	-	-	1/16/32/32	0/3/3/3
2	ADP	J	601	-	-	4/16/32/32	0/3/3/3
2	ADP	D	601	-	-	2/16/32/32	0/3/3/3
2	ADP	G	601	-	-	3/16/32/32	0/3/3/3
2	ADP	A	601	-	-	4/16/32/32	0/3/3/3
2	ADP	K	601	-	-	6/16/32/32	0/3/3/3
2	ADP	B	601	-	-	5/16/32/32	0/3/3/3
2	ADP	F	601	-	-	7/16/32/32	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	602	ADP	C5-C4	4.79	1.47	1.39
2	L	601	ADP	C5-C4	4.79	1.47	1.39
2	I	601	ADP	C5-C4	4.77	1.47	1.39
2	J	601	ADP	C5-C4	4.76	1.47	1.39
2	K	601	ADP	C5-C4	4.74	1.47	1.39
2	C	601	ADP	C5-C4	4.73	1.47	1.39
2	F	601	ADP	C5-C4	4.73	1.47	1.39
2	H	601	ADP	C5-C4	4.73	1.47	1.39
2	G	601	ADP	C5-C4	4.72	1.47	1.39
2	B	601	ADP	C5-C4	4.70	1.47	1.39
2	A	601	ADP	C5-C4	4.70	1.47	1.39
2	D	601	ADP	C5-C4	4.60	1.47	1.39
2	K	601	ADP	C5-C6	2.85	1.48	1.41
2	H	601	ADP	C5-C6	2.85	1.48	1.41
2	J	601	ADP	C5-C6	2.84	1.48	1.41
2	D	601	ADP	C5-C6	2.84	1.48	1.41
2	L	601	ADP	C5-C6	2.83	1.48	1.41
2	C	601	ADP	C5-C6	2.83	1.48	1.41
2	A	601	ADP	C5-C6	2.83	1.48	1.41
2	I	601	ADP	C5-C6	2.82	1.48	1.41
2	F	601	ADP	C5-C6	2.82	1.48	1.41
2	G	601	ADP	C5-C6	2.81	1.48	1.41
2	B	601	ADP	C5-C6	2.80	1.48	1.41
2	C	602	ADP	C5-C6	2.77	1.48	1.41
2	D	601	ADP	C8-N7	2.53	1.36	1.31
2	A	601	ADP	C8-N7	2.51	1.36	1.31
2	L	601	ADP	C8-N7	2.50	1.36	1.31
2	B	601	ADP	C8-N7	2.50	1.36	1.31
2	H	601	ADP	C8-N7	2.48	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	601	ADP	C8-N7	2.47	1.36	1.31
2	F	601	ADP	C8-N7	2.47	1.36	1.31
2	C	601	ADP	C8-N7	2.46	1.36	1.31
2	J	601	ADP	C8-N7	2.45	1.36	1.31
2	I	601	ADP	C8-N7	2.43	1.36	1.31
2	G	601	ADP	C8-N7	2.38	1.36	1.31
2	C	602	ADP	C8-N7	2.34	1.36	1.31
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	G	601	ADP	C5-N7	-2.21	1.35	1.39
2	C	602	ADP	C5-N7	-2.21	1.35	1.39
2	I	601	ADP	C5-N7	-2.20	1.35	1.39
2	J	601	ADP	C5-N7	-2.19	1.35	1.39
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	K	601	ADP	C5-N7	-2.15	1.35	1.39
2	F	601	ADP	C5-N7	-2.14	1.35	1.39
2	H	601	ADP	C5-N7	-2.14	1.35	1.39
2	B	601	ADP	C5-N7	-2.14	1.35	1.39
2	D	601	ADP	C5-N7	-2.14	1.35	1.39
2	A	601	ADP	C5-N7	-2.14	1.35	1.39
2	L	601	ADP	C5-N7	-2.13	1.35	1.39
2	C	601	ADP	C5-N7	-2.11	1.35	1.39
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 (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	ADP	C5-C4-N3	-5.92	118.56	126.72
2	F	601	ADP	C5-C4-N3	-5.85	118.66	126.72
2	C	602	ADP	C5-C4-N3	-5.83	118.68	126.72
2	L	601	ADP	C5-C4-N3	-5.82	118.70	126.72
2	I	601	ADP	C5-C4-N3	-5.78	118.76	126.72
2	C	601	ADP	C5-C4-N3	-5.77	118.77	126.72
2	J	601	ADP	C5-C4-N3	-5.73	118.83	126.72
2	H	601	ADP	C5-C4-N3	-5.72	118.84	126.72
2	K	601	ADP	C5-C4-N3	-5.72	118.84	126.72
2	A	601	ADP	C5-C4-N3	-5.60	119.00	126.72
2	B	601	ADP	C5-C4-N3	-5.56	119.06	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	ADP	C5-C4-N3	-5.56	119.07	126.72
2	C	602	ADP	N3-C4-N9	4.67	135.12	127.17
2	G	601	ADP	N3-C4-N9	4.60	135.00	127.17
2	F	601	ADP	N3-C4-N9	4.53	134.88	127.17
2	I	601	ADP	N3-C4-N9	4.51	134.84	127.17
2	J	601	ADP	N3-C4-N9	4.41	134.66	127.17
2	L	601	ADP	N3-C4-N9	4.41	134.66	127.17
2	C	601	ADP	N3-C4-N9	4.39	134.64	127.17
2	H	601	ADP	N3-C4-N9	4.38	134.62	127.17
2	K	601	ADP	N3-C4-N9	4.34	134.56	127.17
2	B	601	ADP	N3-C4-N9	4.24	134.37	127.17
2	A	601	ADP	N3-C4-N9	4.22	134.34	127.17
2	D	601	ADP	N3-C4-N9	4.15	134.22	127.17
2	A	601	ADP	C4-C5-N7	-3.77	106.28	110.58
2	D	601	ADP	C4-C5-N7	-3.73	106.31	110.58
2	C	601	ADP	C2-N3-C4	3.73	120.94	111.83
2	C	601	ADP	C4-C5-N7	-3.73	106.32	110.58
2	K	601	ADP	C4-C5-N7	-3.71	106.34	110.58
2	H	601	ADP	C2-N3-C4	3.71	120.88	111.83
2	F	601	ADP	C2-N3-C4	3.70	120.88	111.83
2	L	601	ADP	C4-C5-N7	-3.70	106.35	110.58
2	L	601	ADP	C2-N3-C4	3.69	120.84	111.83
2	J	601	ADP	C2-N3-C4	3.67	120.80	111.83
2	K	601	ADP	C2-N3-C4	3.67	120.80	111.83
2	D	601	ADP	C2-N3-C4	3.66	120.77	111.83
2	I	601	ADP	C2-N3-C4	3.66	120.77	111.83
2	C	602	ADP	C2-N3-C4	3.66	120.76	111.83
2	A	601	ADP	C2-N3-C4	3.65	120.75	111.83
2	G	601	ADP	C2-N3-C4	3.65	120.74	111.83
2	B	601	ADP	C2-N3-C4	3.63	120.71	111.83
2	B	601	ADP	C4-C5-N7	-3.62	106.45	110.58
2	H	601	ADP	C4-C5-N7	-3.61	106.45	110.58
2	J	601	ADP	C4-C5-N7	-3.60	106.46	110.58
2	F	601	ADP	C4-C5-N7	-3.60	106.47	110.58
2	G	601	ADP	C4-C5-N7	-3.60	106.47	110.58
2	I	601	ADP	C4-C5-N7	-3.55	106.52	110.58
2	C	602	ADP	C4-C5-N7	-3.41	106.68	110.58
2	H	601	ADP	N3-C2-N1	-3.27	123.64	128.58
2	D	601	ADP	N3-C2-N1	-3.26	123.65	128.58
2	C	601	ADP	N3-C2-N1	-3.24	123.67	128.58
2	B	601	ADP	N3-C2-N1	-3.24	123.69	128.58
2	J	601	ADP	N3-C2-N1	-3.17	123.78	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ADP	N3-C2-N1	-3.17	123.79	128.58
2	F	601	ADP	N3-C2-N1	-3.16	123.80	128.58
2	K	601	ADP	N3-C2-N1	-3.15	123.82	128.58
2	C	602	ADP	N3-C2-N1	-3.15	123.82	128.58
2	L	601	ADP	N3-C2-N1	-3.14	123.83	128.58
2	I	601	ADP	N3-C2-N1	-3.12	123.86	128.58
2	G	601	ADP	N3-C2-N1	-2.96	124.10	128.58
2	A	601	ADP	C5-N7-C8	2.67	107.65	103.45
2	D	601	ADP	C5-N7-C8	2.66	107.63	103.45
2	C	602	ADP	C4-N9-C8	2.65	108.52	105.74
2	C	601	ADP	C5-N7-C8	2.64	107.60	103.45
2	K	601	ADP	C5-N7-C8	2.63	107.59	103.45
2	D	601	ADP	C4-N9-C8	2.63	108.50	105.74
2	I	601	ADP	C4-N9-C8	2.62	108.49	105.74
2	F	601	ADP	C4-N9-C8	2.62	108.49	105.74
2	L	601	ADP	C5-N7-C8	2.61	107.56	103.45
2	C	601	ADP	C4-N9-C8	2.61	108.48	105.74
2	G	601	ADP	C5-N7-C8	2.61	107.55	103.45
2	A	601	ADP	C4-N9-C8	2.61	108.48	105.74
2	B	601	ADP	C4-N9-C8	2.60	108.47	105.74
2	J	601	ADP	C5-N7-C8	2.59	107.51	103.45
2	H	601	ADP	C5-N7-C8	2.58	107.50	103.45
2	K	601	ADP	C4-N9-C8	2.57	108.44	105.74
2	F	601	ADP	C5-N7-C8	2.57	107.49	103.45
2	I	601	ADP	C5-N7-C8	2.56	107.47	103.45
2	H	601	ADP	C4-N9-C8	2.55	108.42	105.74
2	J	601	ADP	C4-N9-C8	2.55	108.42	105.74
2	B	601	ADP	C5-N7-C8	2.55	107.45	103.45
2	G	601	ADP	C4-N9-C8	2.54	108.40	105.74
2	C	602	ADP	C5-N7-C8	2.49	107.37	103.45
2	D	601	ADP	O4'-C1'-N9	2.46	112.82	108.09
2	L	601	ADP	C4-N9-C8	2.44	108.30	105.74
2	A	601	ADP	C6-C5-N7	2.42	136.76	132.09
2	D	601	ADP	C6-C5-N7	2.41	136.74	132.09
2	C	601	ADP	C6-C5-N7	2.35	136.62	132.09
2	A	601	ADP	O4'-C1'-N9	2.34	112.58	108.09
2	J	601	ADP	C3'-C2'-C1'	2.32	105.86	101.46
2	K	601	ADP	C6-C5-N7	2.31	136.55	132.09
2	B	601	ADP	C6-C5-N7	2.31	136.54	132.09
2	H	601	ADP	C6-C5-N7	2.27	136.47	132.09
2	C	602	ADP	C3'-C2'-C1'	2.25	105.72	101.46
2	L	601	ADP	C6-C5-N7	2.23	136.39	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	601	ADP	C6-C5-N7	2.23	136.38	132.09
2	F	601	ADP	O4'-C1'-N9	2.19	112.30	108.09
2	D	601	ADP	N9-C8-N7	-2.18	110.85	113.94
2	I	601	ADP	C6-C5-N7	2.18	136.28	132.09
2	F	601	ADP	C6-C5-N7	2.16	136.26	132.09
2	A	601	ADP	N9-C8-N7	-2.12	110.93	113.94
2	G	601	ADP	C6-C5-N7	2.11	136.16	132.09
2	C	601	ADP	N9-C8-N7	-2.07	111.01	113.94
2	K	601	ADP	N9-C8-N7	-2.05	111.03	113.94
2	B	601	ADP	N9-C8-N7	-2.03	111.06	113.94
2	F	601	ADP	N9-C8-N7	-2.01	111.08	113.94
2	H	601	ADP	N9-C8-N7	-2.01	111.08	113.94
2	C	602	ADP	C6-C5-N7	2.00	135.96	132.09

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
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'

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Mol	Chain	Res	Type	Atoms
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

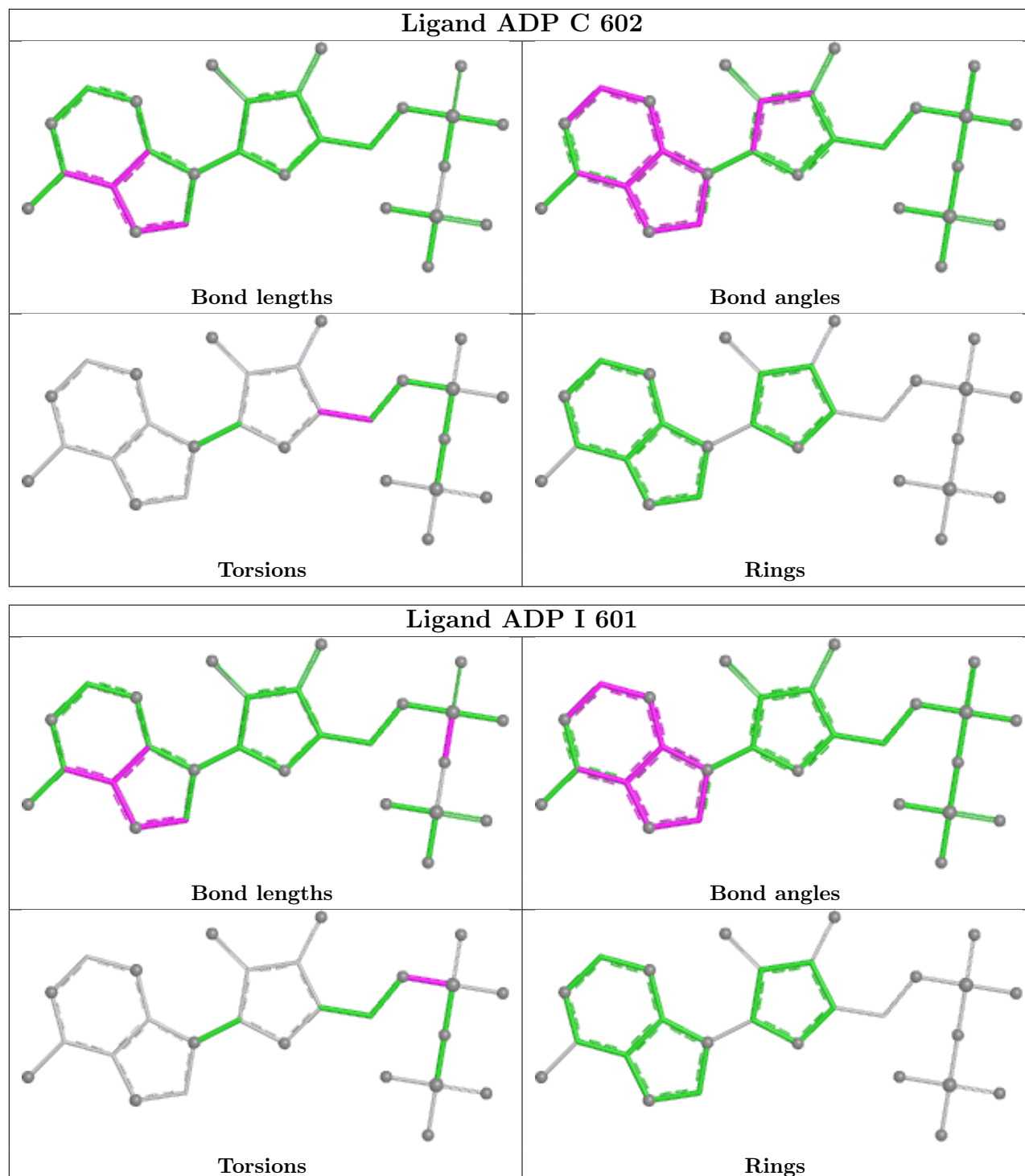
There are no ring outliers.

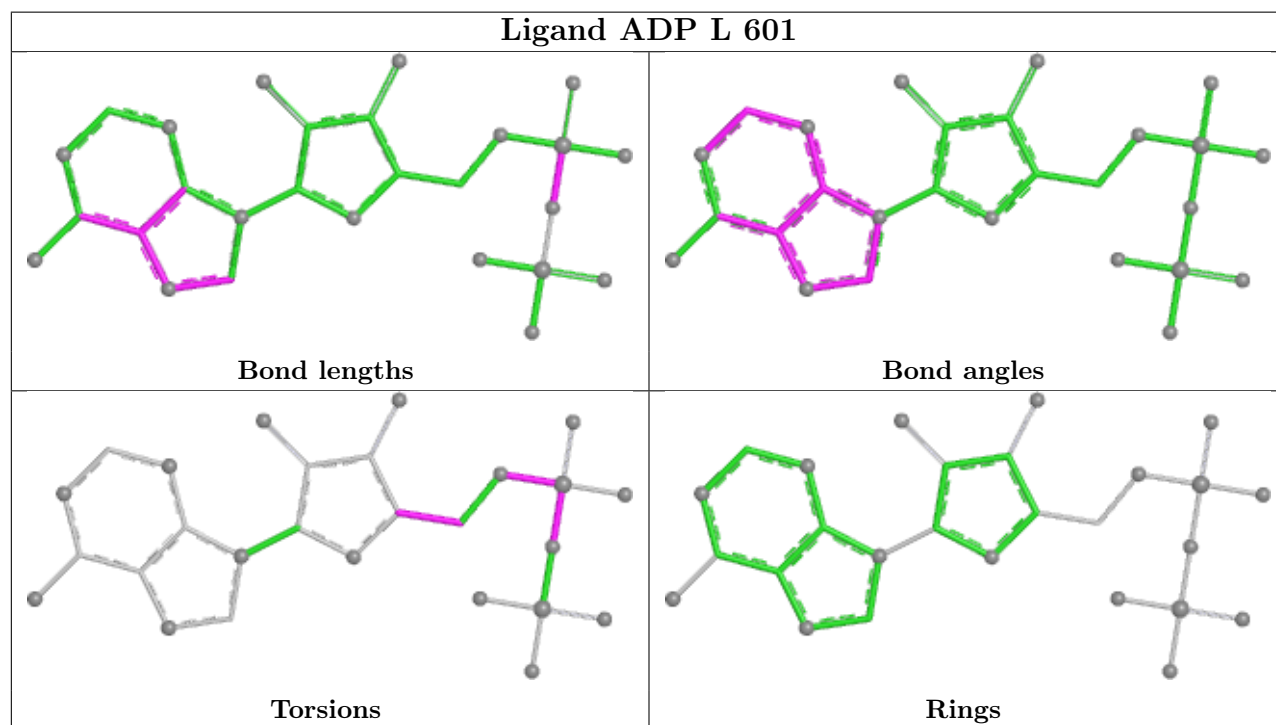
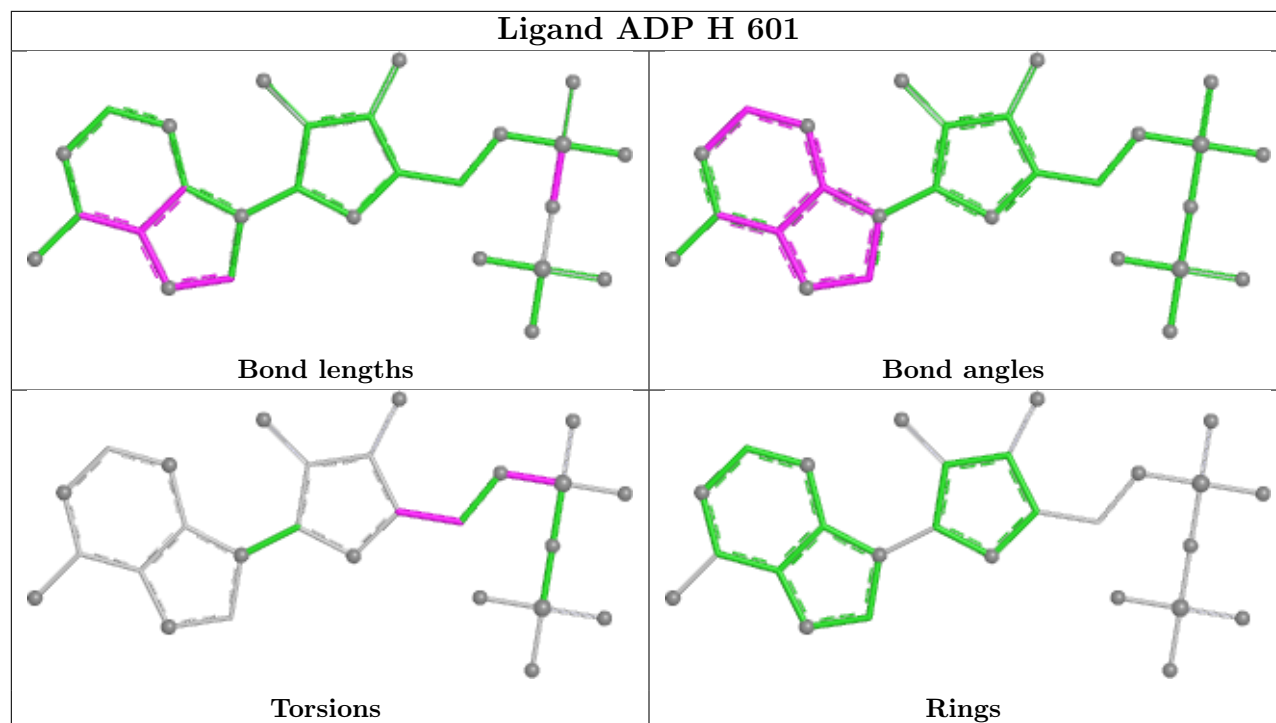
7 monomers are involved in 9 short contacts:

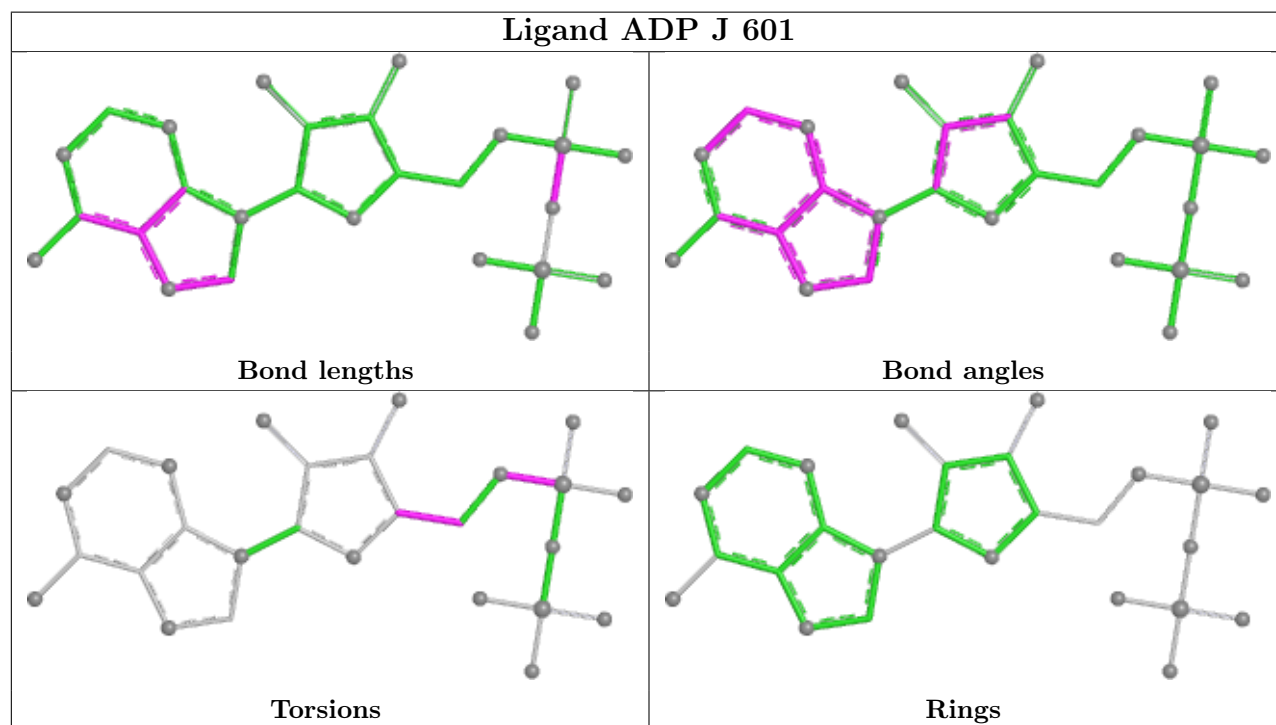
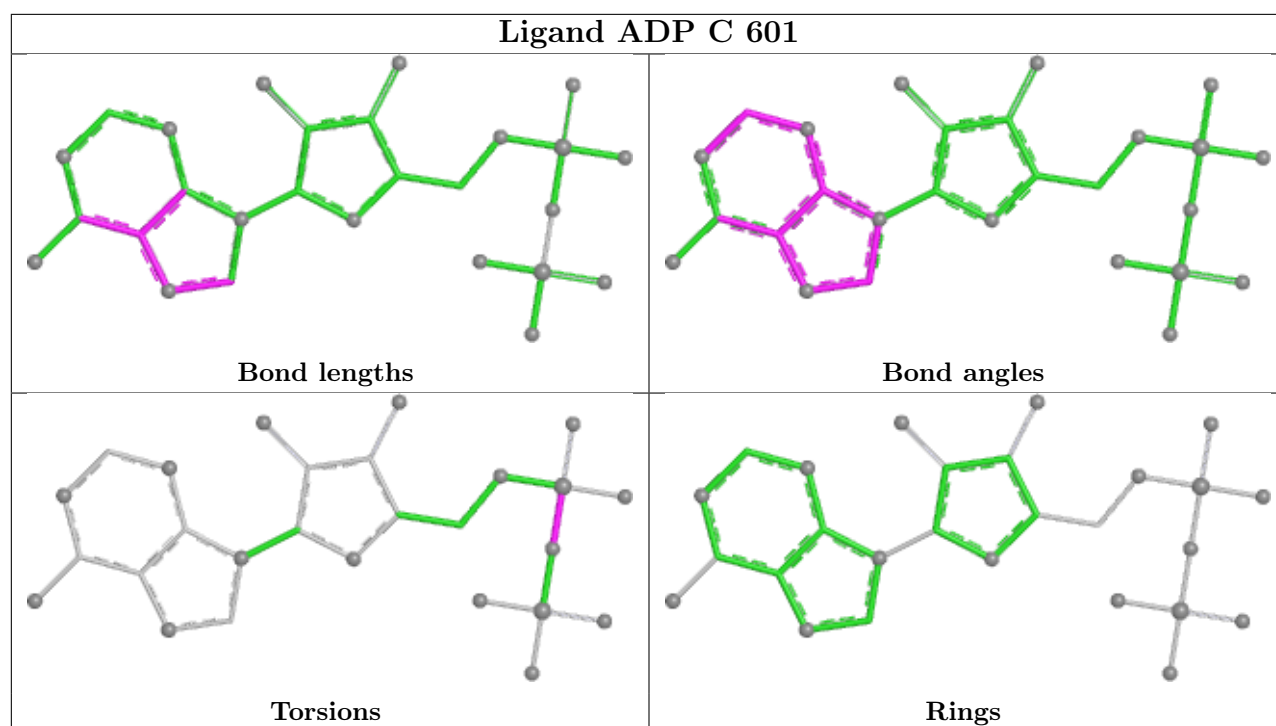
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	ADP	1	0
2	H	601	ADP	2	0
2	L	601	ADP	1	0
2	C	601	ADP	1	0
2	D	601	ADP	1	0
2	B	601	ADP	2	0
2	F	601	ADP	1	0

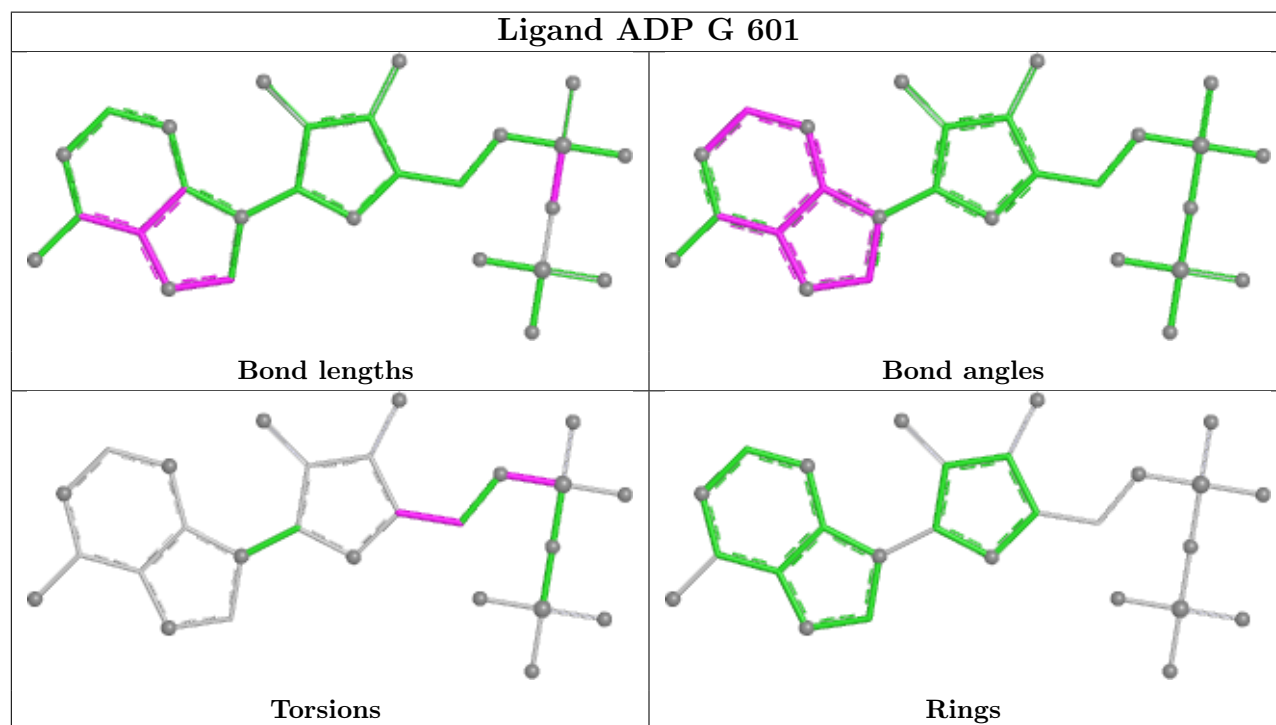
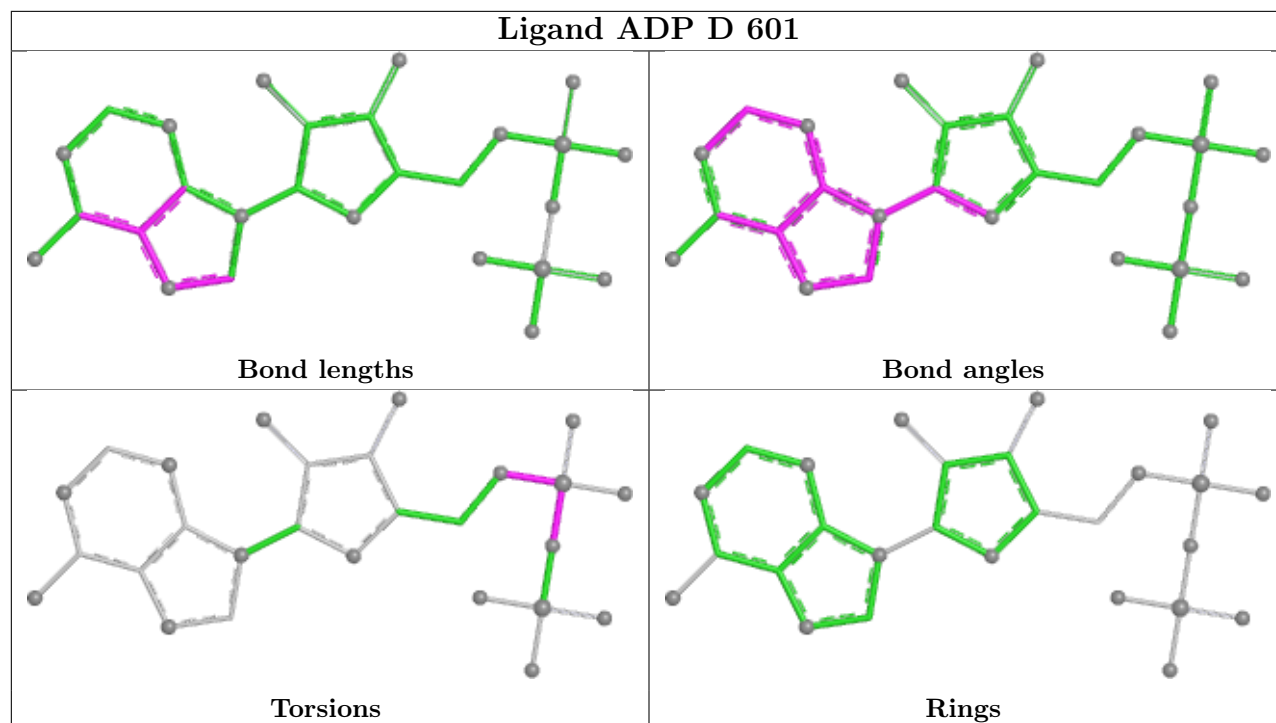
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

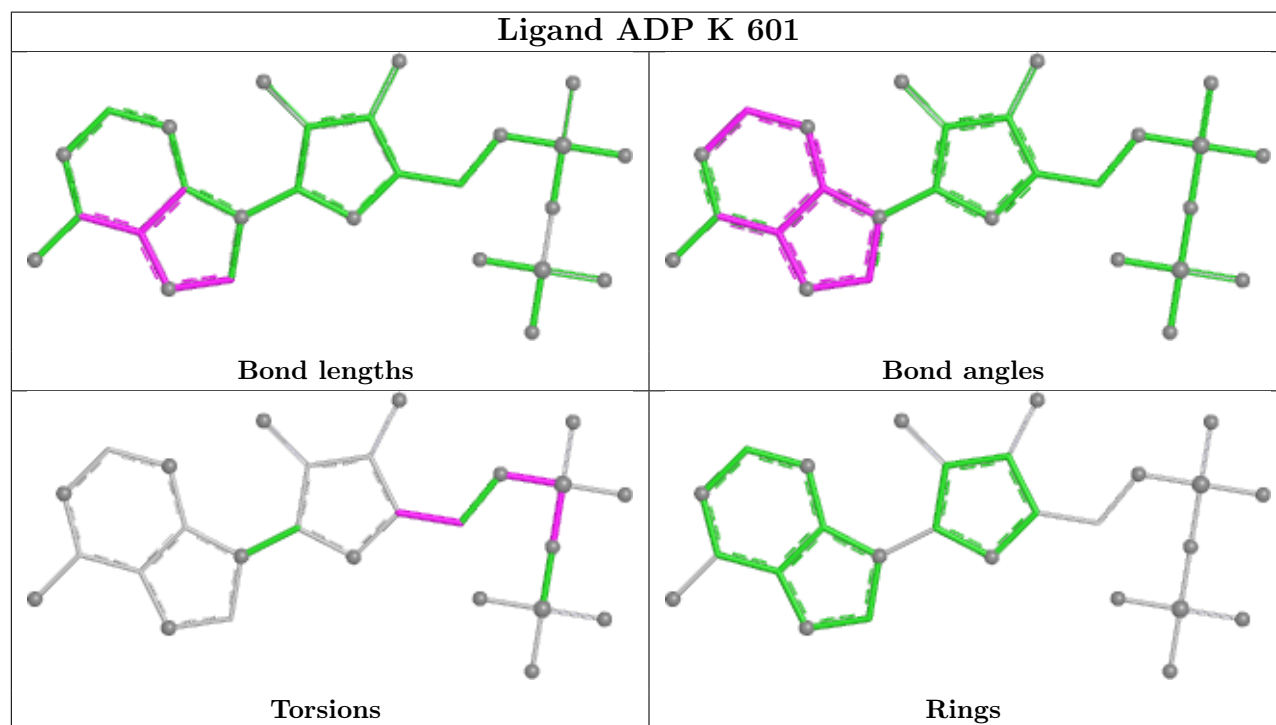
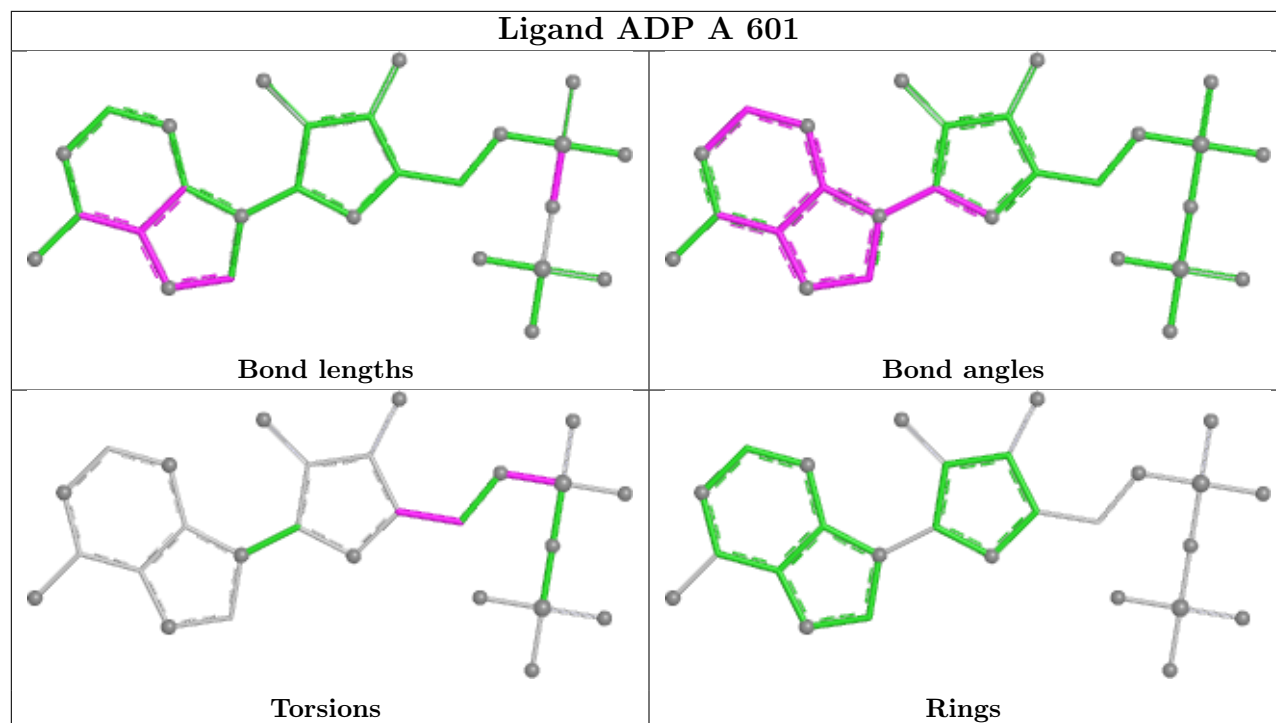
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

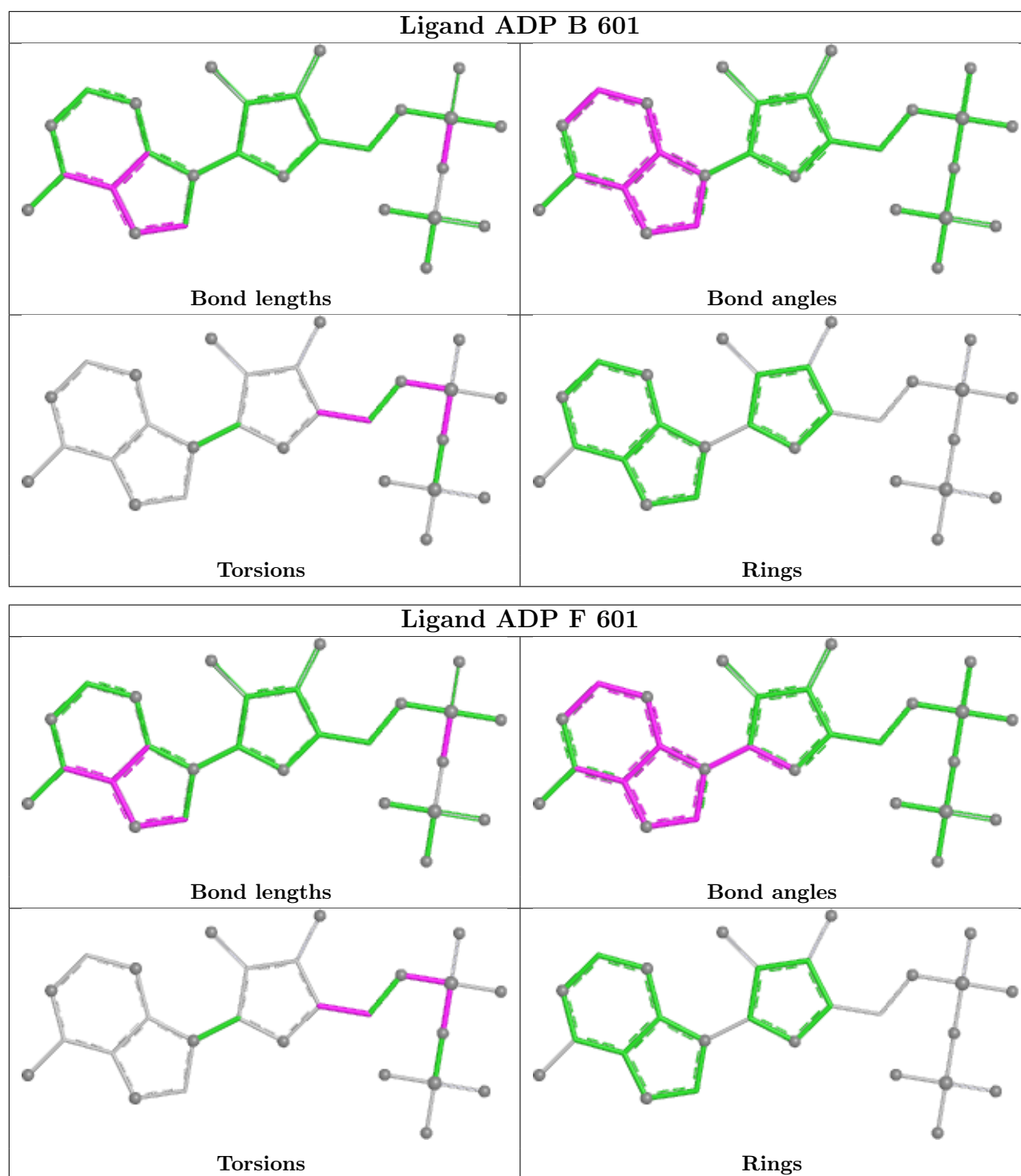












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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%)	-0.13	2 (0%) 88 72	40, 88, 150, 185	0
1	B	496/496 (100%)	-0.18	1 (0%) 91 82	44, 76, 135, 170	0
1	C	496/496 (100%)	-0.01	6 (1%) 76 52	43, 85, 152, 179	0
1	D	496/496 (100%)	-0.15	1 (0%) 91 82	42, 87, 147, 184	0
1	E	496/496 (100%)	-0.09	2 (0%) 88 72	47, 75, 128, 175	0
1	F	496/496 (100%)	-0.20	2 (0%) 88 72	39, 73, 132, 191	0
1	G	496/496 (100%)	-0.20	3 (0%) 85 65	37, 70, 130, 175	0
1	H	496/496 (100%)	-0.11	2 (0%) 88 72	38, 77, 137, 180	0
1	I	496/496 (100%)	-0.01	5 (1%) 79 56	49, 92, 154, 184	0
1	J	496/496 (100%)	-0.17	7 (1%) 73 48	39, 76, 131, 172	0
1	K	496/496 (100%)	-0.03	3 (0%) 85 65	41, 90, 150, 194	0
1	L	496/496 (100%)	-0.07	5 (1%) 79 56	40, 81, 151, 181	0
All	All	5952/5952 (100%)	-0.11	39 (0%) 84 63	37, 80, 146, 194	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	430	ILE	4.8
1	J	243	GLY	3.9
1	A	430	ILE	3.9
1	C	430	ILE	3.8
1	I	498	VAL	3.7
1	F	430	ILE	3.6
1	C	341	ALA	3.5
1	L	501	THR	3.5
1	J	430	ILE	3.4
1	E	430	ILE	3.3
1	K	421	PHE	3.0

Continued on next page...

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Mol	Chain	Res	Type	RSRZ
1	C	351	PRO	2.8
1	L	430	ILE	2.7
1	E	427	THR	2.6
1	A	497	GLY	2.6
1	I	43	ASN	2.6
1	J	240	PRO	2.5
1	C	251	GLY	2.4
1	F	431	VAL	2.4
1	C	421	PHE	2.3
1	I	499	THR	2.3
1	L	315	LEU	2.3
1	B	243	GLY	2.3
1	H	428	ILE	2.2
1	J	242	PHE	2.2
1	K	243	GLY	2.2
1	C	43	ASN	2.2
1	I	32	LEU	2.2
1	J	303	GLY	2.1
1	I	335	ASN	2.1
1	J	245	LYS	2.1
1	K	458	GLU	2.1
1	G	430	ILE	2.1
1	G	87	THR	2.0
1	G	431	VAL	2.0
1	L	498	VAL	2.0
1	J	241	GLY	2.0
1	D	430	ILE	2.0
1	L	45	VAL	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 oligosaccharides in this entry.

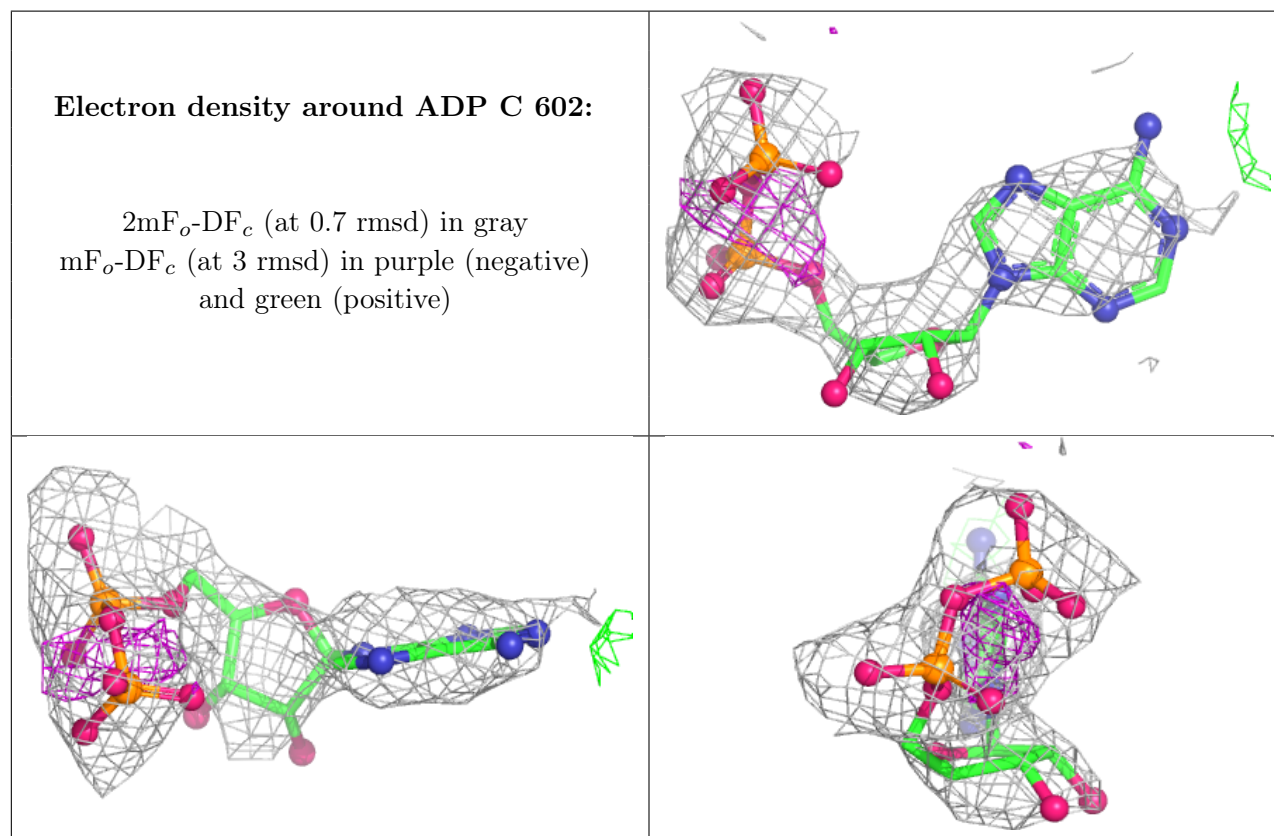
6.4 Ligands [i](#)

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.

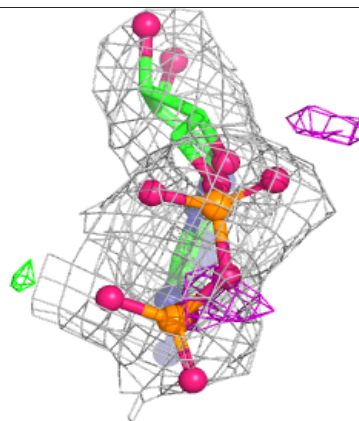
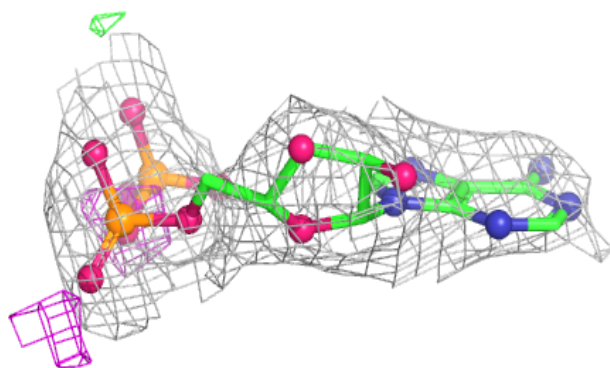
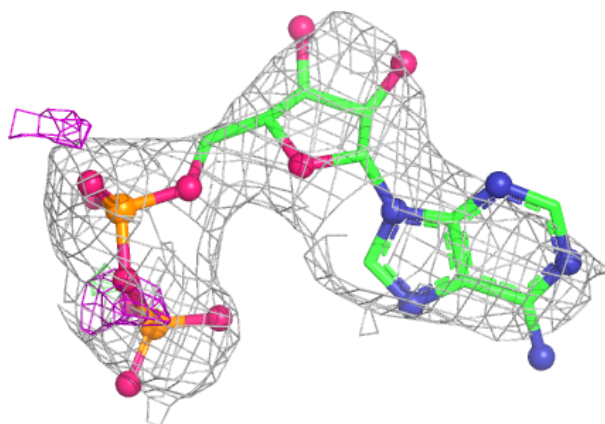
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	C	602	27/27	0.85	0.10	66,91,120,126	0
2	ADP	J	601	27/27	0.86	0.11	64,96,124,149	0
2	ADP	F	601	27/27	0.87	0.10	65,97,122,132	0
2	ADP	A	601	27/27	0.88	0.10	75,97,123,125	0
2	ADP	G	601	27/27	0.89	0.09	66,94,113,122	0
2	ADP	I	601	27/27	0.89	0.09	66,92,124,130	0
2	ADP	B	601	27/27	0.89	0.09	64,79,106,120	0
2	ADP	L	601	27/27	0.90	0.08	56,85,105,113	0
2	ADP	C	601	27/27	0.91	0.08	55,86,112,117	0
2	ADP	D	601	27/27	0.91	0.08	69,90,116,117	0
2	ADP	H	601	27/27	0.91	0.08	65,80,108,121	0
2	ADP	K	601	27/27	0.92	0.09	57,92,109,121	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.

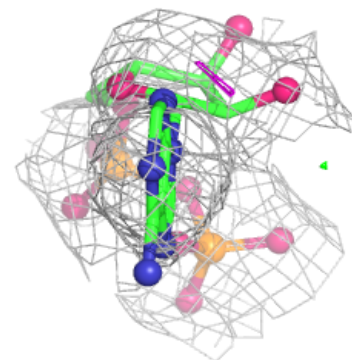
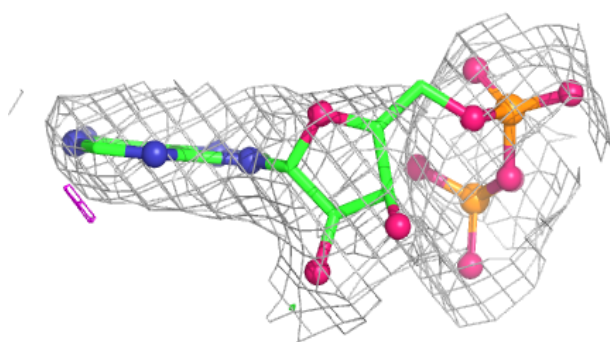
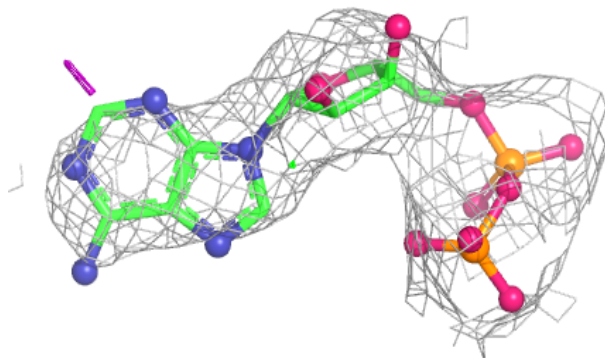


Electron density around ADP J 601:

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

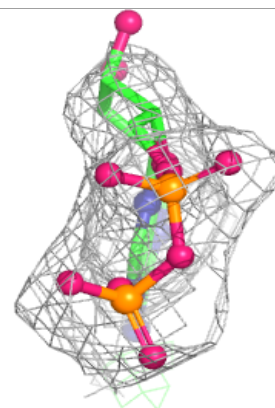
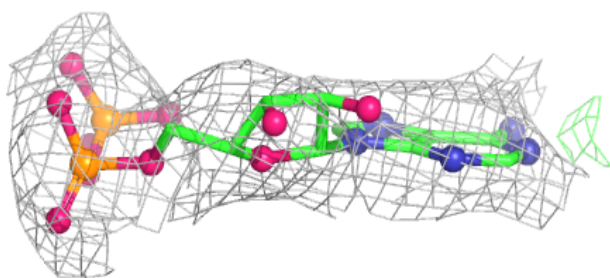
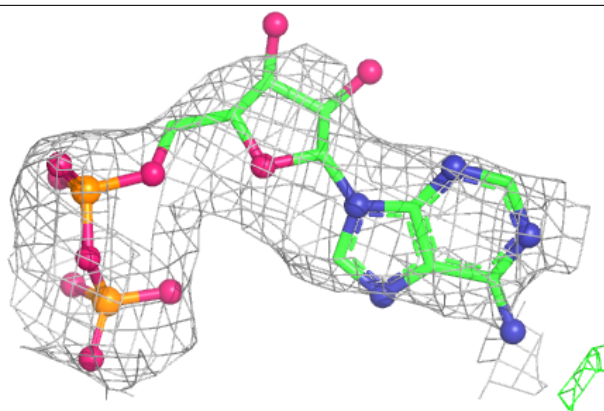
**Electron density around ADP F 601:**

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

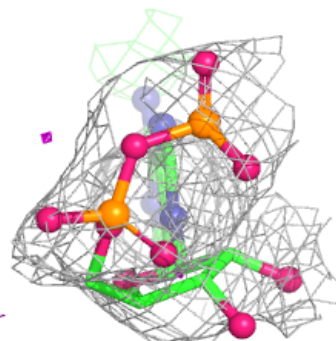
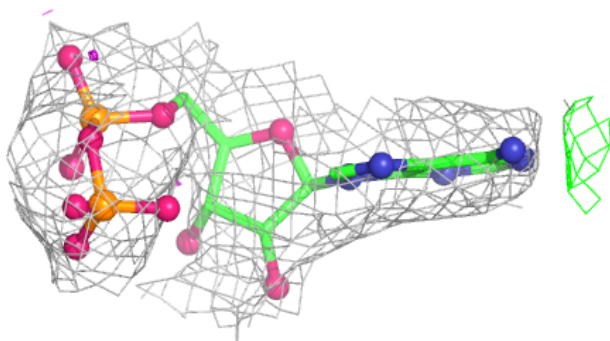
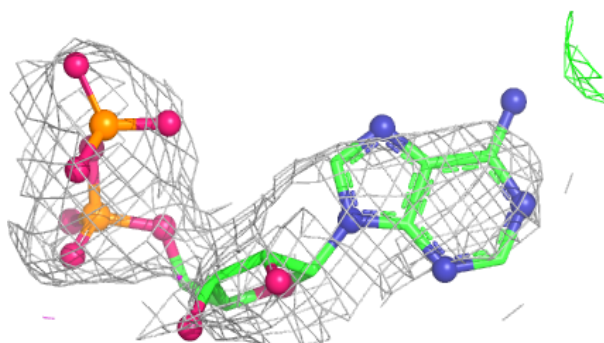


Electron density around ADP A 601:

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

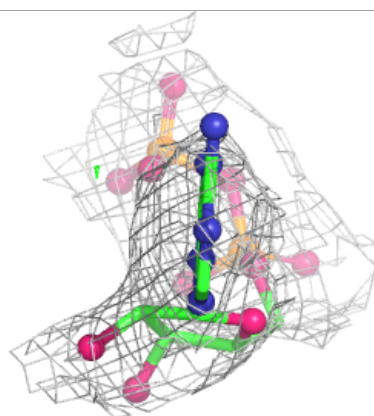
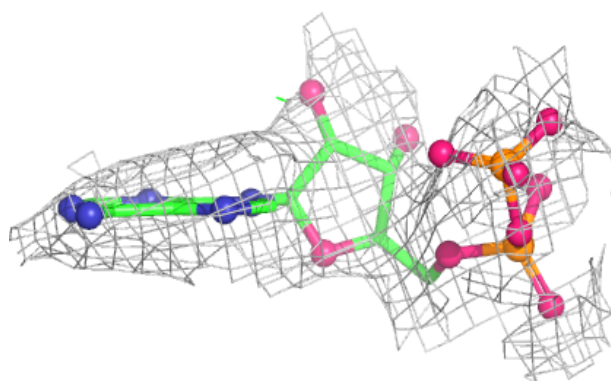
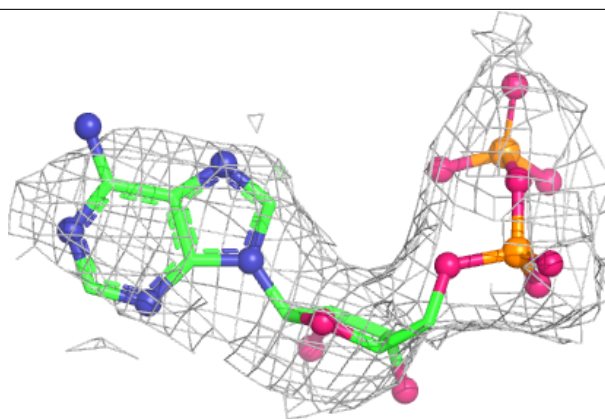
**Electron density around ADP G 601:**

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

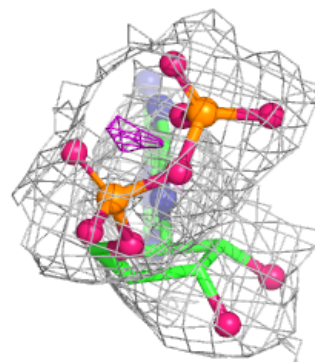
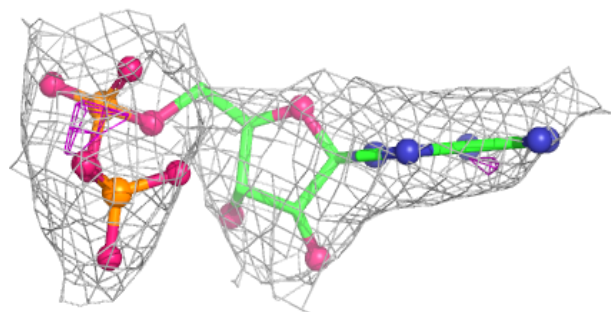
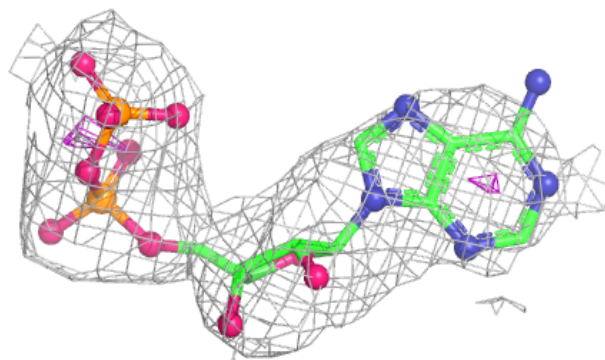


Electron density around ADP I 601:

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

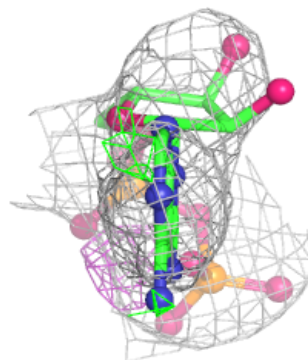
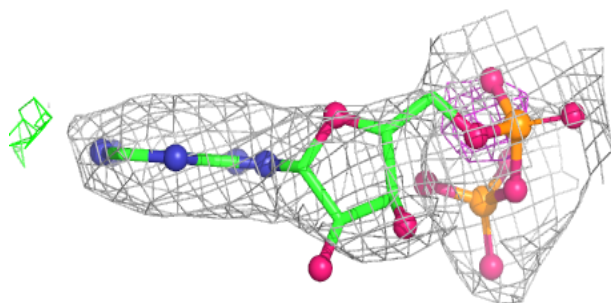
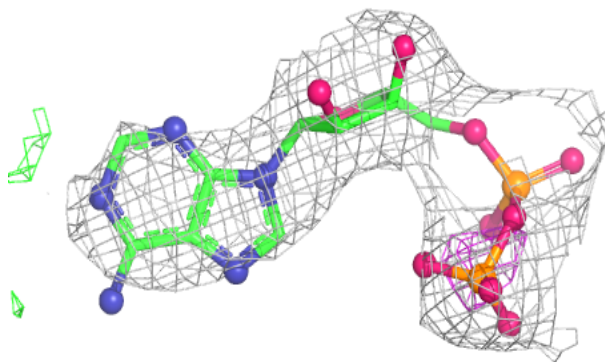
**Electron density around ADP B 601:**

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

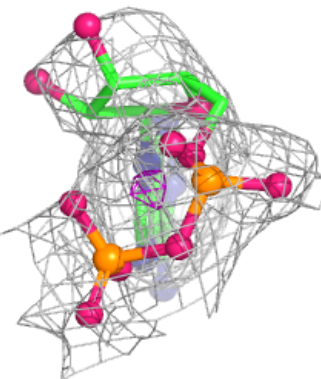
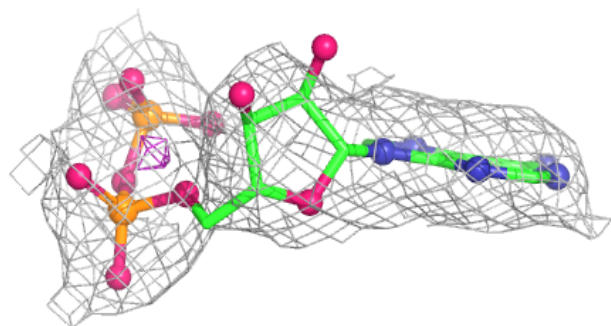
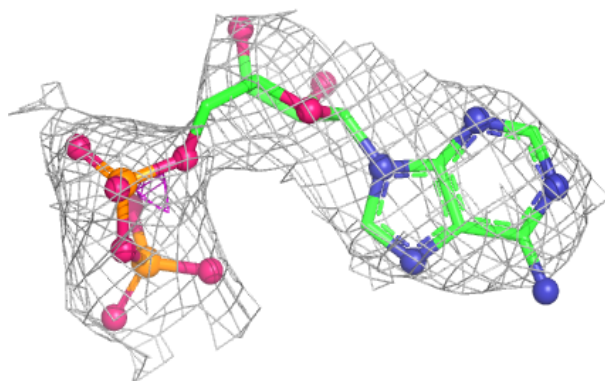


Electron density around ADP L 601:

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

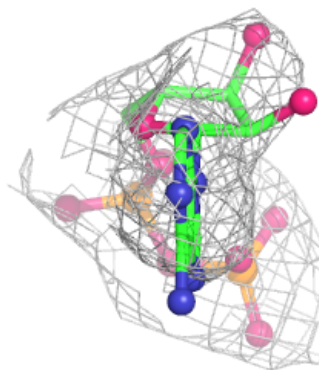
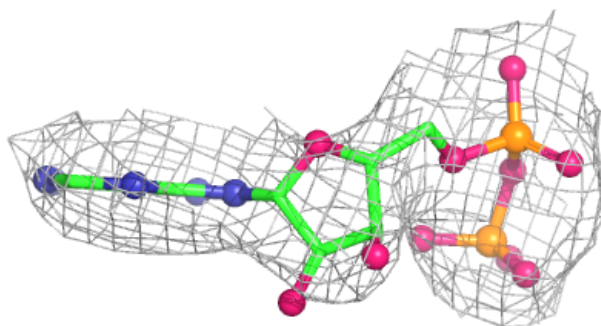
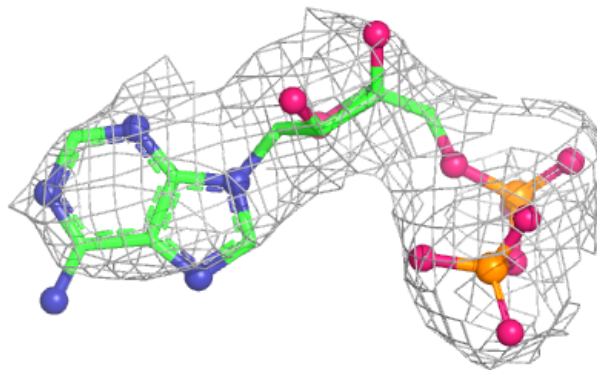
**Electron density around ADP C 601:**

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

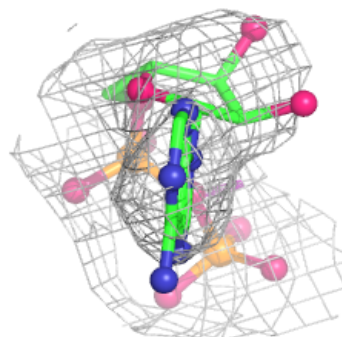
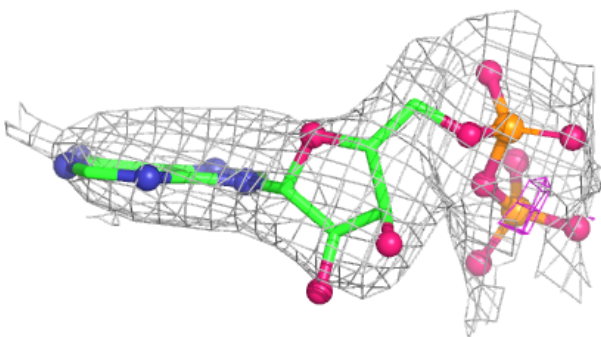
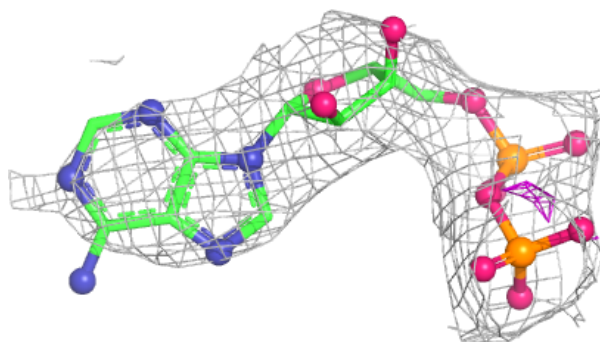


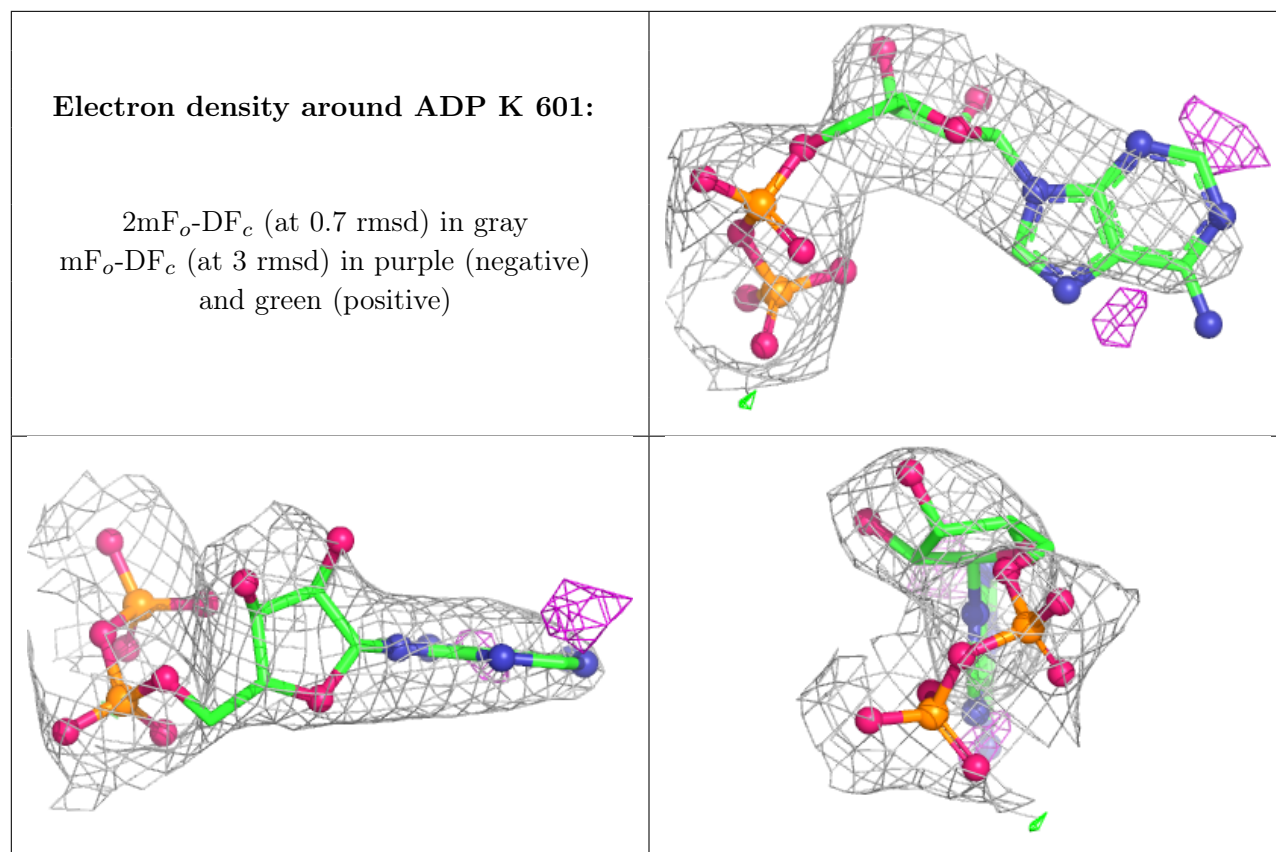
Electron density around ADP D 601:

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

**Electron density around ADP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.