



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2019 – 07:06 PM EST

PDB ID : 1JDB
Title : CARBAMOYL PHOSPHATE SYNTHETASE FROM ESCHERICHIA COLI
Authors : Thoden, J.B.; Holden, H.M.; Wesenberg, G.; Raushel, F.M.; Rayment, I.
Deposited on : 1997-03-25
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

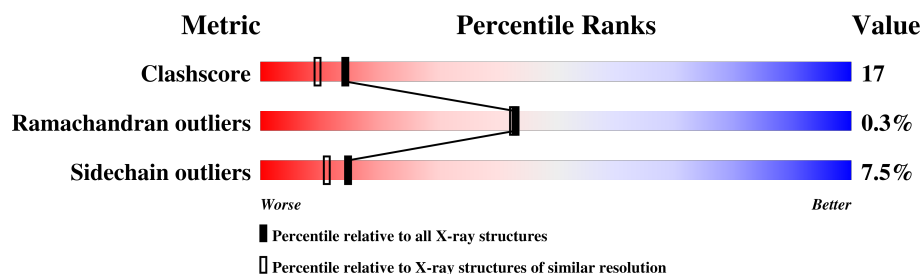
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	1073	64% 27% 6% ..
1	E	1073	61% 30% 7% .
1	H	1073	59% 33% 7% ..
1	K	1073	62% 30% 7% .
2	C	382	51% 39% 8% ..
2	F	382	46% 43% 8% ..
2	I	382	46% 44% 8% ..
2	L	382	58% 34% 7% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	H	1082	-	-	X	-
5	PO4	K	1082	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 49731 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 CARBAMOYL PHOSPHATE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1057	Total	C	N	O	S	0	8	0
			8195	5143	1428	1579	45			
1	E	1057	Total	C	N	O	S	0	13	0
			8223	5160	1440	1577	46			
1	H	1057	Total	C	N	O	S	0	6	0
			8179	5136	1422	1575	46			
1	K	1060	Total	C	N	O	S	0	5	0
			8201	5149	1432	1575	45			

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			
2	F	380	Total	C	N	O	S	0	1	0
			2904	1830	510	554	10			
2	I	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			
2	L	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	183	GLN	GLU	conflict	UNP P00907
F	183	GLN	GLU	conflict	UNP P00907
I	183	GLN	GLU	conflict	UNP P00907
L	183	GLN	GLU	conflict	UNP P00907

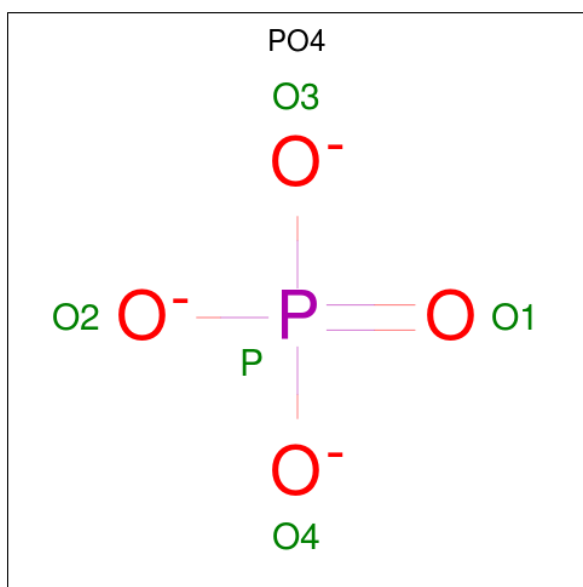
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	4	Total Mn 4 4	0	0
3	B	4	Total Mn 4 4	0	0
3	K	4	Total Mn 4 4	0	0
3	E	4	Total Mn 4 4	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	7	Total K 7 7	0	0
4	E	7	Total K 7 7	0	0
4	H	5	Total K 5 5	0	0
4	B	6	Total K 6 6	0	0
4	I	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	L	1	Total K 1 1	0	0
4	F	1	Total K 1 1	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	E	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	K	1	Total	O	P	0	0
			5	4	1		
5	K	1	Total	O	P	0	0
			5	4	1		
5	K	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

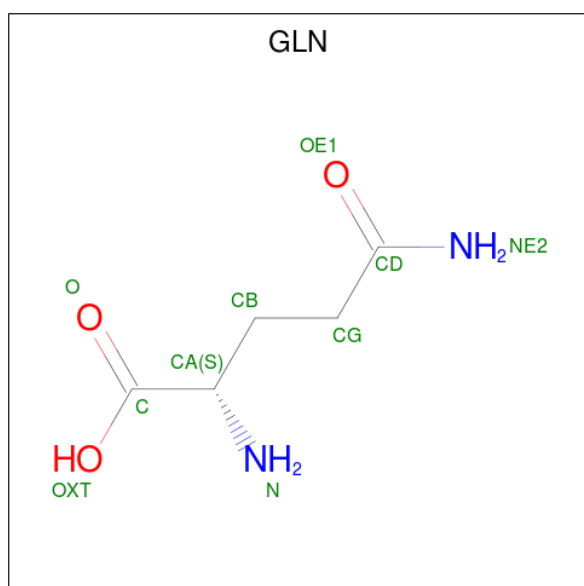
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	6	Total	Cl	0	0
			6	6		
6	E	7	Total	Cl	0	0
			7	7		
6	H	6	Total	Cl	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	6	Total	Cl	0	0
			6	6		
6	I	1	Total	Cl	0	0
			1	1		
6	C	1	Total	Cl	0	0
			1	1		
6	L	1	Total	Cl	0	0
			1	1		
6	F	1	Total	Cl	0	0
			1	1		

- Molecule 7 is GLUTAMINE (three-letter code: GLN) (formula: C₅H₁₀N₂O₃).



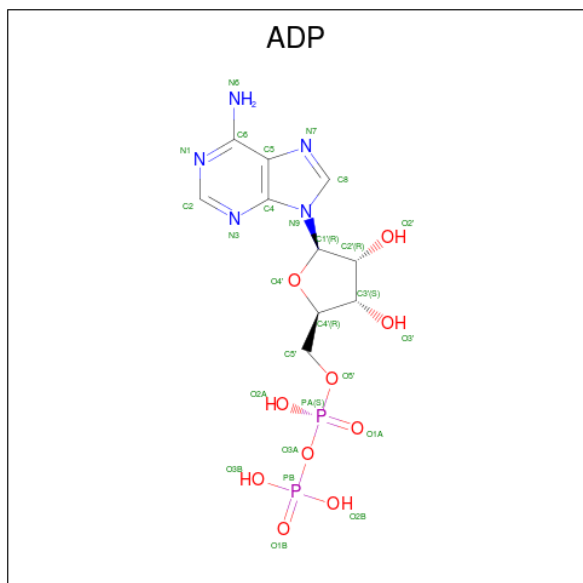
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			10	5	2	3		
7	B	1	Total	C	N	O	0	0
			10	5	2	3		
7	E	1	Total	C	N	O	0	0
			10	5	2	3		
7	E	1	Total	C	N	O	0	0
			10	5	2	3		
7	H	1	Total	C	N	O	0	0
			10	5	2	3		
7	H	1	Total	C	N	O	0	0
			10	5	2	3		

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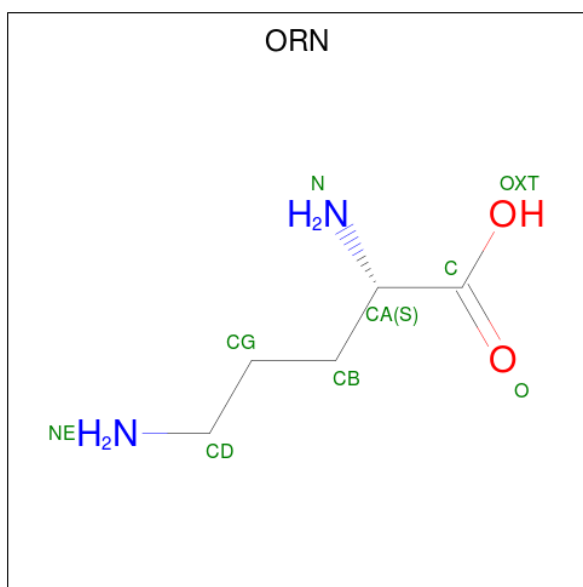
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	K	1	Total	C	N	O	0	0
			10	5	2	3		
7	K	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



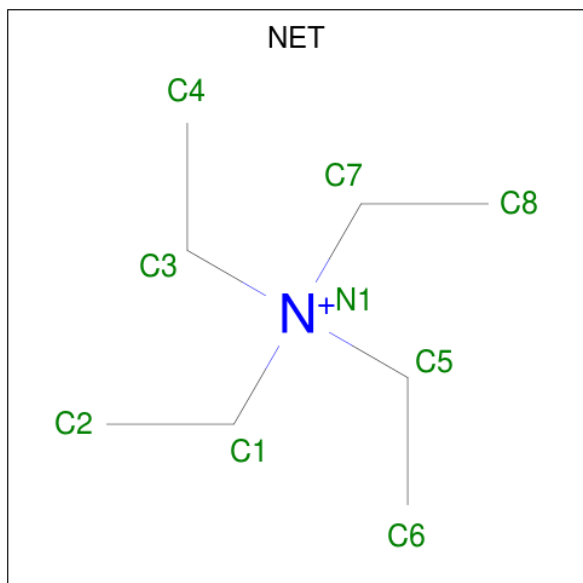
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 9 is L-ornithine (three-letter code: ORN) (formula: $C_5H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total 9	C 5	N 2	O 2	0	0
9	E	1	Total 9	C 5	N 2	O 2	0	0
9	H	1	Total 9	C 5	N 2	O 2	0	0
9	K	1	Total 9	C 5	N 2	O 2	0	0

- Molecule 10 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: $\text{C}_8\text{H}_{20}\text{N}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C N 9 8 1	0	0
10	E	1	Total C N 9 8 1	0	0
10	H	1	Total C N 9 8 1	0	0
10	K	1	Total C N 9 8 1	0	0

- Molecule 11 is water.

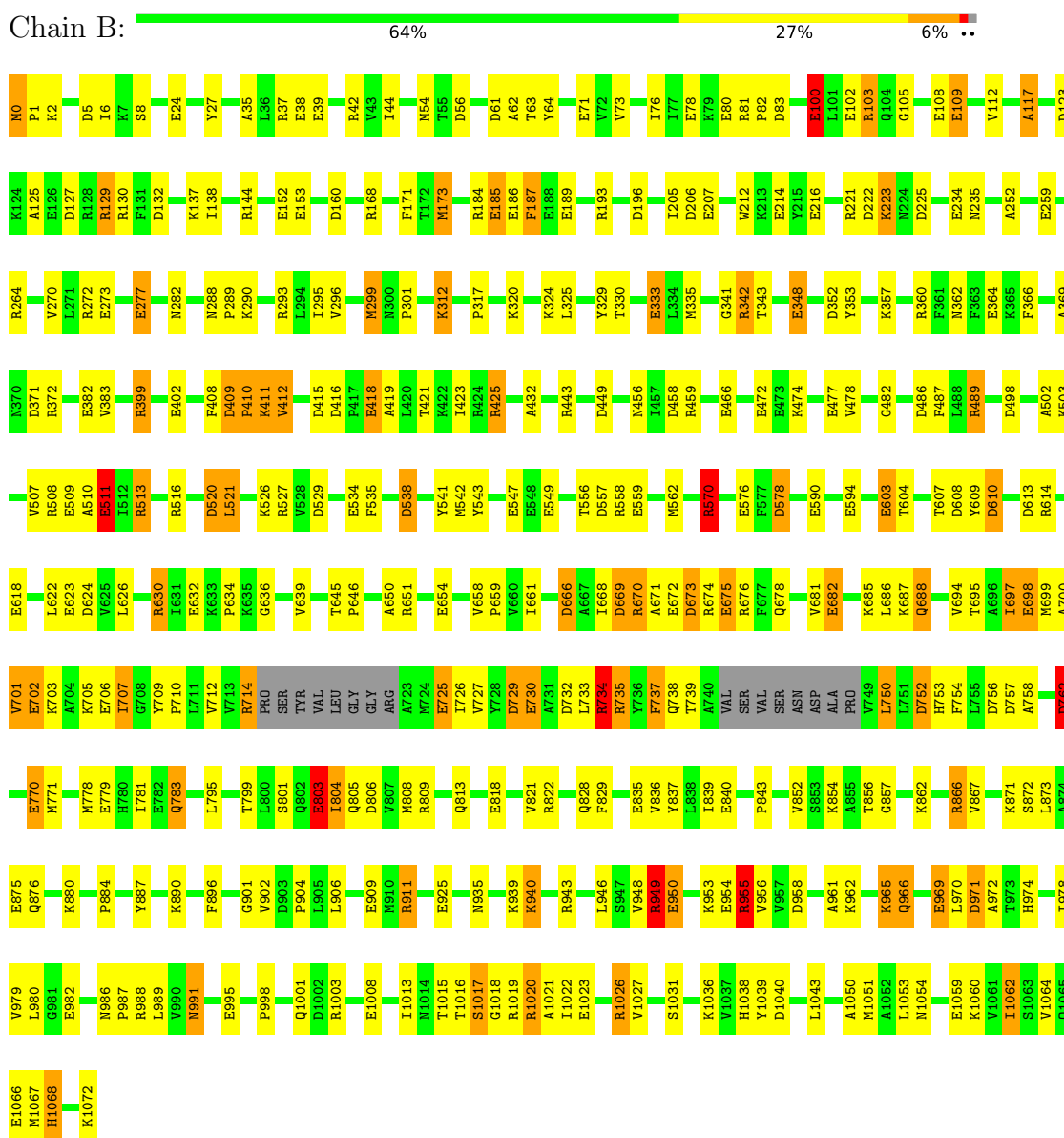
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	970	Total O 970 970	0	0
11	C	241	Total O 241 241	0	0
11	E	1022	Total O 1022 1022	0	0
11	F	210	Total O 210 210	0	0
11	H	942	Total O 942 942	0	0
11	I	235	Total O 235 235	0	0
11	K	980	Total O 980 980	0	0
11	L	257	Total O 257 257	0	0

3 Residue-property plots

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

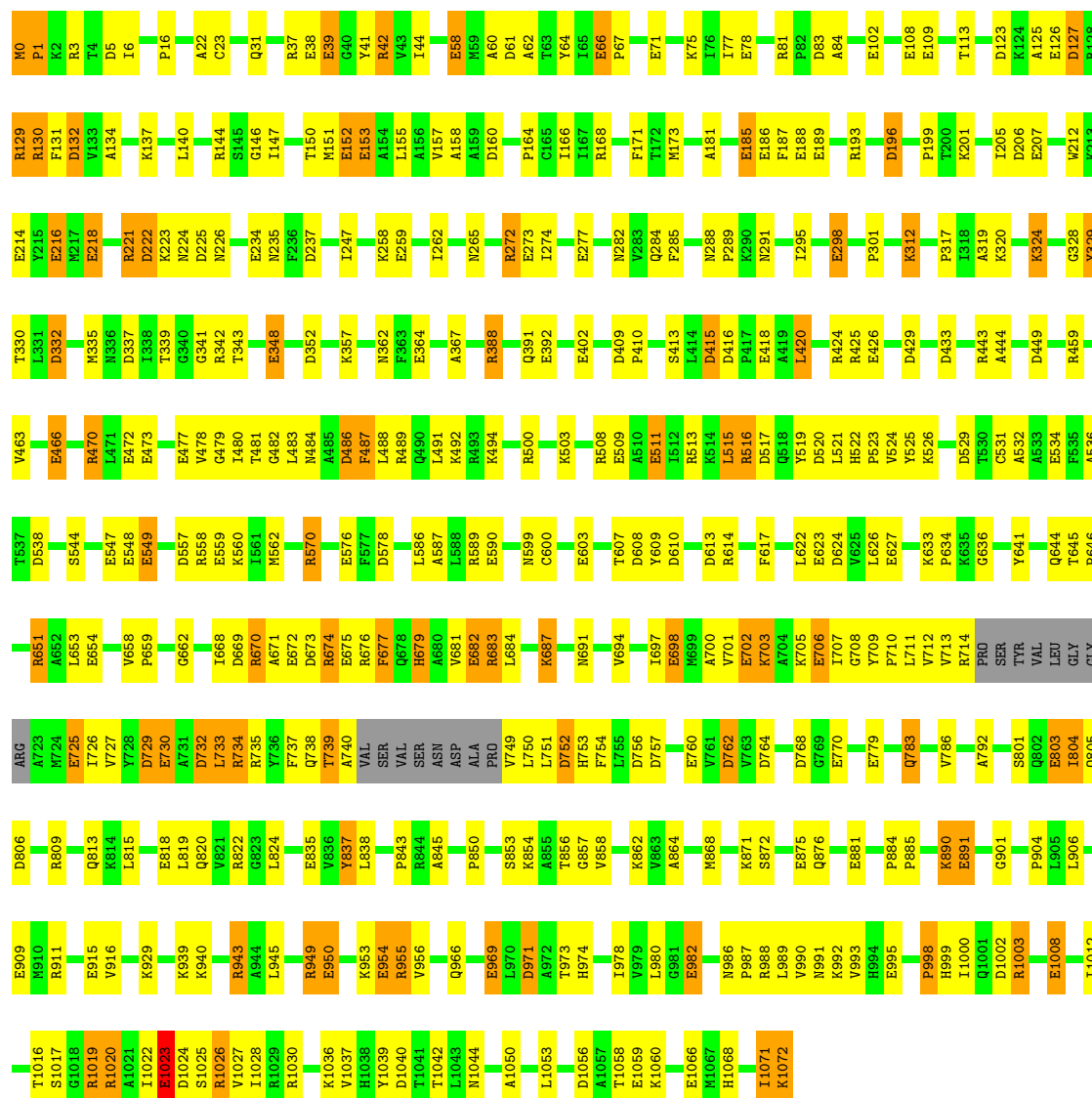
Note EDS was not executed.

• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE



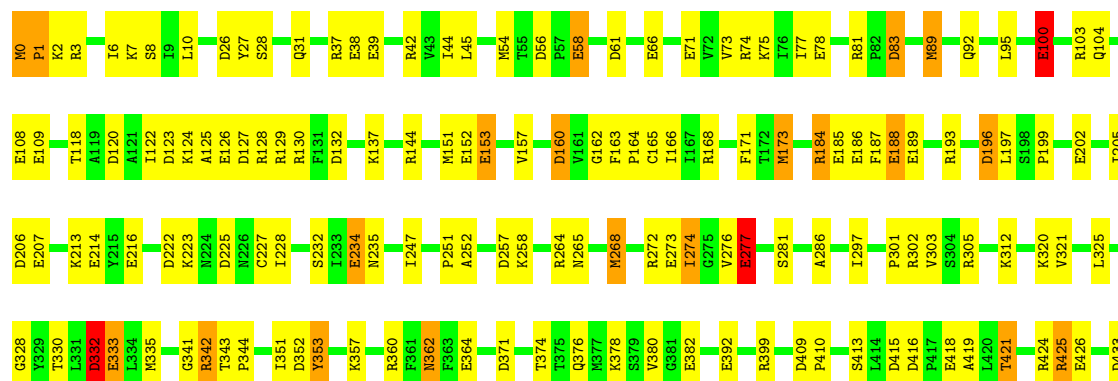
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE

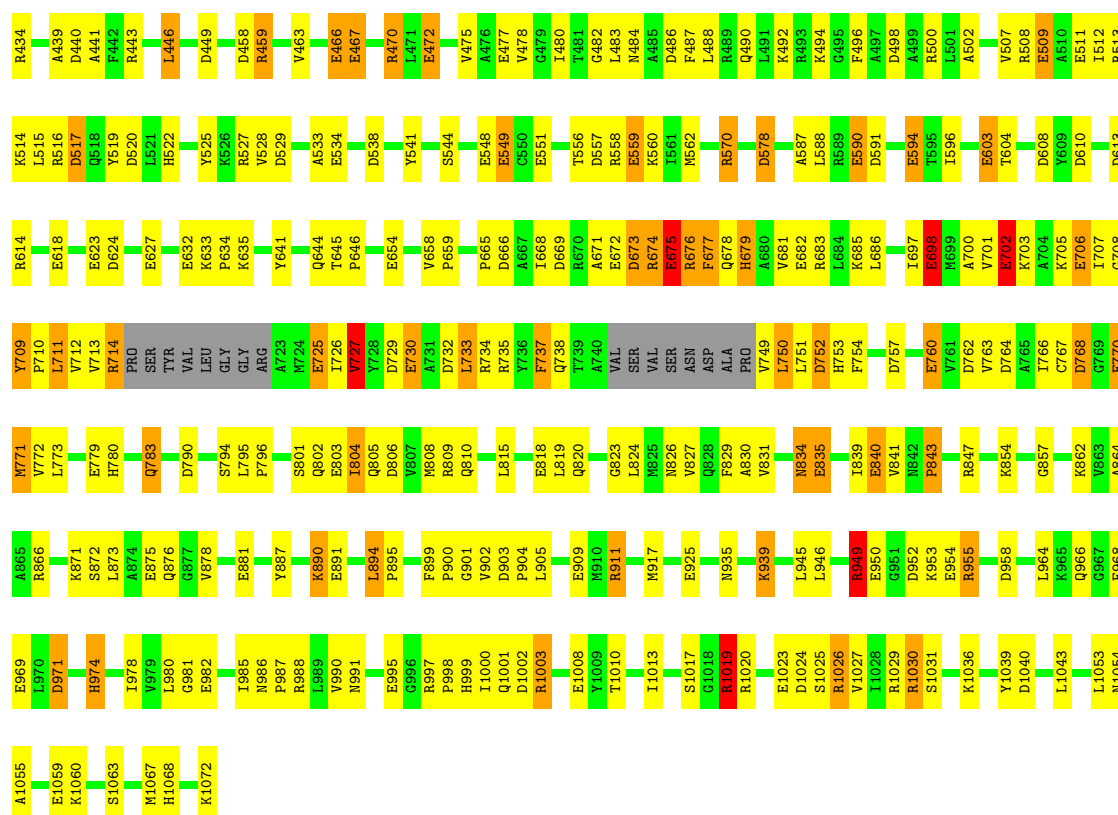
Chain E:



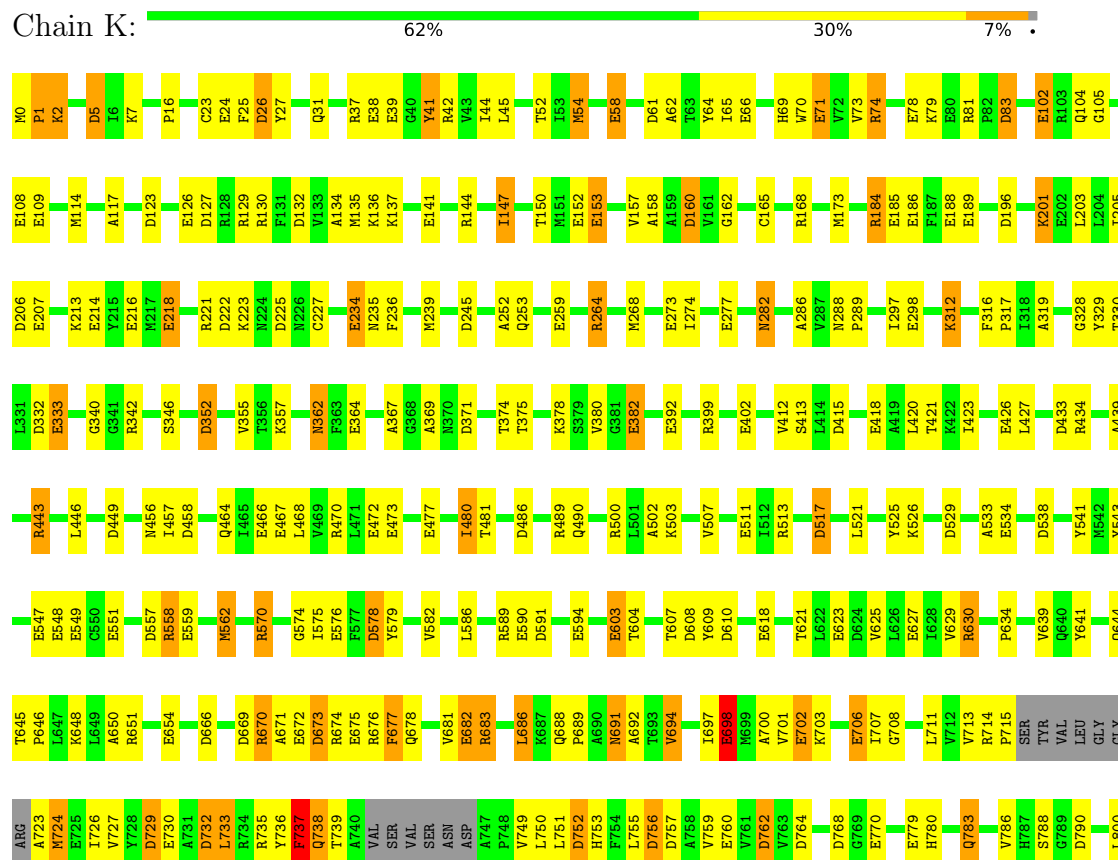
- Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE

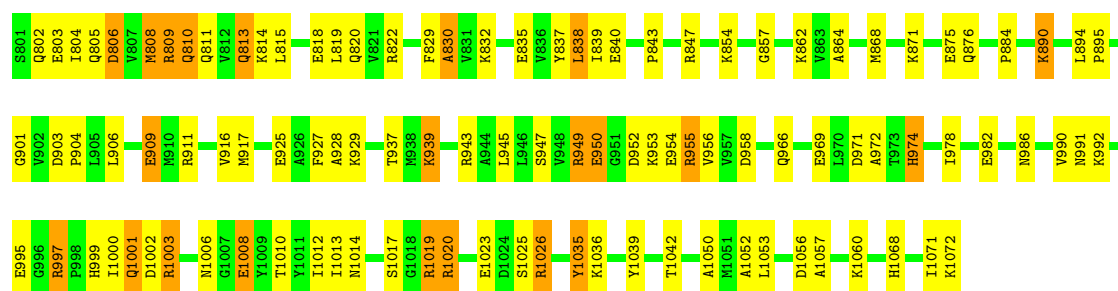
Chain H:



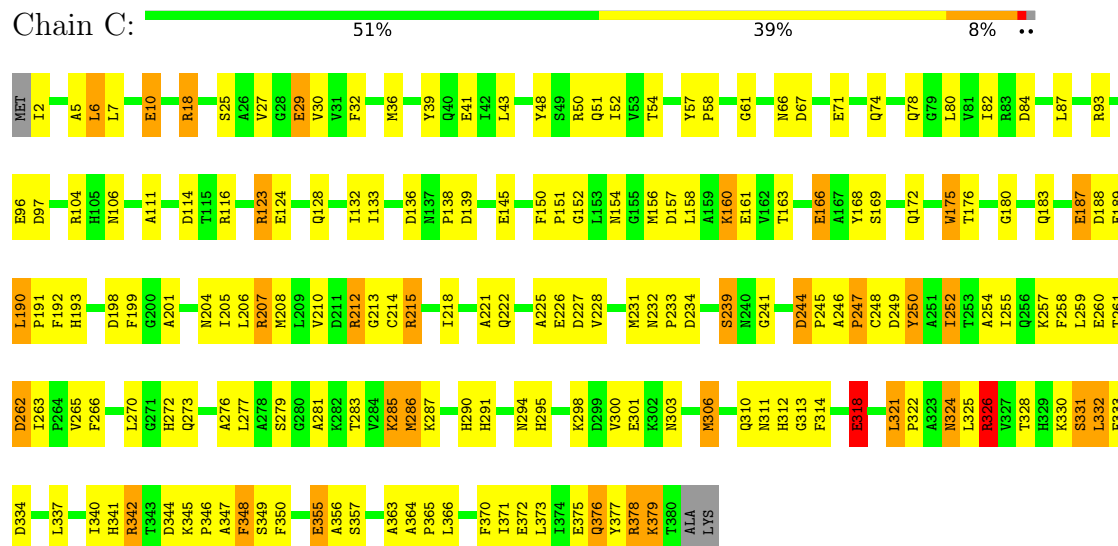


• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE

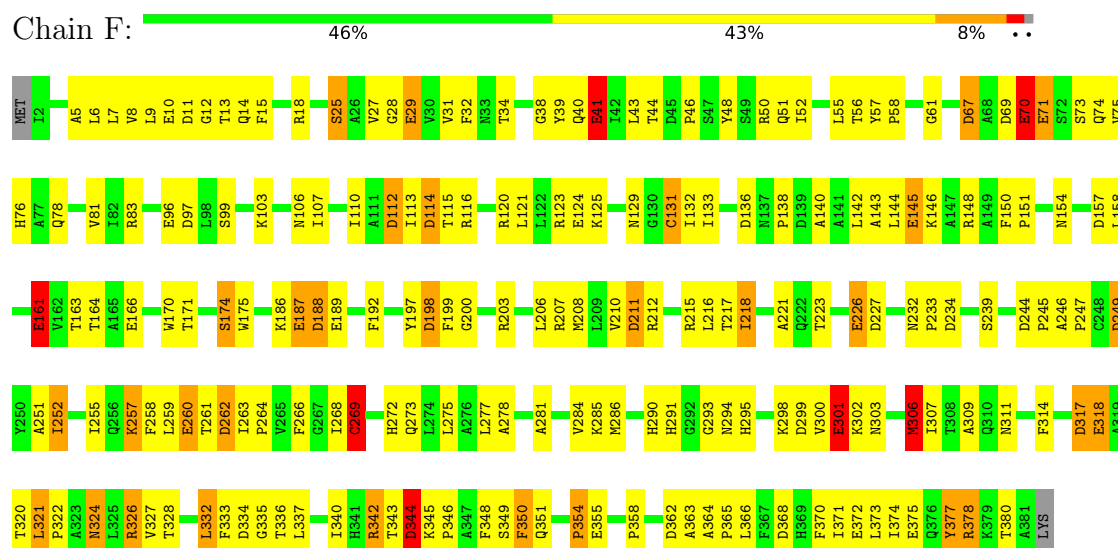




• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE

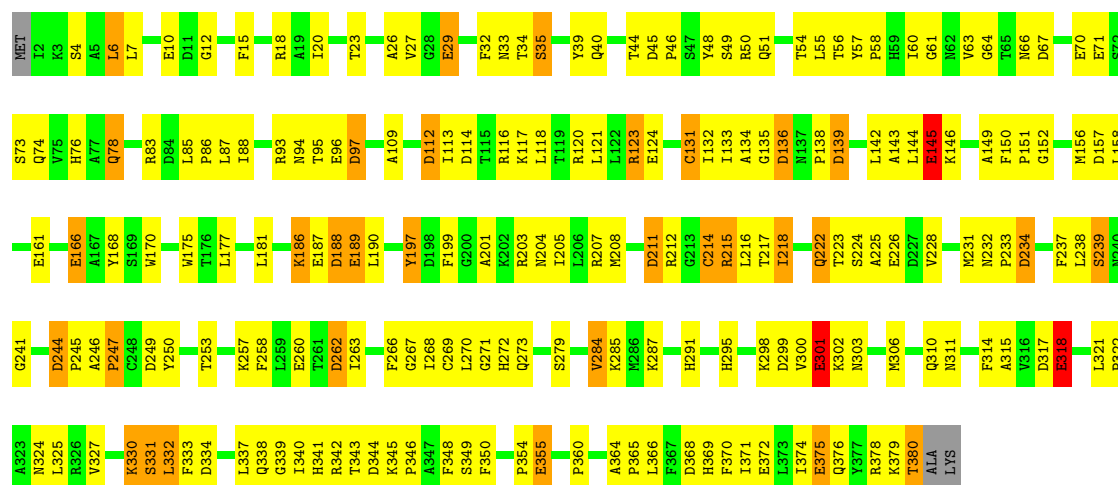


• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE



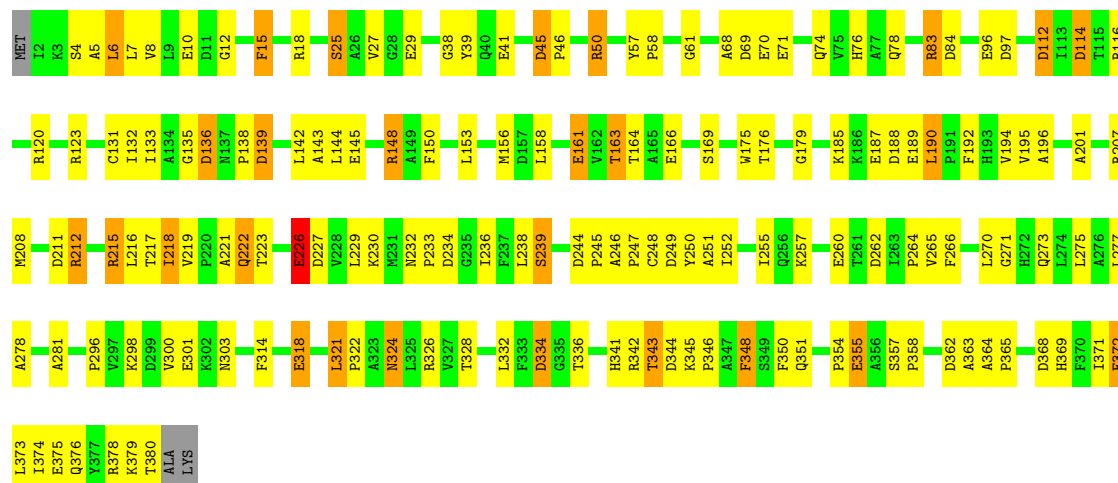
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE





• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE

Chain L: 58% 34% 7% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	143.80Å 167.70Å 323.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	90.0 (30.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	49731	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CL, K, MN, ORN, NET, PO4

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	B	1.00	65/8353 (0.8%)	1.58	143/11292 (1.3%)
1	E	1.01	73/8401 (0.9%)	1.55	132/11352 (1.2%)
1	H	1.00	72/8329 (0.9%)	1.56	149/11259 (1.3%)
1	K	1.02	73/8349 (0.9%)	1.59	154/11289 (1.4%)
2	C	0.89	18/2957 (0.6%)	1.49	42/4016 (1.0%)
2	F	0.87	16/2970 (0.5%)	1.50	34/4034 (0.8%)
2	I	0.87	16/2957 (0.5%)	1.47	33/4016 (0.8%)
2	L	0.89	16/2957 (0.5%)	1.56	51/4016 (1.3%)
All	All	0.98	349/45273 (0.8%)	1.55	738/61274 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	1	0

All (349) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	GLU	CD-OE2	8.36	1.34	1.25
1	E	1008	GLU	CD-OE1	8.23	1.34	1.25
1	B	682	GLU	CD-OE1	8.10	1.34	1.25
1	H	995	GLU	CD-OE2	7.84	1.34	1.25
1	K	995	GLU	CD-OE2	7.74	1.34	1.25
1	E	218	GLU	CD-OE1	7.70	1.34	1.25
1	B	207	GLU	CD-OE1	7.59	1.33	1.25
1	H	1008	GLU	CD-OE1	7.48	1.33	1.25
1	B	511	GLU	CD-OE1	7.41	1.33	1.25
2	I	260	GLU	CD-OE2	7.38	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	594	GLU	CD-OE1	7.30	1.33	1.25
1	E	214	GLU	CD-OE1	7.22	1.33	1.25
1	K	760	GLU	CD-OE1	7.21	1.33	1.25
1	K	477	GLU	CD-OE1	7.19	1.33	1.25
1	E	698	GLU	CD-OE1	7.19	1.33	1.25
1	H	950	GLU	CD-OE2	7.16	1.33	1.25
1	H	38	GLU	CD-OE1	7.15	1.33	1.25
1	B	995	GLU	CD-OE2	7.09	1.33	1.25
1	B	576	GLU	CD-OE1	7.08	1.33	1.25
1	K	549	GLU	CD-OE1	7.04	1.33	1.25
1	K	627	GLU	CD-OE1	7.01	1.33	1.25
1	H	682	GLU	CD-OE1	6.99	1.33	1.25
1	K	216	GLU	CD-OE2	6.99	1.33	1.25
2	L	226	GLU	CD-OE1	6.97	1.33	1.25
1	E	402	GLU	CD-OE2	6.96	1.33	1.25
1	K	58	GLU	CD-OE1	6.94	1.33	1.25
1	E	534	GLU	CD-OE1	6.93	1.33	1.25
2	F	166	GLU	CD-OE2	6.93	1.33	1.25
1	E	216	GLU	CD-OE2	6.93	1.33	1.25
1	B	1008	GLU	CD-OE1	6.92	1.33	1.25
1	E	298	GLU	CD-OE1	-6.89	1.18	1.25
1	E	549	GLU	CD-OE1	6.87	1.33	1.25
1	H	770	GLU	CD-OE1	6.84	1.33	1.25
1	K	982	GLU	CD-OE2	6.84	1.33	1.25
1	H	66	GLU	CD-OE1	6.79	1.33	1.25
1	E	418	GLU	CD-OE1	6.77	1.33	1.25
1	E	185	GLU	CD-OE2	6.75	1.33	1.25
1	E	1023	GLU	CD-OE1	6.73	1.33	1.25
2	I	166	GLU	CD-OE2	6.72	1.33	1.25
1	K	511	GLU	CD-OE1	6.71	1.33	1.25
1	K	698	GLU	CD-OE1	6.68	1.33	1.25
1	B	109	GLU	CD-OE1	6.68	1.32	1.25
1	E	702	GLU	CD-OE1	6.68	1.32	1.25
1	E	875	GLU	CD-OE2	6.67	1.32	1.25
1	B	954	GLU	CD-OE1	6.64	1.32	1.25
1	H	835	GLU	CD-OE2	6.63	1.32	1.25
1	K	954	GLU	CD-OE2	6.61	1.32	1.25
1	B	706	GLU	CD-OE1	6.60	1.32	1.25
1	E	152	GLU	CD-OE1	6.59	1.32	1.25
1	K	770	GLU	CD-OE1	6.59	1.32	1.25
1	K	186	GLU	CD-OE2	6.59	1.32	1.25
2	L	372	GLU	CD-OE1	6.58	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	145	GLU	CD-OE1	6.58	1.32	1.25
1	H	702	GLU	CD-OE1	6.58	1.32	1.25
1	H	277	GLU	CD-OE1	6.58	1.32	1.25
2	I	375	GLU	CD-OE1	6.58	1.32	1.25
1	H	969	GLU	CD-OE1	6.56	1.32	1.25
1	K	277	GLU	CD-OE1	6.56	1.32	1.25
1	B	803	GLU	CD-OE2	6.54	1.32	1.25
1	K	189	GLU	CD-OE1	6.54	1.32	1.25
1	K	1008[A]	GLU	CD-OE1	6.54	1.32	1.25
1	K	1008[B]	GLU	CD-OE1	6.54	1.32	1.25
1	B	80	GLU	CD-OE1	6.53	1.32	1.25
1	H	706	GLU	CD-OE1	6.53	1.32	1.25
1	K	675	GLU	CD-OE2	6.52	1.32	1.25
1	E	995	GLU	CD-OE2	6.49	1.32	1.25
1	H	1023	GLU	CD-OE1	6.47	1.32	1.25
1	B	38	GLU	CD-OE1	6.47	1.32	1.25
2	F	301	GLU	CD-OE1	6.45	1.32	1.25
1	K	473	GLU	CD-OE1	6.45	1.32	1.25
1	H	207	GLU	CD-OE1	6.43	1.32	1.25
1	E	969	GLU	CD-OE1	6.42	1.32	1.25
1	H	760	GLU	CD-OE1	6.41	1.32	1.25
1	K	706	GLU	CD-OE1	6.40	1.32	1.25
1	H	100	GLU	CD-OE1	6.37	1.32	1.25
2	I	161	GLU	CD-OE2	6.36	1.32	1.25
1	B	950	GLU	CD-OE2	6.36	1.32	1.25
1	K	467	GLU	CD-OE1	6.36	1.32	1.25
1	B	108	GLU	CD-OE1	6.34	1.32	1.25
1	K	702	GLU	CD-OE1	6.34	1.32	1.25
2	L	187	GLU	CD-OE1	6.34	1.32	1.25
2	I	355	GLU	CD-OE1	6.33	1.32	1.25
1	H	925	GLU	CD-OE1	6.33	1.32	1.25
1	K	152	GLU	CD-OE1	6.33	1.32	1.25
1	E	603	GLU	CD-OE1	6.33	1.32	1.25
1	H	881	GLU	CD-OE2	6.31	1.32	1.25
1	B	185	GLU	CD-OE1	6.30	1.32	1.25
2	F	226	GLU	CD-OE1	6.30	1.32	1.25
2	C	166	GLU	CD-OE2	6.30	1.32	1.25
2	L	166	GLU	CD-OE1	6.30	1.32	1.25
1	H	71	GLU	CD-OE2	6.27	1.32	1.25
1	B	654	GLU	CD-OE1	6.27	1.32	1.25
2	C	96	GLU	CD-OE2	6.27	1.32	1.25
1	B	186	GLU	CD-OE2	6.27	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	109	GLU	CD-OE2	6.27	1.32	1.25
1	B	466	GLU	CD-OE1	6.26	1.32	1.25
1	B	835	GLU	CD-OE1	6.25	1.32	1.25
2	F	145	GLU	CD-OE1	6.25	1.32	1.25
2	L	145	GLU	CD-OE1	6.24	1.32	1.25
1	B	153	GLU	CD-OE1	6.24	1.32	1.25
2	C	226	GLU	CD-OE1	6.23	1.32	1.25
2	F	41	GLU	CD-OE1	6.23	1.32	1.25
1	E	675	GLU	CD-OE1	6.23	1.32	1.25
1	H	551	GLU	CD-OE2	6.23	1.32	1.25
2	C	10	GLU	CD-OE2	6.22	1.32	1.25
1	H	152	GLU	CD-OE2	6.22	1.32	1.25
2	L	70	GLU	CD-OE1	6.22	1.32	1.25
2	C	375	GLU	CD-OE2	6.21	1.32	1.25
2	C	71	GLU	CD-OE2	6.21	1.32	1.25
1	B	730	GLU	CD-OE1	6.21	1.32	1.25
1	H	214	GLU	CD-OE1	6.21	1.32	1.25
1	H	189	GLU	CD-OE1	6.20	1.32	1.25
1	E	126	GLU	CD-OE1	6.20	1.32	1.25
1	B	672	GLU	CD-OE1	6.15	1.32	1.25
1	K	1023	GLU	CD-OE1	6.14	1.32	1.25
1	K	185	GLU	CD-OE2	6.14	1.32	1.25
1	H	803	GLU	CD-OE2	6.13	1.32	1.25
1	H	627	GLU	CD-OE1	6.13	1.32	1.25
1	H	477	GLU	CD-OE1	6.12	1.32	1.25
2	C	301	GLU	CD-OE1	6.12	1.32	1.25
2	L	301	GLU	CD-OE1	6.11	1.32	1.25
1	K	382	GLU	CD-OE2	6.11	1.32	1.25
1	E	706	GLU	CD-OE1	6.10	1.32	1.25
1	B	364	GLU	CD-OE1	6.09	1.32	1.25
1	H	185[A]	GLU	CD-OE2	6.08	1.32	1.25
1	H	185[B]	GLU	CD-OE2	6.08	1.32	1.25
1	E	186	GLU	CD-OE2	6.08	1.32	1.25
1	H	730	GLU	CD-OE1	6.08	1.32	1.25
1	B	702	GLU	CD-OE1	6.08	1.32	1.25
2	F	70	GLU	CD-OE2	6.07	1.32	1.25
2	F	375	GLU	CD-OE2	6.07	1.32	1.25
1	K	603	GLU	CD-OE1	6.06	1.32	1.25
1	B	1066	GLU	CD-OE1	6.06	1.32	1.25
1	E	477	GLU	CD-OE1	6.06	1.32	1.25
1	E	682	GLU	CD-OE1	6.05	1.32	1.25
1	B	925	GLU	CD-OE1	6.05	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	145	GLU	CD-OE2	6.05	1.32	1.25
1	K	950	GLU	CD-OE2	6.05	1.32	1.25
1	E	348	GLU	CD-OE2	6.05	1.32	1.25
1	B	277	GLU	CD-OE1	6.04	1.32	1.25
1	K	730	GLU	CD-OE1	6.04	1.32	1.25
1	H	875	GLU	CD-OE2	6.04	1.32	1.25
1	E	71	GLU	CD-OE2	6.03	1.32	1.25
1	E	509	GLU	CD-OE1	6.03	1.32	1.25
2	I	372	GLU	CD-OE1	6.02	1.32	1.25
2	F	124	GLU	CD-OE1	6.02	1.32	1.25
1	B	1023	GLU	CD-OE1	6.01	1.32	1.25
1	E	189	GLU	CD-OE1	6.00	1.32	1.25
1	K	418	GLU	CD-OE1	5.99	1.32	1.25
1	K	682	GLU	CD-OE2	5.99	1.32	1.25
2	I	29	GLU	CD-OE2	5.99	1.32	1.25
1	E	818	GLU	CD-OE1	5.98	1.32	1.25
1	K	466	GLU	CD-OE1	5.98	1.32	1.25
1	B	725	GLU	CD-OE1	5.97	1.32	1.25
1	E	473	GLU	CD-OE1	5.95	1.32	1.25
2	I	318	GLU	CD-OE1	5.95	1.32	1.25
1	H	418	GLU	CD-OE1	5.94	1.32	1.25
1	B	982	GLU	CD-OE2	5.93	1.32	1.25
1	K	576	GLU	CD-OE1	5.93	1.32	1.25
1	B	618	GLU	CD-OE1	5.93	1.32	1.25
1	K	207	GLU	CD-OE1	5.92	1.32	1.25
2	C	260	GLU	CD-OE2	5.91	1.32	1.25
1	H	364	GLU	CD-OE1	5.91	1.32	1.25
1	B	632	GLU	CD-OE1	5.91	1.32	1.25
1	E	730	GLU	CD-OE1	5.91	1.32	1.25
1	K	426	GLU	CD-OE2	5.91	1.32	1.25
1	H	392	GLU	CD-OE1	5.90	1.32	1.25
1	K	551	GLU	CD-OE2	5.89	1.32	1.25
1	E	725	GLU	CD-OE1	5.88	1.32	1.25
1	K	875	GLU	CD-OE2	5.86	1.32	1.25
1	E	39	GLU	CD-OE1	5.85	1.32	1.25
1	K	188	GLU	CD-OE1	5.85	1.32	1.25
1	K	835	GLU	CD-OE2	5.85	1.32	1.25
2	L	96	GLU	CD-OE2	5.85	1.32	1.25
1	B	818	GLU	CD-OE1	5.84	1.32	1.25
1	E	770	GLU	CD-OE1	5.84	1.32	1.25
1	H	549	GLU	CD-OE1	5.83	1.32	1.25
1	H	623	GLU	CD-OE1	5.82	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	654	GLU	CD-OE1	5.82	1.32	1.25
1	B	24	GLU	CD-OE1	5.81	1.32	1.25
2	C	372	GLU	CD-OE1	5.80	1.32	1.25
1	B	189	GLU	CD-OE1	5.80	1.32	1.25
2	F	372	GLU	CD-OE2	5.80	1.32	1.25
1	H	954	GLU	CD-OE1	5.80	1.32	1.25
2	L	29	GLU	CD-OE1	5.80	1.32	1.25
2	F	96	GLU	CD-OE2	5.79	1.32	1.25
1	B	603	GLU	CD-OE1	5.79	1.32	1.25
1	K	925	GLU	CD-OE1	5.79	1.32	1.25
1	K	126	GLU	CD-OE1	5.78	1.32	1.25
1	E	58	GLU	CD-OE1	5.78	1.32	1.25
1	E	835	GLU	CD-OE1	5.78	1.32	1.25
1	E	207	GLU	CD-OE1	5.78	1.32	1.25
1	K	141	GLU	CD-OE2	5.78	1.32	1.25
1	H	725	GLU	CD-OE1	5.77	1.32	1.25
1	E	78	GLU	CD-OE2	5.77	1.31	1.25
1	K	402	GLU	CD-OE2	5.77	1.32	1.25
1	H	216	GLU	CD-OE2	5.77	1.31	1.25
1	E	153	GLU	CD-OE1	5.76	1.31	1.25
1	K	66	GLU	CD-OE1	5.76	1.31	1.25
1	K	218	GLU	CD-OE1	5.76	1.31	1.25
2	F	318	GLU	CD-OE1	5.76	1.31	1.25
2	F	260	GLU	CD-OE1	5.75	1.31	1.25
1	B	402	GLU	CD-OE2	5.73	1.31	1.25
1	H	467	GLU	CD-OE1	5.73	1.31	1.25
1	H	818	GLU	CD-OE1	5.71	1.31	1.25
1	H	559	GLU	CD-OE2	5.71	1.31	1.25
1	K	803	GLU	CD-OE2	5.71	1.31	1.25
2	C	189	GLU	CD-OE2	5.71	1.31	1.25
2	L	41	GLU	CD-OE1	5.71	1.31	1.25
1	H	675	GLU	CD-OE1	5.70	1.31	1.25
1	K	108	GLU	CD-OE1	5.70	1.31	1.25
1	B	875	GLU	CD-OE1	5.69	1.31	1.25
2	I	10	GLU	CD-OE2	5.69	1.31	1.25
1	E	891	GLU	CD-OE2	5.68	1.31	1.25
1	K	909	GLU	CD-OE2	5.68	1.31	1.25
1	B	477	GLU	CD-OE1	5.67	1.31	1.25
1	K	548	GLU	CD-OE2	5.65	1.31	1.25
1	B	78	GLU	CD-OE2	5.64	1.31	1.25
1	K	102	GLU	CD-OE1	5.63	1.31	1.25
1	E	277	GLU	CD-OE1	5.62	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	234	GLU	CD-OE1	5.62	1.31	1.25
2	L	355	GLU	CD-OE1	5.62	1.31	1.25
2	C	355	GLU	CD-OE1	5.61	1.31	1.25
1	H	982	GLU	CD-OE2	5.61	1.31	1.25
2	I	187	GLU	CD-OE1	5.61	1.31	1.25
1	K	38	GLU	CD-OE1	5.61	1.31	1.25
2	C	124	GLU	CD-OE1	5.61	1.31	1.25
1	B	770	GLU	CD-OE2	5.60	1.31	1.25
1	E	1059	GLU	CD-OE2	5.60	1.31	1.25
2	C	161	GLU	CD-OE2	5.60	1.31	1.25
2	I	226	GLU	CD-OE1	5.60	1.31	1.25
1	B	698	GLU	CD-OE1	5.59	1.31	1.25
1	E	803	GLU	CD-OE1	5.59	1.31	1.25
1	H	618	GLU	CD-OE1	5.59	1.31	1.25
1	K	559	GLU	CD-OE2	5.59	1.31	1.25
1	H	188	GLU	CD-OE2	5.58	1.31	1.25
1	B	590	GLU	CD-OE1	5.55	1.31	1.25
1	B	969	GLU	CD-OE1	5.55	1.31	1.25
2	C	41	GLU	CD-OE1	5.55	1.31	1.25
1	K	472	GLU	CD-OE1	5.54	1.31	1.25
1	H	109	GLU	CD-OE2	5.54	1.31	1.25
1	H	108	GLU	CD-OE1	5.54	1.31	1.25
1	H	202	GLU	CD-OE2	5.54	1.31	1.25
2	C	29	GLU	CD-OE1	5.54	1.31	1.25
1	E	954[A]	GLU	CD-OE1	5.53	1.31	1.25
1	E	954[B]	GLU	CD-OE1	5.53	1.31	1.25
1	K	333	GLU	CD-OE1	5.53	1.31	1.25
1	E	38	GLU	CD-OE1	5.53	1.31	1.25
1	B	214	GLU	CD-OE1	5.53	1.31	1.25
1	K	214	GLU	CD-OE1	5.53	1.31	1.25
1	K	259	GLU	CD-OE1	5.52	1.31	1.25
1	E	426	GLU	CD-OE2	5.51	1.31	1.25
1	B	549	GLU	CD-OE1	5.51	1.31	1.25
2	L	318	GLU	CD-OE1	5.50	1.31	1.25
1	K	654	GLU	CD-OE1	5.50	1.31	1.25
1	B	348	GLU	CD-OE1	-5.50	1.19	1.25
1	B	102	GLU	CD-OE1	5.49	1.31	1.25
2	F	29	GLU	CD-OE1	5.49	1.31	1.25
1	B	594	GLU	CD-OE1	5.49	1.31	1.25
1	B	779	GLU	CD-OE1	5.49	1.31	1.25
1	H	672	GLU	CD-OE1	5.49	1.31	1.25
1	B	675	GLU	CD-OE1	5.48	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	188	GLU	CD-OE2	5.47	1.31	1.25
1	E	590	GLU	CD-OE1	5.47	1.31	1.25
1	E	1066	GLU	CD-OE1	5.45	1.31	1.25
2	C	318	GLU	CD-OE1	5.45	1.31	1.25
1	E	909	GLU	CD-OE2	5.45	1.31	1.25
2	C	187	GLU	CD-OE1	5.44	1.31	1.25
1	B	39	GLU	CD-OE1	5.44	1.31	1.25
1	E	109	GLU	CD-OE1	5.44	1.31	1.25
1	K	78	GLU	CD-OE2	5.44	1.31	1.25
1	B	259	GLU	CD-OE1	5.43	1.31	1.25
1	E	760	GLU	CD-OE1	5.43	1.31	1.25
1	E	548	GLU	CD-OE2	5.42	1.31	1.25
1	E	466	GLU	CD-OE1	5.42	1.31	1.25
2	L	189	GLU	CD-OE2	5.41	1.31	1.25
1	B	152	GLU	CD-OE1	5.40	1.31	1.25
1	E	392	GLU	CD-OE1	5.39	1.31	1.25
1	H	472	GLU	CD-OE1	5.38	1.31	1.25
1	H	466	GLU	CD-OE1	5.38	1.31	1.25
1	B	100	GLU	CD-OE1	5.38	1.31	1.25
1	H	58	GLU	CD-OE2	5.37	1.31	1.25
1	H	1059	GLU	CD-OE2	5.37	1.31	1.25
1	K	590	GLU	CD-OE1	5.37	1.31	1.25
1	K	969	GLU	CD-OE1	5.35	1.31	1.25
1	H	603	GLU	CD-OE1	5.35	1.31	1.25
1	E	234	GLU	CD-OE1	5.34	1.31	1.25
1	H	234	GLU	CD-OE1	5.34	1.31	1.25
1	H	590	GLU	CD-OE2	5.34	1.31	1.25
2	F	71	GLU	CD-OE2	5.34	1.31	1.25
1	E	102	GLU	CD-OE1	5.33	1.31	1.25
1	B	1059	GLU	CD-OE2	5.33	1.31	1.25
1	K	153	GLU	CD-OE1	5.33	1.31	1.25
1	E	559	GLU	CD-OE2	5.32	1.31	1.25
1	H	779	GLU	CD-OE1	5.32	1.31	1.25
1	B	71	GLU	CD-OE2	5.29	1.31	1.25
2	I	301	GLU	CD-OE1	5.29	1.31	1.25
1	B	725	GLU	CD-OE2	-5.29	1.19	1.25
1	H	39	GLU	CD-OE1	5.28	1.31	1.25
2	L	260	GLU	CD-OE2	5.28	1.31	1.25
1	E	511	GLU	CD-OE1	5.28	1.31	1.25
1	K	24	GLU	CD-OE1	5.27	1.31	1.25
1	B	418[A]	GLU	CD-OE1	5.25	1.31	1.25
1	B	418[B]	GLU	CD-OE1	5.25	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	623	GLU	CD-OE1	5.25	1.31	1.25
1	K	71	GLU	CD-OE2	5.25	1.31	1.25
1	K	840	GLU	CD-OE2	5.25	1.31	1.25
1	K	298	GLU	CD-OE1	-5.25	1.19	1.25
1	E	364	GLU	CD-OE1	5.24	1.31	1.25
1	H	153	GLU	CD-OE1	5.21	1.31	1.25
1	B	909	GLU	CD-OE2	5.20	1.31	1.25
1	E	881	GLU	CD-OE2	5.19	1.31	1.25
1	H	100	GLU	CD-OE2	-5.19	1.20	1.25
2	F	187	GLU	CD-OE2	5.18	1.31	1.25
1	E	472	GLU	CD-OE1	5.18	1.31	1.25
1	E	982	GLU	CD-OE1	5.18	1.31	1.25
1	E	779	GLU	CD-OE1	5.18	1.31	1.25
1	H	509	GLU	CD-OE1	5.17	1.31	1.25
1	H	840	GLU	CD-OE2	5.17	1.31	1.25
1	H	909	GLU	CD-OE2	5.16	1.31	1.25
1	K	392	GLU	CD-OE1	5.16	1.31	1.25
2	L	71	GLU	CD-OE2	5.15	1.31	1.25
1	E	108	GLU	CD-OE1	5.14	1.31	1.25
1	H	78	GLU	CD-OE1	5.14	1.31	1.25
2	I	96	GLU	CD-OE2	5.14	1.31	1.25
1	K	39	GLU	CD-OE1	5.13	1.31	1.25
1	H	186	GLU	CD-OE2	5.12	1.31	1.25
2	I	124	GLU	CD-OE1	5.12	1.31	1.25
1	K	623	GLU	CD-OE1	5.12	1.31	1.25
1	H	698	GLU	CD-OE2	5.12	1.31	1.25
1	H	594	GLU	CD-OE1	5.11	1.31	1.25
1	K	534	GLU	CD-OE1	5.11	1.31	1.25
1	E	654	GLU	CD-OE1	5.11	1.31	1.25
1	K	779	GLU	CD-OE1	5.11	1.31	1.25
1	H	333	GLU	CD-OE1	5.09	1.31	1.25
1	B	623	GLU	CD-OE1	5.09	1.31	1.25
1	E	259	GLU	CD-OE1	5.09	1.31	1.25
1	H	534	GLU	CD-OE1	5.09	1.31	1.25
1	E	915	GLU	CD-OE2	5.09	1.31	1.25
2	L	161	GLU	CD-OE2	5.07	1.31	1.25
1	H	426	GLU	CD-OE2	5.05	1.31	1.25
1	E	950[A]	GLU	CD-OE1	5.04	1.31	1.25
1	E	950[B]	GLU	CD-OE1	5.04	1.31	1.25
1	B	472	GLU	CD-OE1	5.03	1.31	1.25
1	B	333	GLU	CD-OE2	5.03	1.31	1.25
1	E	576	GLU	CD-OE1	5.03	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	189	GLU	CD-OE2	5.03	1.31	1.25
1	H	632	GLU	CD-OE1	5.01	1.31	1.25
2	F	161	GLU	CD-OE2	5.00	1.31	1.25

All (738) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	37	ARG	NE-CZ-NH1	16.23	128.42	120.30
1	E	513	ARG	NE-CZ-NH1	15.09	127.84	120.30
1	K	1003[A]	ARG	NE-CZ-NH1	14.27	127.43	120.30
1	K	1003[B]	ARG	NE-CZ-NH1	14.27	127.43	120.30
1	K	943	ARG	NE-CZ-NH1	14.13	127.37	120.30
1	H	342	ARG	NE-CZ-NH1	13.57	127.08	120.30
1	K	562	MET	CG-SD-CE	-12.88	79.60	100.20
2	I	197	TYR	CB-CG-CD1	-12.45	113.53	121.00
1	H	866	ARG	NE-CZ-NH2	-12.19	114.21	120.30
1	H	911	ARG	NE-CZ-NH2	-12.14	114.23	120.30
1	E	123	ASP	CB-CG-OD2	-12.07	107.44	118.30
1	B	734	ARG	NE-CZ-NH1	12.03	126.32	120.30
1	H	342	ARG	NE-CZ-NH2	-11.91	114.34	120.30
1	B	81	ARG	NE-CZ-NH2	-11.44	114.58	120.30
1	K	130	ARG	NE-CZ-NH1	11.43	126.01	120.30
2	I	207	ARG	NE-CZ-NH1	11.42	126.01	120.30
1	H	81	ARG	NE-CZ-NH1	10.93	125.77	120.30
2	L	123	ARG	NE-CZ-NH1	10.83	125.71	120.30
1	K	670	ARG	NE-CZ-NH2	-10.68	114.96	120.30
2	I	197	TYR	CB-CG-CD2	10.57	127.34	121.00
1	E	513	ARG	NE-CZ-NH2	-10.49	115.06	120.30
1	E	127	ASP	CB-CG-OD2	-10.47	108.88	118.30
1	E	127	ASP	CB-CG-OD1	10.26	127.54	118.30
1	B	225	ASP	CB-CG-OD2	10.26	127.53	118.30
1	E	193	ARG	NE-CZ-NH2	-10.19	115.20	120.30
1	B	614	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	H	74	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	K	168	ARG	NE-CZ-NH2	-10.06	115.27	120.30
1	H	127	ASP	CB-CG-OD2	-10.02	109.28	118.30
2	F	123	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	H	735	ARG	NE-CZ-NH1	9.92	125.26	120.30
1	E	129[A]	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	E	129[B]	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	B	608	ASP	CB-CG-OD1	9.73	127.06	118.30
1	B	887	TYR	CB-CG-CD1	-9.60	115.24	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	949	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	B	127	ASP	CB-CG-OD2	-9.55	109.70	118.30
1	K	123	ASP	CB-CG-OD2	9.50	126.85	118.30
2	C	139	ASP	CB-CG-OD2	-9.45	109.79	118.30
1	B	123	ASP	CB-CG-OD2	9.38	126.74	118.30
2	C	334	ASP	CB-CG-OD1	-9.31	109.92	118.30
1	B	614	ARG	NE-CZ-NH1	9.30	124.95	120.30
2	C	123	ARG	NE-CZ-NH2	-9.30	115.65	120.30
2	I	207	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	K	790	ASP	CB-CG-OD2	-9.22	110.00	118.30
1	E	123	ASP	CB-CG-OD1	9.13	126.51	118.30
1	K	513	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	H	74	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	B	132	ASP	CB-CG-OD1	-9.12	110.09	118.30
1	B	673	ASP	CB-CG-OD1	-9.06	110.15	118.30
1	B	610	ASP	CB-CG-OD1	-9.01	110.19	118.30
1	E	610	ASP	CB-CG-OD1	-9.01	110.19	118.30
1	B	5	ASP	CB-CG-OD1	-8.98	110.21	118.30
1	H	809	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	B	160	ASP	CB-CG-OD1	-8.96	110.24	118.30
1	B	809	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	B	458	ASP	CB-CG-OD2	-8.91	110.28	118.30
1	H	866	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	E	221	ARG	NE-CZ-NH1	8.89	124.74	120.30
1	E	433	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	B	225	ASP	CB-CG-OD1	-8.88	110.31	118.30
1	B	342	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	H	513	ARG	NE-CZ-NH2	-8.87	115.87	120.30
2	C	244	ASP	CB-CG-OD1	-8.84	110.34	118.30
2	L	380	THR	N-CA-CB	-8.81	93.56	110.30
1	E	37	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	B	64	TYR	CB-CG-CD1	-8.75	115.75	121.00
1	K	222	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	H	130	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	B	168	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	K	332	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	K	415	ASP	CB-CG-OD1	-8.71	110.46	118.30
1	E	822	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	E	570	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	B	669	ASP	CB-CG-OD2	8.61	126.05	118.30
2	C	262	ASP	CB-CG-OD2	-8.60	110.56	118.30
1	B	458	ASP	CB-CG-OD1	8.59	126.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	302	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	H	127	ASP	CB-CG-OD1	8.54	125.99	118.30
1	K	221	ARG	NE-CZ-NH1	8.52	124.56	120.30
2	C	139	ASP	CB-CG-OD1	8.52	125.96	118.30
1	E	41	TYR	CB-CG-CD1	-8.51	115.89	121.00
1	K	332	ASP	CB-CG-OD1	8.48	125.93	118.30
2	L	83	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	E	42	ARG	NE-CZ-NH1	8.44	124.52	120.30
2	C	227	ASP	CB-CG-OD2	-8.44	110.71	118.30
1	B	624	ASP	CB-CG-OD2	8.42	125.88	118.30
1	H	168	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	B	670	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	H	557	ASP	CB-CA-C	-8.38	93.64	110.40
1	B	971	ASP	CB-CG-OD2	-8.37	110.76	118.30
1	B	168	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	K	470	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	B	735	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	B	222	ASP	CB-CG-OD2	-8.30	110.83	118.30
2	F	157	ASP	CB-CG-OD2	8.25	125.73	118.30
2	F	262	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	B	735	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	K	589	ARG	NE-CZ-NH1	8.23	124.41	120.30
1	B	673	ASP	CB-CG-OD2	8.22	125.70	118.30
1	H	955	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	H	513	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	B	130	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	H	371	ASP	CB-CG-OD2	-8.15	110.97	118.30
1	K	608	ASP	CB-CG-OD1	8.10	125.59	118.30
2	F	207	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	B	613	ASP	CB-CG-OD1	-8.10	111.01	118.30
1	H	415	ASP	CB-CG-OD1	-8.06	111.04	118.30
1	H	955	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	B	56	ASP	CB-CG-OD2	8.01	125.51	118.30
1	B	132	ASP	CB-CG-OD2	8.00	125.50	118.30
1	B	196	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	H	486	ASP	CB-CG-OD1	7.99	125.49	118.30
1	K	123	ASP	CB-CG-OD1	-7.91	111.18	118.30
1	K	683	ARG	NE-CZ-NH2	-7.89	116.36	120.30
2	L	69	ASP	CB-CG-OD2	7.88	125.39	118.30
1	B	399	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	K	470	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	K	570	ARG	NE-CZ-NH2	-7.84	116.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	127	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	K	670	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	E	443	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	B	425	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	K	752	ASP	CB-CG-OD2	-7.77	111.30	118.30
1	E	520	ASP	CB-CG-OD1	-7.77	111.31	118.30
1	K	5	ASP	CB-CG-OD1	-7.77	111.31	118.30
2	C	326	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	K	458	ASP	CB-CG-OD1	-7.74	111.33	118.30
1	E	608	ASP	CB-CG-OD1	7.74	125.26	118.30
1	E	3	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	B	666	ASP	CB-CG-OD1	-7.73	111.34	118.30
1	K	677	PHE	CB-CG-CD2	-7.72	115.40	120.80
1	E	752	ASP	CB-CG-OD1	7.72	125.25	118.30
1	H	608	ASP	CB-CG-OD1	7.72	125.24	118.30
1	B	123	ASP	CB-CG-OD1	-7.71	111.36	118.30
1	K	768	ASP	CB-CG-OD1	-7.71	111.36	118.30
2	F	249	ASP	CB-CG-OD2	7.70	125.23	118.30
1	B	837	TYR	CB-CG-CD2	-7.69	116.38	121.00
1	H	132	ASP	CB-CG-OD1	-7.66	111.41	118.30
1	H	470	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	E	1003	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	K	5	ASP	CB-CG-OD2	7.62	125.16	118.30
2	L	211	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	K	790	ASP	CB-CG-OD1	7.61	125.15	118.30
1	H	360	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	K	41	TYR	CB-CG-CD2	-7.60	116.44	121.00
1	E	516	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	H	666	ASP	CB-CG-OD1	-7.59	111.47	118.30
1	B	949	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	L	112	ASP	CB-CG-OD2	7.57	125.11	118.30
1	E	614	ARG	NE-CZ-NH2	-7.56	116.52	120.30
2	I	188	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	H	557	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	B	193	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	K	222	ASP	CB-CG-OD1	7.52	125.07	118.30
2	I	157	ASP	CB-CG-OD2	7.51	125.06	118.30
2	I	120	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	K	458	ASP	CB-CG-OD2	7.49	125.04	118.30
1	K	342	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	H	486	ASP	CB-CG-OD2	-7.48	111.57	118.30
2	I	93	ARG	NE-CZ-NH1	7.47	124.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	830	ALA	N-CA-CB	7.47	120.56	110.10
1	K	608	ASP	CB-CG-OD2	-7.47	111.58	118.30
2	C	207	ARG	NE-CZ-NH1	7.46	124.03	120.30
2	L	344	ASP	CB-CG-OD1	-7.46	111.59	118.30
1	H	83	ASP	CB-CG-OD1	-7.45	111.59	118.30
1	K	822	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	E	517	ASP	CB-CG-OD2	-7.45	111.60	118.30
2	I	262	ASP	CB-CG-OD2	-7.43	111.62	118.30
1	K	706	GLU	CB-CA-C	7.42	125.25	110.40
2	F	211	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	K	591	ASP	CB-CG-OD2	7.42	124.98	118.30
1	H	89	MET	CA-CB-CG	7.41	125.89	113.30
1	B	887	TYR	CB-CG-CD2	7.40	125.44	121.00
1	K	225	ASP	CB-CG-OD1	-7.40	111.64	118.30
1	K	610	ASP	CB-CG-OD2	7.40	124.96	118.30
1	K	37	ARG	NE-CZ-NH1	7.40	124.00	120.30
2	F	192	PHE	CB-CG-CD1	-7.38	115.64	120.80
1	H	613	ASP	CB-CG-OD1	-7.37	111.67	118.30
2	F	269	CYS	CB-CA-C	7.36	125.11	110.40
1	K	806	ASP	CB-CG-OD1	-7.35	111.68	118.30
1	H	790	ASP	CB-CG-OD2	-7.35	111.69	118.30
2	C	348	PHE	CB-CG-CD2	-7.33	115.67	120.80
1	B	196	ASP	CB-CG-OD1	7.31	124.88	118.30
1	H	56	ASP	CB-CG-OD2	7.31	124.88	118.30
2	F	5	ALA	N-CA-CB	7.31	120.33	110.10
1	K	847	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	K	666	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	K	1056	ASP	CB-CG-OD2	7.28	124.85	118.30
2	C	244	ASP	CB-CG-OD2	7.26	124.83	118.30
2	L	212	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	E	486	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	H	103	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	H	184	ARG	N-CA-CB	-7.20	97.64	110.60
2	L	5	ALA	N-CA-CB	7.20	120.18	110.10
2	L	139	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	E	168	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	K	127	ASP	CB-CG-OD1	7.19	124.77	118.30
1	K	168	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	H	911	ARG	NE-CZ-NH1	7.18	123.89	120.30
2	L	97	ASP	CB-CG-OD1	-7.18	111.84	118.30
1	E	225	ASP	CB-CG-OD2	7.17	124.75	118.30
1	H	409	ASP	CB-CG-OD2	7.17	124.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	538	ASP	CB-CG-OD1	-7.13	111.88	118.30
2	I	97	ASP	CB-CG-OD1	-7.12	111.89	118.30
2	L	112	ASP	CB-CG-OD1	-7.12	111.89	118.30
2	F	249	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	H	128	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	B	187	PHE	CB-CG-CD2	7.10	125.77	120.80
1	E	735	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	E	670	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	E	41	TYR	CB-CG-CD2	7.08	125.25	121.00
2	F	244	ASP	CB-CG-OD1	-7.07	111.94	118.30
1	K	1003[A]	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	K	1003[B]	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	E	237	ASP	CB-CG-OD1	7.05	124.65	118.30
1	H	459	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	K	764	ASP	CB-CG-OD2	7.05	124.64	118.30
1	E	272	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	E	624	ASP	CB-CG-OD2	7.02	124.62	118.30
2	I	211	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	E	433	ASP	CB-CG-OD1	7.00	124.60	118.30
1	E	809	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	K	1056	ASP	CB-CG-OD1	-6.96	112.03	118.30
2	C	250	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	H	903	ASP	CB-CG-OD1	-6.95	112.04	118.30
1	K	132	ASP	CB-CG-OD1	-6.94	112.05	118.30
1	E	538	ASP	CB-CG-OD1	-6.94	112.06	118.30
2	F	348	PHE	CB-CG-CD2	-6.93	115.95	120.80
1	H	958	ASP	CB-CG-OD2	-6.93	112.07	118.30
2	L	348	PHE	CB-CG-CD1	6.92	125.65	120.80
1	H	971	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	610	ASP	CB-CG-OD2	6.92	124.53	118.30
1	E	132	ASP	CB-CG-OD1	6.92	124.52	118.30
1	K	806	ASP	CB-CG-OD2	6.92	124.53	118.30
1	E	131	PHE	CB-CG-CD1	6.92	125.64	120.80
1	K	562	MET	CB-CA-C	-6.90	96.59	110.40
1	E	329	TYR	CB-CG-CD1	-6.90	116.86	121.00
1	H	729	ASP	CB-CG-OD1	-6.89	112.10	118.30
1	E	144[A]	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	E	144[B]	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	E	752	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	H	56	ASP	CB-CG-OD1	-6.88	112.11	118.30
2	L	120	ARG	NE-CZ-NH1	6.87	123.73	120.30
2	F	342	ARG	NE-CZ-NH1	6.87	123.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	486	ASP	CB-CG-OD1	6.87	124.48	118.30
2	L	148	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	K	1020	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	H	409	ASP	CB-CG-OD1	-6.84	112.15	118.30
1	H	61	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	E	487	PHE	CB-CG-CD2	-6.82	116.03	120.80
2	C	286	MET	CG-SD-CE	-6.80	89.32	100.20
1	E	3	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	E	5	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	K	768	ASP	CB-CG-OD2	6.78	124.40	118.30
1	E	538	ASP	CB-CG-OD2	6.78	124.40	118.30
2	L	114	ASP	CB-CG-OD2	6.77	124.39	118.30
1	H	123	ASP	CB-CG-OD1	-6.77	112.21	118.30
1	H	529	ASP	CB-CG-OD1	6.76	124.39	118.30
1	H	120	ASP	CB-CG-OD1	-6.76	112.22	118.30
1	B	459	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	C	262	ASP	CB-CG-OD1	6.74	124.37	118.30
1	K	81	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	I	97	ASP	CB-CG-OD2	6.73	124.36	118.30
2	L	234	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	B	160	ASP	CB-CG-OD2	6.73	124.36	118.30
1	B	486	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	H	669	ASP	CB-CG-OD1	-6.70	112.27	118.30
1	B	127	ASP	CB-CG-OD1	6.69	124.32	118.30
2	I	262	ASP	CB-CG-OD1	6.67	124.30	118.30
2	F	211	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	624	ASP	CB-CG-OD1	-6.66	112.30	118.30
1	E	225	ASP	CB-CG-OD1	-6.66	112.30	118.30
2	I	74	GLN	CB-CA-C	-6.66	97.09	110.40
1	H	520	ASP	CB-CG-OD1	-6.64	112.33	118.30
1	H	949	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	C	212	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	E	670	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	E	757	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	489	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	E	352	ASP	CB-CG-OD2	6.61	124.24	118.30
1	H	58	GLU	N-CA-CB	-6.60	98.71	110.60
1	E	415	ASP	CB-CG-OD1	-6.60	112.36	118.30
1	E	764	ASP	CB-CG-OD2	6.60	124.24	118.30
1	K	434	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	K	160	ASP	CB-CG-OD1	-6.59	112.37	118.30
2	C	123	ARG	NE-CZ-NH1	6.57	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	344	ASP	CB-CG-OD1	-6.56	112.40	118.30
2	F	70	GLU	N-CA-CB	6.55	122.39	110.60
2	C	348	PHE	CB-CG-CD1	6.54	125.38	120.80
1	B	371	ASP	CB-CG-OD1	6.53	124.18	118.30
2	C	67	ASP	CB-CG-OD2	6.53	124.17	118.30
1	E	332	ASP	CB-CG-OD1	6.52	124.17	118.30
1	E	520	ASP	CB-CG-OD2	6.52	124.17	118.30
1	K	756	ASP	CB-CG-OD1	-6.52	112.43	118.30
1	H	83	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	83	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	K	415	ASP	CB-CG-OD2	6.48	124.13	118.30
1	K	221	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	E	42	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	H	613	ASP	CB-CG-OD2	6.47	124.13	118.30
1	H	608	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	E	943	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	K	762	ASP	CB-CG-OD2	6.44	124.10	118.30
1	K	809	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	I	136	ASP	CB-CG-OD1	-6.44	112.50	118.30
1	K	196	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	B	353	TYR	CB-CG-CD1	6.43	124.86	121.00
1	H	425	ARG	NE-CZ-NH1	6.43	123.52	120.30
2	C	334	ASP	CB-CG-OD2	6.43	124.09	118.30
1	K	529	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	B	37	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	K	433	ASP	CB-CG-OD1	6.41	124.07	118.30
1	K	666	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	1040	ASP	CB-CG-OD2	6.39	124.06	118.30
1	K	74	ARG	NE-CZ-NH1	6.39	123.50	120.30
2	F	192	PHE	CB-CG-CD2	6.39	125.27	120.80
1	H	666	ASP	CB-CG-OD2	6.37	124.03	118.30
1	K	997	ARG	NE-CZ-NH2	-6.37	117.12	120.30
2	F	223	THR	CA-CB-CG2	6.36	121.30	112.40
2	C	136	ASP	CB-CG-OD1	-6.35	112.58	118.30
1	H	752	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	K	1003[A]	ARG	CD-NE-CZ	6.34	132.48	123.60
1	K	1003[B]	ARG	CD-NE-CZ	6.34	132.48	123.60
1	E	449	ASP	CB-CG-OD1	-6.33	112.61	118.30
1	E	651	ARG	NE-CZ-NH1	6.33	123.46	120.30
2	F	262	ASP	CB-CG-OD1	6.33	123.99	118.30
1	B	608	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	E	449	ASP	CB-CG-OD2	6.31	123.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	97	ASP	CB-CG-OD2	6.31	123.98	118.30
1	E	424	ARG	NE-CZ-NH2	-6.31	117.15	120.30
1	H	458	ASP	CB-CG-OD2	-6.30	112.63	118.30
2	I	112	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	B	425	ARG	NE-CZ-NH1	6.29	123.45	120.30
2	L	114	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	B	206	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	H	26	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	399	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	E	329	TYR	CB-CG-CD2	6.28	124.77	121.00
1	K	952	ASP	CB-CG-OD2	6.27	123.95	118.30
1	B	669	ASP	CB-CG-OD1	-6.27	112.66	118.30
1	H	757	ASP	CB-CG-OD2	6.27	123.94	118.30
1	K	570	ARG	CB-CA-C	-6.26	97.87	110.40
2	L	207	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	513	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	K	486	ASP	CB-CG-OD1	6.25	123.92	118.30
1	K	443	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	E	949	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	K	449	ASP	CB-CG-OD2	6.24	123.91	118.30
2	F	120	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	H	415	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	5	ASP	CB-CG-OD2	6.22	123.90	118.30
1	B	730	GLU	CG-CD-OE2	6.22	130.73	118.30
1	B	415	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	61	ASP	CB-CG-OD1	6.21	123.89	118.30
1	E	998	PRO	N-CA-CB	6.21	110.75	103.30
1	E	837	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	E	949	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	H	225	ASP	CB-CG-OD2	6.20	123.88	118.30
1	H	529	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	C	188	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	1051	MET	CB-CA-C	-6.19	98.02	110.40
1	K	809	ARG	NE-CZ-NH2	-6.19	117.20	120.30
2	L	139	ASP	CB-CG-OD1	6.19	123.87	118.30
1	E	613	ASP	CB-CG-OD2	6.19	123.87	118.30
1	H	1003	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	911[A]	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	911[B]	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	C	6	LEU	N-CA-CB	-6.18	98.05	110.40
1	K	757	ASP	CB-CG-OD2	6.17	123.85	118.30
2	L	262	ASP	CB-CG-OD2	-6.17	112.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	42	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	K	245	ASP	CB-CG-OD2	6.16	123.84	118.30
1	K	729	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	432	ALA	CB-CA-C	-6.16	100.87	110.10
1	E	613	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	H	120	ASP	CB-CG-OD2	6.15	123.84	118.30
1	E	1056	ASP	CB-CG-OD2	6.14	123.83	118.30
1	H	434	ARG	NE-CZ-NH2	6.14	123.37	120.30
2	F	198	ASP	CB-CG-OD2	6.13	123.82	118.30
2	I	93	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	B	372	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	K	538	ASP	CB-CG-OD1	-6.13	112.79	118.30
1	B	409	ASP	CB-CG-OD2	6.12	123.81	118.30
1	K	724	MET	CG-SD-CE	6.12	110.00	100.20
2	F	377	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	E	130	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	E	429[A]	ASP	CB-CG-OD1	-6.12	112.80	118.30
1	E	429[B]	ASP	CB-CG-OD1	-6.12	112.80	118.30
1	K	757	ASP	CB-CG-OD1	-6.12	112.80	118.30
1	H	847	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	E	762	ASP	CB-CG-OD1	-6.11	112.80	118.30
2	L	10	GLU	CB-CA-C	-6.10	98.19	110.40
2	I	112	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	756	ASP	CB-CG-OD1	-6.08	112.83	118.30
2	L	15	PHE	CB-CG-CD2	-6.08	116.55	120.80
1	E	608	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	K	669	ASP	CB-CG-OD1	-6.07	112.84	118.30
1	K	669	ASP	CB-CG-OD2	6.06	123.76	118.30
1	E	352	ASP	CB-CG-OD1	-6.06	112.85	118.30
1	B	171	PHE	CB-CG-CD2	-6.06	116.56	120.80
2	C	331	SER	N-CA-CB	6.05	119.58	110.50
1	E	515	LEU	CB-CG-CD2	-6.05	100.71	111.00
1	E	756	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	B	729	ASP	CB-CG-OD1	-6.05	112.85	118.30
1	E	971	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	H	729	ASP	CB-CG-OD2	6.05	123.74	118.30
1	H	809	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	E	60	ALA	N-CA-CB	6.05	118.56	110.10
1	H	538	ASP	CB-CG-OD2	6.04	123.74	118.30
1	K	206	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	B	520[A]	ASP	CA-CB-CG	6.03	126.67	113.40
1	B	520[B]	ASP	CA-CB-CG	6.03	126.67	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	245	ASP	CB-CG-OD1	-6.03	112.88	118.30
1	K	955	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	H	709	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	K	557	ASP	CB-CG-OD2	6.03	123.72	118.30
1	H	206	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	H	103	ARG	NE-CZ-NH2	-6.00	117.30	120.30
2	C	5	ALA	N-CA-CB	6.00	118.50	110.10
2	L	15	PHE	CB-CG-CD1	6.00	125.00	120.80
1	H	305	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	K	225	ASP	CB-CG-OD2	5.98	123.68	118.30
1	K	557	ASP	CB-CG-OD1	-5.97	112.92	118.30
2	L	163	THR	CA-CB-CG2	-5.97	104.05	112.40
1	K	952	ASP	CB-CG-OD1	-5.96	112.93	118.30
2	C	67	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	K	443	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	B	578	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	B	962	LYS	CA-CB-CG	-5.94	100.33	113.40
2	C	377	TYR	CB-CG-CD1	-5.94	117.44	121.00
1	H	184	ARG	C-N-CA	5.94	136.55	121.70
1	H	257	ASP	CB-CG-OD2	5.93	123.64	118.30
1	K	610	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	B	737	PHE	CB-CG-CD2	-5.92	116.65	120.80
1	K	500	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	E	5	ASP	CB-CG-OD2	5.91	123.62	118.30
1	E	610	ASP	CB-CG-OD2	5.91	123.62	118.30
1	H	1040	ASP	CB-CG-OD2	5.91	123.62	118.30
1	E	388	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	H	533	ALA	N-CA-CB	5.90	118.36	110.10
2	L	18	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	K	808	MET	CG-SD-CE	-5.90	90.76	100.20
1	B	1026	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	H	790	ASP	CB-CG-OD1	5.89	123.60	118.30
1	E	424	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	557	ASP	N-CA-CB	-5.88	100.02	110.60
2	L	378	ARG	CB-CA-C	-5.88	98.65	110.40
1	B	1068	HIS	N-CA-CB	-5.87	100.03	110.60
2	L	97	ASP	CB-CG-OD2	5.87	123.58	118.30
1	H	160	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	B	752	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	E	673	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	E	729	ASP	CB-CG-OD2	5.86	123.58	118.30
2	C	84	ASP	CB-CG-OD1	5.86	123.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	184	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	H	332	ASP	CB-CG-OD1	5.86	123.58	118.30
1	H	498	ASP	CB-CG-OD2	5.86	123.58	118.30
1	H	917	MET	CG-SD-CE	5.85	109.56	100.20
1	E	222	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	B	1068	HIS	CA-CB-CG	-5.85	103.66	113.60
1	E	272	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	H	709	TYR	CB-CG-CD1	5.84	124.50	121.00
1	B	971	ASP	CB-CA-C	-5.83	98.73	110.40
1	H	268	MET	CG-SD-CE	-5.83	90.87	100.20
1	K	203	LEU	CB-CA-C	-5.83	99.12	110.20
1	H	440	ASP	CB-CG-OD1	-5.83	113.06	118.30
2	F	67	ASP	CB-CG-OD1	-5.83	113.06	118.30
2	C	18	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	E	500	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	117	ALA	N-CA-CB	5.82	118.24	110.10
1	K	618	GLU	N-CA-CB	-5.81	100.14	110.60
2	F	317	ASP	CB-CG-OD1	-5.81	113.07	118.30
2	I	139	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	911[A]	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	911[B]	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	538	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	409	ASP	CB-CG-OD1	-5.79	113.08	118.30
1	B	83	ASP	CB-CG-OD2	5.78	123.50	118.30
2	L	69	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	H	971	ASP	CB-CG-OD1	5.76	123.49	118.30
1	K	958	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	B	1038	HIS	CA-CB-CG	-5.76	103.80	113.60
2	L	348	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	K	135	MET	CG-SD-CE	5.76	109.41	100.20
1	B	277	GLU	N-CA-CB	5.75	120.96	110.60
1	E	416	ASP	CB-CA-C	5.75	121.90	110.40
1	H	538	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	B	714	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	C	36	MET	N-CA-CB	5.73	120.92	110.60
2	C	342	ARG	NE-CZ-NH1	5.73	123.16	120.30
2	C	227	ASP	CB-CG-OD1	5.73	123.45	118.30
1	E	332	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	K	489	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	K	1035	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	K	25	PHE	CB-CG-CD1	-5.72	116.79	120.80
1	B	487	PHE	CB-CG-CD2	-5.72	116.80	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	83	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	B	1003	ARG	NE-CZ-NH1	5.71	123.15	120.30
2	L	344	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	762	ASP	CB-CG-OD1	-5.70	113.17	118.30
2	I	234	ASP	CB-CG-OD1	5.70	123.43	118.30
1	E	683	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	H	272	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	449	ASP	CB-CG-OD1	-5.69	113.18	118.30
2	I	266	PHE	CB-CG-CD1	5.68	124.78	120.80
1	H	433	ASP	CB-CG-OD1	5.68	123.41	118.30
1	E	37	ARG	CD-NE-CZ	5.67	131.54	123.60
1	K	517	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	H	232	SER	N-CA-CB	5.66	118.99	110.50
1	H	1026	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	K	673	ASP	CB-CG-OD1	5.65	123.38	118.30
2	C	97	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	K	500	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	H	130	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	C	84	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	K	26	ASP	CB-CG-OD2	5.63	123.37	118.30
1	E	470	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	I	244	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	E	337	ASP	CB-CG-OD1	-5.62	113.25	118.30
1	H	342	ARG	CG-CD-NE	-5.61	100.01	111.80
1	K	369	ALA	N-CA-CB	-5.61	102.25	110.10
1	E	669	ASP	CB-CG-OD2	5.61	123.35	118.30
1	H	129	ARG	NE-CZ-NH1	5.61	123.10	120.30
2	L	262	ASP	CB-CG-OD1	5.61	123.34	118.30
2	L	342	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	H	185[A]	GLU	O-C-N	5.59	131.64	122.70
1	H	185[B]	GLU	O-C-N	5.59	131.64	122.70
2	F	350	PHE	CB-CG-CD2	-5.59	116.89	120.80
1	H	196	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	C	136	ASP	CB-CG-OD2	5.58	123.32	118.30
1	H	332	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	K	433	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	E	160	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	B	498	ASP	CB-CG-OD2	5.56	123.31	118.30
1	E	61	ASP	CB-CG-OD1	5.56	123.31	118.30
2	F	306	MET	N-CA-CB	5.56	120.61	110.60
1	H	433	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	E	1040	ASP	CB-CG-OD2	5.55	123.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	74	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	K	673	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	K	42	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	H	206	ASP	CB-CG-OD2	5.54	123.29	118.30
2	L	136	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	B	661	ILE	CA-CB-CG2	-5.54	99.83	110.90
1	B	752	ASP	CB-CG-OD1	5.54	123.28	118.30
1	K	355	VAL	CA-CB-CG1	-5.54	102.60	110.90
1	E	529	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	B	666	ASP	CB-CG-OD2	5.53	123.28	118.30
1	H	727	VAL	CA-CB-CG2	-5.53	102.60	110.90
1	H	520	ASP	CB-CG-OD2	5.51	123.26	118.30
2	L	227	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	H	917	MET	N-CA-CB	5.51	120.51	110.60
2	F	344	ASP	CB-CG-OD2	5.50	123.25	118.30
2	I	344	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	E	1024	ASP	CB-CG-OD2	5.50	123.25	118.30
1	H	610	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	757[A]	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	757[B]	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	129[A]	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	129[B]	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	293	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	K	579	TYR	CB-CG-CD2	-5.49	117.71	121.00
2	C	378	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	K	489	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	H	470	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	516	ARG	NE-CZ-NH1	5.47	123.03	120.30
2	I	334	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	B	958	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	K	83	ASP	CB-CG-OD2	5.46	123.21	118.30
1	K	399	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	103	ARG	NE-CZ-NH1	5.45	123.03	120.30
2	I	123	ARG	NE-CZ-NH1	5.45	123.02	120.30
2	L	45	ASP	CB-CG-OD2	5.45	123.20	118.30
2	C	10	GLU	CB-CA-C	-5.44	99.52	110.40
1	E	1024	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	B	299	MET	CG-SD-CE	-5.44	91.50	100.20
1	K	352	ASP	CB-CG-OD2	5.44	123.19	118.30
2	L	84	ASP	CB-CG-OD1	5.43	123.19	118.30
1	H	61	ASP	CB-CG-OD1	5.43	123.18	118.30
1	K	130	ARG	NE-CZ-NH2	-5.43	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1024	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	K	997	ARG	N-CA-CB	-5.42	100.83	110.60
2	F	227	ASP	CB-CG-OD2	5.42	123.18	118.30
1	E	486	ASP	CB-CG-OD1	5.41	123.17	118.30
1	H	903	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	415	ASP	CB-CG-OD1	-5.41	113.44	118.30
1	E	735	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	H	517[A]	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	H	517[B]	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	H	184	ARG	N-CA-C	5.40	125.58	111.00
1	B	729	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	570	ARG	CB-CA-C	-5.39	99.61	110.40
1	H	714	ARG	CA-C-O	-5.39	108.77	120.10
2	L	215	ARG	N-CA-CB	5.39	120.31	110.60
1	E	66	GLU	CG-CD-OE2	5.39	129.08	118.30
1	B	570	ARG	CD-NE-CZ	-5.39	116.06	123.60
1	E	768	ASP	CB-CG-OD2	5.39	123.15	118.30
2	L	68	ALA	N-CA-CB	5.39	117.64	110.10
1	E	285	PHE	CB-CG-CD2	-5.38	117.03	120.80
1	K	37	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	H	991	ASN	CB-CA-C	-5.37	99.66	110.40
1	B	529	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	H	449	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	K	982	GLU	OE1-CD-OE2	5.37	129.74	123.30
1	E	367	ALA	CB-CA-C	5.37	118.15	110.10
1	E	206	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	E	429[A]	ASP	CB-CG-OD2	5.36	123.12	118.30
1	E	429[B]	ASP	CB-CG-OD2	5.36	123.12	118.30
1	H	556	THR	N-CA-CB	-5.35	100.13	110.30
1	H	673	ASP	CB-CG-OD2	-5.35	113.48	118.30
2	F	11	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	B	991	ASN	CB-CA-C	-5.35	99.70	110.40
1	K	1035	TYR	CA-CB-CG	-5.33	103.28	113.40
1	H	735	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	E	83	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	H	222	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	56	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	B	529	ASP	CB-CG-OD1	5.31	123.08	118.30
1	H	676	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	558	ARG	NE-CZ-NH2	-5.31	117.64	120.30
2	I	114	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	H	618	GLU	N-CA-CB	-5.30	101.05	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	972	ALA	N-CA-CB	5.30	117.52	110.10
1	B	578	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	866	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	H	222	ASP	CB-CG-OD1	5.30	123.07	118.30
2	C	188	ASP	CB-CG-OD1	-5.29	113.53	118.30
1	K	837	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	E	409	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	H	887	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	K	503	LYS	CB-CA-C	-5.27	99.85	110.40
1	K	591	ASP	CB-CG-OD1	-5.27	113.56	118.30
2	L	368	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	264	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	F	97	ASP	CB-CG-OD2	5.27	123.04	118.30
1	E	757	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	B	955	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	K	786	VAL	N-CA-C	-5.26	96.81	111.00
1	E	196	ASP	CB-CG-OD1	5.25	123.03	118.30
1	E	64	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	K	253	GLN	CB-CA-C	-5.25	99.91	110.40
1	K	677	PHE	CB-CG-CD1	5.25	124.47	120.80
2	L	362	ASP	CB-CG-OD2	5.24	123.01	118.30
2	I	214	CYS	CB-CA-C	-5.23	99.94	110.40
1	E	247	ILE	N-CA-C	-5.22	96.89	111.00
1	H	624	ASP	CB-CG-OD2	5.22	123.00	118.30
1	K	342	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	E	160	ASP	CB-CG-OD2	5.22	123.00	118.30
2	L	343	THR	CA-CB-CG2	-5.22	105.09	112.40
1	E	570	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	E	756	ASP	CB-CG-OD2	5.22	122.99	118.30
1	K	630	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	B	64	TYR	CB-CG-CD2	5.20	124.12	121.00
1	H	971	ASP	N-CA-CB	5.20	119.95	110.60
2	L	223	THR	CA-CB-CG2	-5.20	105.13	112.40
1	H	123	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	786	VAL	N-CA-C	-5.19	96.99	111.00
2	C	212	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	K	132	ASP	CB-CG-OD2	5.19	122.97	118.30
1	K	971	ASP	N-CA-CB	5.19	119.93	110.60
2	F	114	ASP	CB-CG-OD1	-5.18	113.63	118.30
2	F	112	ASP	CB-CG-OD2	5.18	122.96	118.30
2	F	97	ASP	CB-CG-OD1	-5.18	113.64	118.30
2	I	188	ASP	CB-CG-OD1	5.18	122.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1000	ILE	CB-CA-C	-5.17	101.25	111.60
1	H	768	ASP	CB-CG-OD2	5.17	122.95	118.30
1	H	459	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	H	527	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	K	399	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	K	686	LEU	N-CA-CB	5.16	120.72	110.40
1	E	1023	GLU	CB-CA-C	-5.16	100.09	110.40
1	K	578	ASP	CB-CG-OD2	5.15	122.94	118.30
1	H	496	PHE	CB-CG-CD1	-5.15	117.20	120.80
1	K	206	ASP	CB-CG-OD2	5.15	122.93	118.30
1	H	1019	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	K	927	PHE	CB-CG-CD1	5.15	124.40	120.80
1	B	971	ASP	N-CA-CB	5.15	119.86	110.60
1	H	58	GLU	CA-CB-CG	-5.15	102.08	113.40
1	H	764	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	H	1055	ALA	N-CA-CB	5.14	117.30	110.10
1	H	247	ILE	N-CA-C	-5.14	97.13	111.00
1	K	61	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	K	525	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	B	806	ASP	CB-CG-OD1	-5.13	113.68	118.30
2	L	5	ALA	CB-CA-C	5.13	117.80	110.10
1	K	847	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	C	306	MET	N-CA-CB	5.12	119.82	110.60
2	L	249	ASP	CB-CG-OD2	5.12	122.91	118.30
1	H	508	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	L	234	ASP	CB-CG-OD1	5.11	122.90	118.30
1	E	337	ASP	CB-CA-C	-5.11	100.18	110.40
2	L	314	PHE	CB-CG-CD2	-5.11	117.22	120.80
2	L	334	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	E	1037	VAL	CA-CB-CG2	-5.11	103.24	110.90
1	H	578	ASP	CB-CG-OD2	5.11	122.90	118.30
1	H	806	ASP	CB-CG-OD2	5.11	122.90	118.30
2	L	196	ALA	N-CA-CB	-5.11	102.95	110.10
1	E	845	ALA	CB-CA-C	-5.11	102.44	110.10
1	H	353	TYR	CB-CG-CD1	5.11	124.06	121.00
1	B	762	ASP	CB-CG-OD2	5.10	122.89	118.30
1	K	54	MET	CG-SD-CE	5.10	108.36	100.20
1	K	735	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	H	26	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	H	342	ARG	CB-CA-C	5.09	120.59	110.40
2	L	84	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	342	ARG	NE-CZ-NH1	5.09	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	1071	ILE	CB-CA-C	5.09	121.78	111.60
1	K	371	ASP	CB-CG-OD1	5.08	122.87	118.30
2	L	217	THR	CA-CB-CG2	-5.08	105.28	112.40
1	E	729	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	E	792	ALA	N-CA-C	-5.08	97.29	111.00
1	E	487	PHE	CB-CG-CD1	5.08	124.35	120.80
2	C	190	LEU	CB-CA-C	5.08	119.84	110.20
1	E	677	PHE	CB-CG-CD2	-5.07	117.25	120.80
2	I	317	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	757[A]	ASP	CB-CG-OD1	-5.06	113.74	118.30
1	B	757[B]	ASP	CB-CG-OD1	-5.06	113.74	118.30
1	B	630	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	411	LYS	N-CA-CB	-5.06	101.50	110.60
1	K	683	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	998	PRO	N-CA-CB	5.05	109.36	103.30
2	I	139	ASP	CB-CG-OD2	-5.05	113.76	118.30
2	C	377	TYR	CB-CG-CD2	5.05	124.03	121.00
1	H	118	THR	CA-CB-CG2	-5.04	105.34	112.40
1	K	538	ASP	CB-CG-OD2	5.04	122.84	118.30
2	I	330	LYS	CB-CA-C	-5.04	100.32	110.40
1	B	329	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	H	1040	ASP	CB-CG-OD1	-5.03	113.78	118.30
2	I	211	ASP	CB-CG-OD1	5.03	122.83	118.30
1	B	222	ASP	CB-CG-OD1	5.02	122.82	118.30
1	E	806	ASP	CB-CG-OD1	-5.02	113.78	118.30
2	F	354	PRO	N-CA-CB	5.02	109.32	103.30
1	H	591	ASP	CB-CG-OD1	-5.02	113.78	118.30
2	I	244	ASP	CB-CG-OD2	5.02	122.82	118.30
1	K	264	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	487	PHE	CB-CG-CD1	5.01	124.31	120.80
1	E	578	ASP	CB-CG-OD1	-5.01	113.79	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	338	ILE	CA

There are no planarity outliers.

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	B	8195	0	8221	207	0
1	E	8223	0	8265	280	0
1	H	8179	0	8215	257	0
1	K	8201	0	8241	225	0
2	C	2895	0	2863	134	0
2	F	2904	0	2868	154	0
2	I	2895	0	2863	153	0
2	L	2895	0	2863	95	0
3	B	4	0	0	0	0
3	E	4	0	0	0	0
3	H	4	0	0	0	0
3	K	4	0	0	0	0
4	B	6	0	0	0	0
4	C	1	0	0	0	0
4	E	7	0	0	0	0
4	F	1	0	0	0	0
4	H	5	0	0	0	0
4	I	1	0	0	0	0
4	K	7	0	0	0	0
4	L	1	0	0	0	0
5	B	10	0	0	1	0
5	E	10	0	0	1	0
5	H	10	0	0	2	0
5	K	15	0	0	2	0
6	B	6	0	0	1	0
6	C	1	0	0	0	0
6	E	7	0	0	1	0
6	F	1	0	0	0	0
6	H	6	0	0	1	0
6	I	1	0	0	1	0
6	K	6	0	0	0	0
6	L	1	0	0	0	0
7	B	20	0	14	0	0
7	E	20	0	14	1	0
7	H	20	0	14	2	0
7	K	20	0	14	1	0
8	B	54	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	54	0	24	1	0
8	H	54	0	24	0	0
8	K	54	0	24	1	0
9	B	9	0	11	4	0
9	E	9	0	11	3	0
9	H	9	0	11	0	0
9	K	9	0	11	1	0
10	B	9	0	20	1	0
10	E	9	0	20	0	0
10	H	9	0	20	2	0
10	K	9	0	20	0	0
11	B	970	0	0	19	1
11	C	241	0	0	6	0
11	E	1022	0	0	30	1
11	F	210	0	0	6	0
11	H	942	0	0	28	0
11	I	235	0	0	5	0
11	K	980	0	0	21	0
11	L	257	0	0	6	0
All	All	49731	0	44675	1485	1

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 17.

All (1485) 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:E:0:MET:HB3	1:E:223:LYS:HE3	1.22	1.17
1:H:701:VAL:HG12	1:H:705:LYS:HE3	1.31	1.05
2:I:133:ILE:HG22	2:I:138:PRO:HB3	1.31	1.04
1:B:702:GLU:HA	1:B:705:LYS:HD2	1.38	1.04
1:H:673:ASP:HB3	1:H:676:ARG:HB2	1.37	1.03
2:I:133:ILE:HD12	2:I:143:ALA:HB2	1.42	1.02
1:H:674:ARG:H	1:H:674:ARG:HD2	1.23	1.00
1:E:480:ILE:HD12	1:E:483:LEU:HD12	1.44	0.97
1:H:783:GLN:H	1:H:783:GLN:NE2	1.60	0.97
1:B:0:MET:H1	1:B:223:LYS:HZ2	0.97	0.96
1:K:810[A]:GLN:HE21	1:K:814:LYS:NZ	1.61	0.96
1:K:157:VAL:HG11	1:K:205:ILE:HB	1.48	0.96
1:E:697:ILE:H	1:E:697:ILE:HD12	1.27	0.95
2:C:261:THR:HG21	2:C:263:ILE:HG13	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:738:GLN:HE21	1:K:739:THR:N	1.65	0.94
1:H:783:GLN:H	1:H:783:GLN:HE21	0.96	0.93
1:K:674:ARG:H	1:K:674:ARG:HD2	1.32	0.93
1:B:701:VAL:HG12	1:B:705:LYS:HE3	1.48	0.92
1:K:810[A]:GLN:HE21	1:K:814:LYS:HZ2	1.10	0.91
1:E:701:VAL:HG12	1:E:705:LYS:HE3	1.48	0.91
2:C:285:LYS:HG3	2:C:314:PHE:CE2	2.06	0.90
1:E:783:GLN:NE2	1:E:783:GLN:H	1.70	0.89
1:H:702:GLU:HA	1:H:705:LYS:HD2	1.53	0.89
1:E:702:GLU:HA	1:E:705:LYS:HD2	1.51	0.89
1:B:0:MET:H1	1:B:223:LYS:NZ	1.71	0.89
1:B:562:MET:CE	1:B:634:PRO:HG3	2.04	0.88
2:I:285:LYS:HG3	2:I:314:PHE:CE1	2.09	0.88
2:F:27:VAL:HG22	2:F:131:CYS:HB2	1.53	0.88
1:K:0:MET:HG3	1:K:1:PRO:HD2	1.56	0.87
2:C:228:VAL:HA	2:C:231:MET:HE3	1.57	0.87
1:H:562:MET:HE3	1:H:634:PRO:HG3	1.56	0.87
1:H:733:LEU:HD22	1:H:737:PHE:HD2	1.39	0.87
1:E:1020[B]:ARG:HH11	1:E:1020[B]:ARG:HG2	1.37	0.87
2:C:261:THR:CG2	2:C:263:ILE:HG13	2.05	0.86
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.10	0.86
2:I:215:ARG:HH11	2:I:215:ARG:HG3	1.38	0.85
2:C:261:THR:HG22	2:C:263:ILE:H	1.41	0.85
1:B:783:GLN:HE21	1:B:783:GLN:H	1.23	0.85
1:K:562:MET:HE3	1:K:634:PRO:HG3	1.58	0.85
1:E:783:GLN:HE21	1:E:783:GLN:H	1.19	0.85
1:B:0:MET:N	1:B:223:LYS:HZ2	1.73	0.85
1:B:701:VAL:HG13	1:B:730:GLU:HG3	1.58	0.85
1:E:0:MET:HB3	1:E:223:LYS:CE	2.05	0.85
2:I:133:ILE:CG2	2:I:138:PRO:HB3	2.06	0.84
1:B:783:GLN:NE2	1:B:783:GLN:H	1.75	0.84
2:L:324:ASN:HD22	2:L:324:ASN:H	1.22	0.84
2:I:57:TYR:CD1	2:I:58:PRO:HD2	2.13	0.84
2:I:201:ALA:HB2	2:I:239:SER:HB2	1.58	0.84
2:F:322:PRO:HB2	2:F:324:ASN:ND2	1.91	0.84
2:F:187:GLU:HG2	2:F:215:ARG:CD	2.08	0.84
1:B:906:LEU:HD11	9:B:1095:ORN:HD3	1.58	0.83
1:E:508[B]:ARG:HH11	1:E:508[B]:ARG:HB2	1.43	0.83
1:H:562:MET:CE	1:H:634:PRO:HG3	2.07	0.83
1:H:711:LEU:HD11	1:H:751:LEU:HD23	1.58	0.83
2:L:322:PRO:HB2	2:L:324:ASN:ND2	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:587:ALA:HB2	1:H:862:LYS:HG2	1.61	0.82
1:E:674:ARG:HD2	1:E:674:ARG:H	1.43	0.82
1:H:480:ILE:CD1	1:H:507:VAL:HG11	2.10	0.82
2:F:324:ASN:H	2:F:324:ASN:HD22	1.28	0.82
1:E:420:LEU:HD11	1:E:444:ALA:HB1	1.60	0.82
1:H:783:GLN:N	1:H:783:GLN:HE21	1.76	0.81
1:E:687:LYS:HE2	1:E:837:TYR:CE2	2.14	0.81
2:I:201:ALA:HB2	2:I:239:SER:CB	2.09	0.81
1:B:0:MET:N	1:B:223:LYS:NZ	2.28	0.81
2:F:246:ALA:HB3	2:F:247:PRO:HD3	1.63	0.81
1:K:74:ARG:HH11	1:K:74:ARG:HG2	1.46	0.81
2:F:285:LYS:HG3	2:F:314:PHE:CE1	2.16	0.80
2:L:345:LYS:HB3	2:L:346:PRO:HD2	1.62	0.80
1:E:974:HIS:HD1	1:H:974:HIS:HD1	0.84	0.79
2:C:192:PHE:HD1	2:C:378:ARG:HH11	1.28	0.79
2:C:193:HIS:CD2	2:C:215:ARG:HD2	2.17	0.79
1:H:733:LEU:HD22	1:H:737:PHE:CD2	2.17	0.79
1:E:801:SER:O	1:E:805:GLN:HG3	1.83	0.78
2:I:54:THR:HG21	2:I:118:LEU:HD23	1.63	0.78
1:H:673:ASP:HB3	1:H:676:ARG:CB	2.12	0.78
1:E:662:GLY:CA	1:E:868:MET:HG2	2.14	0.78
2:I:324:ASN:O	2:I:343:THR:HG23	1.84	0.78
2:C:322:PRO:HB2	2:C:324:ASN:ND2	1.99	0.78
2:L:194:VAL:HB	2:L:216:LEU:HD23	1.66	0.78
1:H:707:ILE:HG23	1:H:753:HIS:HB2	1.66	0.77
1:K:697:ILE:HD12	1:K:697:ILE:H	1.49	0.77
1:E:342[B]:ARG:HH12	1:E:536:ALA:HB3	1.48	0.77
1:E:1072:LYS:HA	1:E:1072:LYS:HE3	1.65	0.77
1:E:31:GLN:OE1	1:E:319:ALA:HB3	1.84	0.77
2:L:300:VAL:HG22	2:L:328:THR:O	1.85	0.77
1:H:674:ARG:H	1:H:674:ARG:CD	1.95	0.77
1:H:760:GLU:HG2	1:H:780:HIS:CE1	2.19	0.77
1:E:1020[B]:ARG:NH2	1:E:1023:GLU:HG3	1.99	0.77
1:K:966:GLN:HG2	1:K:1053:LEU:HD13	1.67	0.77
2:F:71:GLU:O	2:F:203:ARG:HG3	1.83	0.77
2:I:322:PRO:HB2	2:I:324:ASN:OD1	1.84	0.77
1:E:1023:GLU:HB3	11:E:2061:HOH:O	1.85	0.76
2:F:318:GLU:HA	2:F:321:LEU:HD22	1.67	0.76
1:K:759:VAL:HG11	1:K:800:LEU:HD21	1.67	0.76
1:E:489:ARG:HG3	1:E:521:LEU:HD21	1.66	0.76
1:E:737:PHE:HZ	1:E:749:VAL:HG11	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1036:LYS:HA	11:H:1828:HOH:O	1.85	0.76
1:B:1036:LYS:HE2	11:B:1330:HOH:O	1.85	0.76
1:E:1072:LYS:HA	1:E:1072:LYS:CE	2.15	0.76
1:E:258:LYS:O	1:E:262:ILE:HG13	1.86	0.76
1:H:28[B]:SER:OG	1:H:303:VAL:HG21	1.83	0.76
1:H:480:ILE:HD13	1:H:507:VAL:HG11	1.67	0.76
2:L:298:LYS:HE2	2:L:303:ASN:OD1	1.86	0.76
1:E:547:GLU:OE2	2:F:114:ASP:HA	1.85	0.76
2:F:187:GLU:HG2	2:F:215:ARG:HD3	1.68	0.76
1:K:990:VAL:HB	1:K:1003[A]:ARG:NH1	2.00	0.76
1:K:783:GLN:HE21	1:K:783:GLN:H	1.34	0.75
2:C:157:ASP:OD1	2:C:160:LYS:HG2	1.87	0.75
1:E:312:LYS:HE2	1:E:607:THR:O	1.86	0.75
1:E:980:LEU:CD1	1:E:987:PRO:HG3	2.17	0.74
2:F:75:VAL:HG11	2:F:107:ILE:HG13	1.69	0.74
1:E:703:LYS:O	1:E:706:GLU:HB3	1.87	0.74
1:E:1019:ARG:O	1:E:1023:GLU:HG2	1.88	0.74
1:B:416:ASP:HB3	1:B:419:ALA:HB2	1.70	0.74
1:H:712:VAL:HG23	1:H:754:PHE:HB2	1.69	0.74
1:H:673:ASP:CB	1:H:676:ARG:HB2	2.14	0.74
2:L:50:ARG:HH21	2:L:150:PHE:HE1	1.37	0.73
1:H:701:VAL:HG13	1:H:730:GLU:HG3	1.68	0.73
2:L:318:GLU:HG2	11:L:4685:HOH:O	1.88	0.73
2:I:152:GLY:O	2:I:156:MET:HE3	1.89	0.73
1:K:674:ARG:H	1:K:674:ARG:CD	2.02	0.73
1:E:980:LEU:HD12	1:E:987:PRO:HG3	1.71	0.73
1:K:810[A]:GLN:NE2	1:K:814:LYS:NZ	2.36	0.73
1:E:966[B]:GLN:HG3	1:E:1053:LEU:HD13	1.70	0.72
1:K:999:HIS:HD2	1:K:1002:ASP:H	1.36	0.72
2:I:208:MET:HE3	11:I:3149:HOH:O	1.89	0.72
1:K:694:VAL:HG12	1:K:703:LYS:HD3	1.72	0.72
1:B:366:PHE:HB3	1:B:902:VAL:HG21	1.71	0.72
1:H:478:VAL:CG2	1:H:482:GLY:HA3	2.20	0.72
2:C:228:VAL:HA	2:C:231:MET:CE	2.19	0.71
2:F:187:GLU:HG2	2:F:215:ARG:HD2	1.72	0.71
2:I:27:VAL:HG22	2:I:131:CYS:HB2	1.70	0.71
2:C:318:GLU:HB2	2:C:337:LEU:HD22	1.73	0.71
1:E:904:PRO:HB2	1:E:1039:TYR:OH	1.89	0.71
1:K:904:PRO:HB2	1:K:1039:TYR:OH	1.90	0.71
1:B:991:ASN:ND2	1:K:974:HIS:HE2	1.88	0.71
2:F:186:LYS:O	2:F:189:GLU:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:937:THR:O	1:K:939:LYS:HE3	1.89	0.71
1:H:980:LEU:HD12	1:H:987:PRO:HG3	1.72	0.71
1:B:872:SER:O	1:B:876:GLN:HG3	1.91	0.70
1:B:534:GLU:HG2	1:B:535:PHE:CE1	2.25	0.70
1:B:896:PHE:HB3	11:B:1730:HOH:O	1.91	0.70
1:E:674:ARG:CD	1:E:674:ARG:H	2.01	0.70
1:H:480:ILE:HD12	1:H:507:VAL:HG21	1.73	0.70
1:E:342[B]:ARG:HH12	1:E:536:ALA:CA	2.04	0.70
1:E:549:GLU:HG3	11:E:1670:HOH:O	1.91	0.70
2:C:277:LEU:HD23	2:C:281:ALA:O	1.92	0.70
1:E:0:MET:HG3	1:E:1:PRO:N	2.07	0.70
1:E:1020[B]:ARG:CZ	1:E:1023:GLU:HG3	2.21	0.70
1:B:681:VAL:HG11	1:B:688:GLN:NE2	2.07	0.69
1:B:730:GLU:OE2	1:B:734:ARG:NH2	2.25	0.69
2:C:206:LEU:O	2:C:210:VAL:HG23	1.92	0.69
1:E:342[B]:ARG:HH12	1:E:536:ALA:CB	2.05	0.69
2:L:324:ASN:O	2:L:343:THR:HG23	1.92	0.69
2:C:225:ALA:O	2:C:228:VAL:HB	1.92	0.69
1:E:515:LEU:HD21	1:E:519:TYR:CE2	2.27	0.69
2:F:27:VAL:O	2:F:78:GLN:HG2	1.92	0.69
2:L:324:ASN:HD22	2:L:324:ASN:N	1.89	0.69
1:E:478:VAL:HG23	1:E:479:GLY:O	1.92	0.69
1:H:478:VAL:HB	1:H:482:GLY:HA3	1.75	0.69
1:K:884:PRO:HG2	11:K:1704:HOH:O	1.91	0.69
1:H:674:ARG:N	1:H:674:ARG:HD2	2.04	0.69
1:E:562:MET:SD	1:E:634:PRO:HG3	2.33	0.68
1:E:459:ARG:O	1:E:463:VAL:HG22	1.93	0.68
2:I:190:LEU:HB2	2:I:215:ARG:HB3	1.74	0.68
2:C:341:HIS:CD2	2:C:348:PHE:HB3	2.28	0.68
1:H:701:VAL:O	1:H:705:LYS:HG3	1.93	0.68
2:F:327:VAL:HG13	2:F:337:LEU:CD1	2.24	0.68
1:K:810[A]:GLN:NE2	1:K:814:LYS:HZ2	1.88	0.68
1:B:317:PRO:HG3	1:B:609:TYR:OH	1.93	0.68
1:H:725:GLU:OE2	1:H:1019:ARG:HD3	1.93	0.68
2:I:197:TYR:HB3	2:I:199:PHE:CZ	2.28	0.68
1:H:946:LEU:N	1:H:946:LEU:HD12	2.08	0.68
1:K:64:TYR:OH	1:K:79:LYS:HE2	1.93	0.68
1:B:562:MET:HE2	1:B:634:PRO:HG3	1.75	0.68
2:F:234:ASP:OD1	2:F:378:ARG:HD2	1.94	0.68
1:K:681:VAL:HG11	1:K:688:GLN:HE21	1.58	0.68
1:B:697:ILE:H	1:B:697:ILE:HD12	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:365:PRO:HA	2:F:368[A]:ASP:OD2	1.94	0.68
1:K:0:MET:N	1:K:330:THR:HG23	2.09	0.68
1:H:251:PRO:HD3	1:H:351:ILE:HD11	1.77	0.67
2:L:57:TYR:CD1	2:L:58:PRO:HD2	2.29	0.67
2:F:275:LEU:HD22	2:F:349:SER:HB3	1.76	0.67
1:H:905:LEU:HD13	1:H:1029:ARG:CD	2.24	0.67
1:B:562:MET:HE3	1:B:634:PRO:HG3	1.76	0.67
1:E:515:LEU:HD21	1:E:519:TYR:HE2	1.59	0.67
2:F:307:ILE:O	2:F:362:ASP:HB2	1.94	0.67
1:E:488:LEU:CD2	1:E:515:LEU:HD22	2.25	0.67
1:E:871:LYS:HD3	1:E:876:GLN:HG2	1.75	0.67
1:B:695:THR:H	1:B:699:MET:HE2	1.59	0.67
1:E:929:LYS:HE3	11:E:1316:HOH:O	1.95	0.66
1:K:157:VAL:CG1	1:K:205:ILE:HB	2.23	0.66
1:E:671:ALA:HB3	1:E:843:PRO:HG3	1.77	0.66
1:K:999:HIS:CD2	1:K:1002:ASP:H	2.14	0.66
1:H:904:PRO:HB2	1:H:1039:TYR:OH	1.95	0.66
1:H:362:ASN:OD1	1:H:380:VAL:HG21	1.96	0.66
2:I:215:ARG:HG3	2:I:215:ARG:NH1	2.06	0.66
2:I:291:HIS:HA	2:I:310:GLN:O	1.95	0.66
1:K:223:LYS:NZ	11:K:1138:HOH:O	2.28	0.66
2:L:78:GLN:NE2	11:L:4658:HOH:O	2.27	0.66
1:B:129[A]:ARG:NH1	11:B:1258:HOH:O	2.29	0.66
2:C:123:ARG:O	2:C:287:LYS:HE2	1.95	0.66
1:E:662:GLY:HA3	1:E:868:MET:HG2	1.77	0.66
2:C:266:PHE:HA	2:C:348:PHE:O	1.95	0.66
2:F:268:ILE:HD11	2:F:354:PRO:HG2	1.77	0.66
1:E:152:GLU:HB2	11:E:2337:HOH:O	1.95	0.66
2:I:186:LYS:HB2	2:I:189:GLU:OE2	1.95	0.66
2:I:374:ILE:O	2:I:378:ARG:HG3	1.96	0.66
1:K:939:LYS:HG3	1:K:1010:THR:HB	1.78	0.66
1:E:0:MET:HG3	1:E:1:PRO:CD	2.26	0.65
1:B:330:THR:OG1	1:B:333:GLU:HG3	1.96	0.65
1:E:391:GLN:OE1	1:E:494:LYS:HD2	1.96	0.65
1:E:645:THR:HB	1:E:646:PRO:HD3	1.78	0.65
1:K:673:ASP:HB3	1:K:676:ARG:HB2	1.77	0.65
1:K:708:GLY:O	1:K:753:HIS:ND1	2.29	0.65
1:B:735:ARG:O	1:B:739:THR:HG23	1.97	0.65
2:C:192:PHE:O	2:C:215:ARG:HG3	1.95	0.65
2:C:6:LEU:HD12	2:C:7:LEU:N	2.11	0.65
1:H:658:VAL:HG13	1:H:659:PRO:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:133:ILE:HD12	2:I:143:ALA:CB	2.24	0.65
1:K:992:LYS:NZ	5:K:1082:PO4:O1	2.29	0.65
1:B:714:ARG:HB2	1:B:750:LEU:HB2	1.78	0.65
1:K:674:ARG:N	1:K:674:ARG:HD2	2.09	0.65
1:E:153:GLU:O	1:E:157:VAL:HG23	1.95	0.65
1:E:750:LEU:O	1:E:751:LEU:HD12	1.96	0.65
2:F:272:HIS:ND1	2:F:349:SER:OG	2.30	0.65
1:H:673:ASP:OD2	1:H:676:ARG:HB2	1.97	0.65
1:B:732:ASP:O	1:B:735:ARG:HB3	1.97	0.65
2:I:215:ARG:NH1	11:I:3589:HOH:O	2.29	0.65
1:H:467:GLU:OE1	2:I:87:LEU:HD11	1.97	0.65
2:I:168:TYR:CE2	2:I:218:ILE:HG12	2.31	0.65
2:I:44:THR:HG21	2:I:70:GLU:HG2	1.77	0.65
1:K:953:LYS:NZ	5:K:1082:PO4:O4	2.30	0.65
1:H:100:GLU:HA	1:H:100:GLU:OE1	1.95	0.65
1:H:671:ALA:HB3	1:H:843:PRO:HG3	1.79	0.65
1:H:971:ASP:OD1	1:H:988:ARG:HB3	1.96	0.65
1:E:420:LEU:CD1	1:E:444:ALA:HB1	2.26	0.64
2:C:318:GLU:CB	2:C:337:LEU:HD22	2.25	0.64
1:E:725:GLU:OE2	1:E:1019:ARG:HD3	1.97	0.64
2:F:144:LEU:O	2:F:148:ARG:HG3	1.97	0.64
1:K:909:GLU:HG2	11:K:2060:HOH:O	1.97	0.64
2:C:57:TYR:CD1	2:C:58:PRO:HD2	2.32	0.64
1:H:443:ARG:NH2	1:H:472:GLU:OE1	2.31	0.64
1:K:227:CYS:O	1:K:268:MET:HE1	1.97	0.64
1:K:673:ASP:OD2	1:K:676:ARG:HG3	1.97	0.64
1:B:901:GLY:O	1:B:1026:ARG:NH2	2.30	0.64
1:B:701:VAL:O	1:B:705:LYS:HG3	1.98	0.64
2:C:249:ASP:OD1	2:C:250:TYR:N	2.30	0.64
2:I:33:ASN:OD1	2:I:35:SER:HB2	1.96	0.64
1:K:904:PRO:HB2	1:K:1039:TYR:HH	1.60	0.64
2:L:27:VAL:O	2:L:78:GLN:HG2	1.97	0.64
1:B:342:ARG:NH2	1:B:538:ASP:OD2	2.29	0.64
1:E:171:PHE:HB3	1:E:199:PRO:HG2	1.78	0.64
1:H:675:GLU:O	1:H:679:HIS:ND1	2.30	0.64
1:H:953:LYS:NZ	5:H:1082:PO4:O4	2.29	0.64
2:L:218:ILE:N	2:L:218:ILE:HD13	2.12	0.64
1:B:904:PRO:HB2	1:B:1039:TYR:OH	1.97	0.64
2:I:6:LEU:HD23	2:I:7:LEU:H	1.61	0.64
1:K:890:LYS:NZ	11:K:1679:HOH:O	2.31	0.64
1:B:953:LYS:HA	1:B:956:VAL:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:783:GLN:NE2	1:K:783:GLN:H	1.95	0.63
2:C:78:GLN:NE2	11:C:578:HOH:O	2.30	0.63
1:B:489:ARG:HA	1:B:521:LEU:HD21	1.80	0.63
2:F:327:VAL:HG13	2:F:337:LEU:HD11	1.79	0.63
1:H:862:LYS:HE2	11:H:1617:HOH:O	1.97	0.63
2:C:261:THR:HG22	2:C:263:ILE:N	2.10	0.63
1:E:950[A]:GLU:OE2	1:E:953:LYS:HE3	1.97	0.63
1:K:694:VAL:HG21	1:K:700:ALA:HA	1.80	0.63
1:H:671:ALA:CB	1:H:843:PRO:HG3	2.28	0.63
2:I:225:ALA:HA	2:I:258:PHE:CE1	2.33	0.63
1:B:966[B]:GLN:OE1	1:B:1054:ASN:ND2	2.31	0.63
1:H:1003:ARG:NE	11:H:1812:HOH:O	2.30	0.63
1:K:201:LYS:NZ	11:K:1982:HOH:O	2.30	0.63
1:B:409:ASP:OD2	1:B:503:LYS:NZ	2.30	0.63
1:B:502:ALA:HB1	1:B:507:VAL:O	1.98	0.63
2:C:261:THR:HG22	2:C:262:ASP:H	1.63	0.63
2:L:201:ALA:HB2	2:L:239:SER:CB	2.29	0.63
2:C:258:PHE:O	2:C:261:THR:HB	1.98	0.63
2:F:14:GLN:NE2	2:F:140:ALA:HB1	2.14	0.63
1:E:223:LYS:HE2	1:E:328:GLY:O	1.99	0.62
1:E:694:VAL:HG21	1:E:700:ALA:HA	1.82	0.62
2:L:194:VAL:HB	2:L:216:LEU:CD2	2.30	0.62
2:L:322:PRO:HB2	2:L:324:ASN:HD21	1.61	0.62
1:E:737:PHE:CZ	1:E:749:VAL:HG11	2.33	0.62
2:I:34:THR:HA	2:I:56:THR:OG1	2.00	0.62
2:F:245:PRO:HG3	2:F:273:GLN:OE1	2.00	0.62
1:H:343:THR:HB	11:H:1461:HOH:O	1.98	0.62
1:K:750:LEU:O	1:K:751:LEU:HD12	1.98	0.62
1:E:339:THR:O	1:E:342[B]:ARG:HG2	2.00	0.62
2:F:322:PRO:HB2	2:F:324:ASN:HD22	1.62	0.62
1:H:902:VAL:HG13	11:H:1882:HOH:O	1.99	0.62
1:B:801:SER:OG	1:B:804:ILE:HB	2.00	0.62
1:E:966[A]:GLN:HG2	1:E:1053:LEU:HD13	1.82	0.62
1:E:709:TYR:HB3	1:E:710:PRO:HA	1.82	0.62
2:F:10:GLU:OE1	2:F:129:ASN:N	2.30	0.62
2:I:318:GLU:O	2:I:321:LEU:HB2	1.99	0.62
1:E:42:ARG:NH1	11:E:2039:HOH:O	2.29	0.62
1:H:321:VAL:O	1:H:325:LEU:HD13	2.00	0.62
2:I:279:SER:HB2	2:I:325:LEU:HD11	1.82	0.62
1:H:857:GLY:HA2	1:H:1068:HIS:CE1	2.35	0.61
1:H:480:ILE:HD12	1:H:507:VAL:HG11	1.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:733:LEU:HD22	1:K:737:PHE:HD2	1.65	0.61
1:K:986:ASN:ND2	11:K:1103:HOH:O	2.32	0.61
1:E:697:ILE:N	1:E:697:ILE:HD12	2.09	0.61
1:H:399:ARG:HD3	11:H:1502:HOH:O	2.00	0.61
2:C:190:LEU:HB2	2:C:215:ARG:HB3	1.82	0.61
1:H:872:SER:O	1:H:876:GLN:HG3	2.00	0.61
1:H:990:VAL:HG23	1:H:1003:ARG:NH1	2.15	0.61
1:K:713:VAL:HG11	1:K:736:TYR:CE2	2.35	0.61
2:C:222:GLN:NE2	11:C:508:HOH:O	2.29	0.61
1:H:1054:ASN:ND2	11:H:1793:HOH:O	2.30	0.61
1:K:562:MET:CE	1:K:634:PRO:HG3	2.29	0.61
1:B:320:LYS:NZ	1:B:610:ASP:OD2	2.33	0.61
2:C:193:HIS:HD2	2:C:215:ARG:HD2	1.65	0.61
1:H:677:PHE:O	1:H:681:VAL:HG23	2.01	0.61
2:L:334:ASP:OD1	2:L:336:THR:HG23	2.00	0.61
1:H:808:MET:HG2	1:H:829:PHE:CD2	2.35	0.61
1:E:342[B]:ARG:NH1	1:E:536:ALA:N	2.49	0.61
2:F:300:VAL:HG23	2:F:301:GLU:N	2.15	0.61
1:K:357:LYS:HE3	11:K:1434:HOH:O	1.99	0.61
1:K:644:GLN:HE21	1:K:648:LYS:NZ	1.99	0.61
1:E:998:PRO:HB3	1:E:1002:ASP:OD2	2.01	0.61
1:E:488:LEU:HD22	1:E:515:LEU:HD22	1.82	0.60
2:I:228:VAL:HA	2:I:231:MET:CE	2.32	0.60
1:K:929:LYS:NZ	1:K:1057:ALA:O	2.32	0.60
1:B:357:LYS:HE3	11:B:1424:HOH:O	2.02	0.60
2:F:6:LEU:HD21	2:F:8:VAL:HG23	1.83	0.60
1:B:578:ASP:OD2	1:B:604:THR:HB	2.01	0.60
2:F:298:LYS:NZ	2:F:303:ASN:OD1	2.29	0.60
1:E:526:LYS:NZ	1:E:549:GLU:O	2.29	0.60
1:H:196:ASP:OD2	1:H:1036:LYS:NZ	2.30	0.60
1:B:730:GLU:CD	1:B:734:ARG:HH21	2.05	0.60
1:E:783:GLN:N	1:E:783:GLN:HE21	1.96	0.60
1:K:724:MET:HG2	1:K:909:GLU:OE2	2.01	0.60
1:E:523:PRO:HD2	1:E:627:GLU:OE1	2.02	0.60
1:H:702:GLU:O	1:H:705:LYS:HB2	2.02	0.60
1:H:771:MET:HG2	1:H:873:LEU:HD12	1.83	0.60
2:L:248:CYS:O	2:L:252:ILE:HG13	2.01	0.60
1:B:857:GLY:HA2	1:B:1068:HIS:CE1	2.37	0.59
2:F:263:ILE:HG12	2:F:377:TYR:OH	2.02	0.59
1:B:456:ASN:ND2	11:B:1344:HOH:O	2.34	0.59
1:E:0:MET:O	1:E:329:TYR:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:ILE:O	1:B:700:ALA:N	2.35	0.59
1:E:701:VAL:O	1:E:705:LYS:HG3	2.03	0.59
2:F:74:GLN:NE2	11:F:1834:HOH:O	2.34	0.59
2:I:228:VAL:HA	2:I:231:MET:HE3	1.84	0.59
1:B:1018:GLY:O	1:B:1022:ILE:HG13	2.03	0.59
1:B:399:ARG:HD3	11:B:1493:HOH:O	2.03	0.59
1:E:712:VAL:HG23	1:E:754:PHE:HB2	1.84	0.59
1:B:1062:ILE:HD13	1:B:1067:MET:HG3	1.84	0.59
1:B:508:ARG:NH1	1:B:510:ALA:HB3	2.18	0.59
2:F:295:HIS:CE1	2:F:333:PHE:HD2	2.21	0.59
2:F:67:ASP:O	2:F:70:GLU:HG3	2.03	0.59
2:I:350:PHE:HD2	2:I:354:PRO:HD3	1.65	0.59
1:K:691:ASN:ND2	1:K:691:ASN:N	2.51	0.59
1:K:697:ILE:O	1:K:700:ALA:HB3	2.03	0.59
2:F:218:ILE:HD13	2:F:218:ILE:N	2.16	0.59
2:I:135:GLY:O	2:I:138:PRO:HD3	2.02	0.59
1:K:738:GLN:HE21	1:K:738:GLN:C	2.06	0.59
1:K:547:GLU:OE2	2:L:114:ASP:HA	2.02	0.59
2:F:252:ILE:HG22	2:F:278:ALA:HA	1.85	0.59
2:I:146:LYS:HA	2:I:149:ALA:HB3	1.82	0.59
1:E:804:ILE:HG22	1:E:805:GLN:N	2.17	0.59
2:F:306:MET:HB2	2:F:362:ASP:HB3	1.85	0.59
1:K:715:PRO:HD3	1:K:724:MET:HB3	1.85	0.59
11:H:1587:HOH:O	2:I:295:HIS:HD2	1.85	0.59
1:K:857:GLY:HA2	1:K:1068:HIS:CE1	2.38	0.59
2:L:163:THR:OG1	2:L:164:THR:N	2.34	0.59
2:C:212:ARG:HG3	2:C:212:ARG:HH11	1.67	0.58
2:C:277:LEU:HA	2:C:281:ALA:O	2.03	0.58
1:E:1071:ILE:O	1:E:1072:LYS:HB2	2.02	0.58
1:B:668:ILE:HA	1:B:843:PRO:HG2	1.84	0.58
1:K:162:GLY:O	1:K:165:CYS:HB3	2.03	0.58
1:B:707:ILE:HG23	1:B:753:HIS:HB2	1.84	0.58
2:C:163:THR:HG21	2:C:221:ALA:HB3	1.85	0.58
2:C:298:LYS:NZ	11:C:410:HOH:O	2.36	0.58
1:E:973:THR:HB	1:E:992:LYS:HE3	1.84	0.58
1:H:939:LYS:HG3	1:H:1010:THR:HB	1.85	0.58
1:H:42:ARG:HD2	11:H:1964:HOH:O	2.02	0.58
1:K:0:MET:O	1:K:329:TYR:HA	2.03	0.58
1:K:813:GLN:NE2	11:K:1950:HOH:O	2.35	0.58
1:B:989:LEU:HD23	1:K:978:ILE:HG12	1.85	0.58
1:E:342[B]:ARG:NH1	1:E:536:ALA:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:578:ASP:OD2	1:K:604:THR:HB	2.03	0.58
1:B:527:ARG:HG2	1:B:542:MET:HG2	1.85	0.58
1:E:709:TYR:OH	1:E:733:LEU:HD12	2.04	0.58
1:K:756:ASP:O	1:K:832:LYS:HE3	2.03	0.58
2:C:261:THR:HG22	2:C:262:ASP:N	2.19	0.58
2:F:6:LEU:HD21	2:F:8:VAL:CG2	2.34	0.58
1:H:1063:SER:O	1:H:1067:MET:HG3	2.04	0.58
2:I:27:VAL:O	2:I:78:GLN:HG3	2.03	0.58
1:E:697:ILE:H	1:E:697:ILE:CD1	2.04	0.58
1:K:218:GLU:OE2	1:K:282:ASN:HB2	2.04	0.58
1:B:0:MET:HA	1:B:223:LYS:HE3	1.86	0.58
2:F:286:MET:HE1	2:F:290:HIS:CD2	2.39	0.58
1:H:641:TYR:OH	1:H:864:ALA:HB3	2.03	0.58
1:B:694:VAL:HG13	1:B:699:MET:HB3	1.85	0.57
1:H:492:LYS:HE2	1:H:516:ARG:HD3	1.86	0.57
1:H:710:PRO:HG2	1:H:754:PHE:HD2	1.69	0.57
2:F:158:LEU:O	2:F:161:GLU:HB2	2.04	0.57
2:F:31:VAL:HG11	2:F:51:GLN:OE1	2.05	0.57
2:I:46:PRO:HA	2:I:76:HIS:CG	2.39	0.57
1:K:1050:ALA:O	1:K:1053:LEU:HB2	2.04	0.57
1:B:288:ASN:OD1	1:B:289:PRO:HD2	2.03	0.57
1:E:662:GLY:HA2	1:E:868:MET:HG2	1.85	0.57
2:L:264:PRO:HA	2:L:346:PRO:HB2	1.86	0.57
2:L:364:ALA:N	2:L:365:PRO:HD2	2.19	0.57
1:E:150:THR:OG1	1:E:153:GLU:HG3	2.04	0.57
1:E:151:MET:O	1:E:155:LEU:HD12	2.05	0.57
2:F:174:SER:HB2	2:F:211:ASP:OD2	2.04	0.57
2:F:252:ILE:HG22	2:F:278:ALA:CA	2.34	0.57
1:H:507:VAL:HB	1:H:511[A]:GLU:OE1	2.03	0.57
2:L:266:PHE:HA	2:L:348:PHE:O	2.05	0.57
1:B:418[B]:GLU:CD	1:H:421:THR:HG21	2.24	0.57
2:F:50:ARG:HD3	11:F:2254:HOH:O	2.05	0.57
1:K:58:GLU:HB3	11:K:1209:HOH:O	2.04	0.57
2:C:279:SER:O	2:C:322:PRO:HG3	2.03	0.57
1:E:701:VAL:HG12	1:E:705:LYS:CE	2.28	0.57
1:E:714:ARG:HB2	1:E:750:LEU:HB2	1.87	0.57
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.38	0.57
2:F:344:ASP:OD1	2:F:344:ASP:N	2.30	0.57
1:K:681:VAL:HG11	1:K:688:GLN:NE2	2.19	0.57
2:C:376:GLN:HA	2:C:379:LYS:HE2	1.86	0.57
1:E:0:MET:HG3	1:E:1:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:186:LYS:N	2:F:189:GLU:OE1	2.30	0.57
1:H:999:HIS:CD2	1:H:1002:ASP:H	2.23	0.57
1:H:274:ILE:HG22	1:H:276:VAL:HG23	1.87	0.57
1:E:727:VAL:CG1	1:E:732:ASP:HB3	2.35	0.57
1:H:37:ARG:HH11	1:H:37:ARG:HG3	1.69	0.57
1:H:73:VAL:O	1:H:77:ILE:HG13	2.05	0.57
2:I:348:PHE:CZ	2:I:369:HIS:HB3	2.40	0.57
2:L:133:ILE:HD12	2:L:143:ALA:HB2	1.87	0.57
1:B:714:ARG:CB	1:B:750:LEU:HB2	2.34	0.57
2:C:175:TRP:HA	2:C:180:GLY:O	2.05	0.57
1:E:16:PRO:HG3	1:E:916:VAL:CG1	2.35	0.57
2:I:6:LEU:HD23	2:I:7:LEU:N	2.20	0.57
1:B:733:LEU:HG	1:B:737:PHE:CD2	2.39	0.56
2:C:133:ILE:HG22	2:C:138:PRO:HB3	1.87	0.56
1:E:335:MET:HB3	1:E:341:GLY:HA2	1.85	0.56
1:E:725:GLU:HG3	1:E:726:ILE:H	1.70	0.56
1:E:694:VAL:O	1:E:749:VAL:HB	2.05	0.56
2:F:208:MET:SD	2:F:355:GLU:HA	2.45	0.56
1:H:808:MET:HG2	1:H:829:PHE:CE2	2.41	0.56
2:I:199:PHE:O	2:I:241:GLY:HA3	2.05	0.56
1:B:725:GLU:HG2	1:B:726:ILE:N	2.21	0.56
1:B:884:PRO:HG2	11:B:1692:HOH:O	2.03	0.56
2:C:201:ALA:HB2	2:C:239:SER:CB	2.35	0.56
1:E:906:LEU:HD11	9:E:1097:ORN:HD3	1.87	0.56
1:H:277:GLU:HB3	11:H:1380:HOH:O	2.05	0.56
1:E:727:VAL:HG12	1:E:732:ASP:HB3	1.87	0.56
1:K:738:GLN:HE21	1:K:739:THR:CA	2.19	0.56
1:E:978:ILE:O	1:E:982:GLU:HG3	2.05	0.56
2:I:238:LEU:HB2	2:I:267:GLY:HA2	1.86	0.56
2:I:40:GLN:HE21	2:I:70:GLU:HG3	1.71	0.56
2:C:66:ASN:HB3	2:C:93:ARG:O	2.04	0.56
1:E:0:MET:CG	1:E:1:PRO:HD2	2.36	0.56
2:L:350:PHE:HD2	2:L:354:PRO:HD3	1.71	0.56
1:E:813:GLN:NE2	11:E:1950:HOH:O	2.38	0.56
1:H:227:CYS:SG	1:H:268:MET:HG2	2.46	0.56
1:H:478:VAL:CB	1:H:482:GLY:HA3	2.35	0.56
2:I:201:ALA:CB	2:I:239:SER:HB2	2.33	0.56
1:E:0:MET:N	1:E:330:THR:HG23	2.20	0.56
1:H:727:VAL:HG12	1:H:732:ASP:HB3	1.86	0.56
1:B:212:TRP:CZ3	1:B:295:ILE:HD12	2.41	0.56
1:B:27:TYR:CE1	1:B:312:LYS:HE3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:ARG:HD2	11:C:587:HOH:O	2.05	0.56
1:E:470:ARG:HB2	11:E:2200:HOH:O	2.05	0.56
1:H:935:ASN:HB2	11:H:1147:HOH:O	2.05	0.56
2:I:371:ILE:O	2:I:375:GLU:HG3	2.05	0.56
2:C:261:THR:CG2	2:C:262:ASP:H	2.18	0.56
2:C:291:HIS:HD2	11:C:453:HOH:O	1.89	0.56
2:I:40:GLN:NE2	2:I:70:GLU:HG3	2.21	0.56
1:B:727:VAL:HG21	1:B:733:LEU:CD1	2.36	0.55
2:I:29:GLU:OE1	2:I:285:LYS:NZ	2.30	0.55
1:K:780:HIS:HE1	1:K:788:SER:HB3	1.71	0.55
1:B:1016:THR:HG21	1:B:1022:ILE:HA	1.86	0.55
2:C:6:LEU:HD12	2:C:7:LEU:H	1.70	0.55
1:K:733:LEU:O	1:K:737:PHE:HB2	2.05	0.55
2:C:205:ILE:HG13	2:C:355:GLU:HG3	1.87	0.55
2:C:232:ASN:N	2:C:233:PRO:HD3	2.22	0.55
1:E:134:ALA:O	1:E:137:LYS:HB3	2.07	0.55
2:F:133:ILE:HD12	2:F:143:ALA:HB2	1.88	0.55
2:F:318:GLU:CA	2:F:321:LEU:HD22	2.35	0.55
1:H:711:LEU:CD1	1:H:751:LEU:HD23	2.32	0.55
1:H:905:LEU:HD13	1:H:1029:ARG:HD2	1.88	0.55
2:C:356:ALA:HB3	11:C:556:HOH:O	2.05	0.55
1:H:674:ARG:O	1:H:678:GLN:HG2	2.07	0.55
1:H:713:VAL:HG21	1:H:727:VAL:HG21	1.89	0.55
1:B:783:GLN:HE21	1:B:783:GLN:N	2.00	0.55
1:E:749:VAL:HG12	1:E:751:LEU:CD1	2.36	0.55
1:H:184:ARG:O	1:H:188:GLU:HG3	2.07	0.55
1:H:986:ASN:ND2	11:H:1104:HOH:O	2.40	0.55
2:I:365:PRO:O	2:I:368:ASP:HB2	2.06	0.55
1:E:216:GLU:HG2	1:E:284:GLN:HG2	1.88	0.55
1:H:558:ARG:NH2	11:H:1915:HOH:O	2.38	0.55
1:E:492:LYS:HE2	1:E:516:ARG:HD3	1.89	0.55
2:F:206:LEU:O	2:F:210:VAL:HG23	2.06	0.55
2:F:232:ASN:N	2:F:233:PRO:HD3	2.21	0.55
2:F:46:PRO:HA	2:F:76:HIS:CG	2.41	0.55
1:H:570:ARG:N	1:H:570:ARG:HD3	2.22	0.55
1:K:1025:SER:HB3	7:K:1093:GLN:HA	1.88	0.55
1:K:317:PRO:HG3	1:K:609:TYR:OH	2.07	0.55
1:K:689:PRO:HG3	1:K:755:LEU:HD11	1.89	0.55
2:C:255:ILE:HA	2:C:258:PHE:HD2	1.72	0.54
1:H:949:ARG:HB3	11:H:1785:HOH:O	2.07	0.54
2:I:212:ARG:HB3	2:I:371:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:0:MET:HB3	1:K:223:LYS:HE3	1.88	0.54
2:C:228:VAL:HG11	2:C:258:PHE:CE1	2.43	0.54
1:E:1027:VAL:HG13	1:E:1028:ILE:N	2.22	0.54
1:H:332:ASP:OD1	1:H:332:ASP:N	2.39	0.54
1:H:645:THR:HB	1:H:646:PRO:HD3	1.89	0.54
1:H:707:ILE:CG2	1:H:753:HIS:HB2	2.36	0.54
1:H:773:LEU:HD22	1:H:878:VAL:HG12	1.88	0.54
1:K:1036:LYS:NZ	11:K:1324:HOH:O	2.39	0.54
2:L:222:GLN:HG3	2:L:250:TYR:CE2	2.43	0.54
1:B:474:LYS:O	1:B:478:VAL:HG13	2.07	0.54
1:B:803:GLU:HB3	11:B:1695:HOH:O	2.07	0.54
1:E:1020[B]:ARG:NH2	1:E:1023:GLU:OE2	2.40	0.54
2:F:186:LYS:HB2	2:F:189:GLU:OE1	2.07	0.54
1:H:0:MET:H2	1:H:1:PRO:HD3	1.72	0.54
2:I:6:LEU:O	2:I:132:ILE:HA	2.08	0.54
1:K:0:MET:HB3	1:K:223:LYS:CE	2.37	0.54
2:L:50:ARG:NH1	11:L:4668:HOH:O	2.41	0.54
2:C:254:ALA:O	2:C:257:LYS:HB2	2.08	0.54
1:K:671:ALA:CB	1:K:843:PRO:HG3	2.38	0.54
1:B:821:VAL:O	1:B:822:ARG:HD3	2.08	0.54
1:E:0:MET:H3	1:E:330:THR:HG23	1.73	0.54
1:K:698:GLU:OE1	1:K:698:GLU:HA	2.06	0.54
1:E:729:ASP:OD1	1:E:732:ASP:HB2	2.07	0.54
2:L:232:ASN:N	2:L:233:PRO:HD3	2.23	0.54
1:B:729:ASP:H	1:B:732:ASP:HB2	1.73	0.54
2:C:222:GLN:HA	2:C:250:TYR:CD2	2.43	0.54
2:F:299:ASP:OD2	2:F:302:LYS:HD2	2.07	0.54
1:H:166:ILE:HD12	1:H:166:ILE:N	2.23	0.54
1:E:522:HIS:HB3	1:E:523:PRO:HD2	1.90	0.54
2:F:133:ILE:HG22	2:F:138:PRO:HB3	1.90	0.54
2:F:298:LYS:NZ	11:F:1569:HOH:O	2.31	0.54
2:I:238:LEU:O	2:I:271:GLY:HA3	2.07	0.54
1:K:953:LYS:O	1:K:956:VAL:HG12	2.08	0.54
1:H:342:ARG:NH2	11:H:1876:HOH:O	2.40	0.54
2:I:244:ASP:OD1	2:I:245:PRO:HD2	2.08	0.54
1:K:749:VAL:HG12	1:K:751:LEU:HD13	1.89	0.54
2:L:195:VAL:HG13	2:L:219:VAL:HG13	1.89	0.54
1:H:658:VAL:CG1	1:H:659:PRO:HD2	2.37	0.54
2:I:299:ASP:OD2	2:I:302:LYS:HD2	2.08	0.54
1:K:639:VAL:HG21	1:K:650:ALA:HB2	1.89	0.54
1:B:636:GLY:HA2	1:B:659:PRO:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:121:LEU:HD11	2:F:125:LYS:HD2	1.90	0.53
2:F:6:LEU:CD2	2:F:8:VAL:HG23	2.38	0.53
1:E:127:ASP:OD1	1:E:129[B]:ARG:HB3	2.07	0.53
1:E:980:LEU:HD13	1:E:987:PRO:HG3	1.89	0.53
2:L:277:LEU:HD23	2:L:281:ALA:O	2.08	0.53
1:B:1016:THR:HG22	1:B:1017:SER:N	2.22	0.53
1:B:953:LYS:O	1:B:956:VAL:HG12	2.09	0.53
1:E:342[B]:ARG:HH12	1:E:536:ALA:N	2.05	0.53
1:E:694:VAL:HG21	1:E:700:ALA:CA	2.38	0.53
2:F:150:PHE:CD1	2:F:151:PRO:HD2	2.43	0.53
2:F:29:GLU:OE2	2:F:285:LYS:NZ	2.31	0.53
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.73	0.53
1:H:184:ARG:HA	1:H:187:PHE:HB3	1.90	0.53
2:I:205:ILE:HG13	2:I:355:GLU:HG3	1.89	0.53
1:K:352:ASP:OD2	2:L:116:ARG:HD2	2.09	0.53
2:C:201:ALA:HB2	2:C:239:SER:HB2	1.90	0.53
1:H:95:LEU:HD22	1:H:122:ILE:HD13	1.89	0.53
1:H:163:PHE:HA	1:H:164:PRO:C	2.28	0.53
1:B:508:ARG:HB2	1:B:511:GLU:OE1	2.08	0.53
1:B:710:PRO:HG2	1:B:754:PHE:HD2	1.72	0.53
1:B:272:ARG:NH1	11:B:1380:HOH:O	2.39	0.53
1:B:727:VAL:CG1	1:B:732:ASP:HB3	2.39	0.53
1:K:749:VAL:HG12	1:K:751:LEU:CD1	2.38	0.53
1:B:673:ASP:OD1	1:B:675:GLU:HB2	2.09	0.53
2:C:168:TYR:CE2	2:C:218:ILE:HG13	2.43	0.53
1:H:562:MET:HE3	1:H:634:PRO:CG	2.33	0.53
2:I:215:ARG:C	2:I:216:LEU:HD23	2.29	0.53
2:L:369:HIS:O	2:L:373:LEU:HG	2.09	0.53
1:E:1003:ARG:NE	11:E:2092:HOH:O	2.25	0.53
1:E:1025:SER:HB3	7:E:1093:GLN:HA	1.90	0.53
2:I:298:LYS:NZ	11:I:2813:HOH:O	2.40	0.53
2:I:355:GLU:N	2:I:355:GLU:OE1	2.36	0.53
1:E:677:PHE:O	1:E:681:VAL:HG23	2.09	0.53
1:H:560:LYS:HG2	1:H:594:GLU:OE1	2.09	0.53
2:L:355:GLU:N	2:L:355:GLU:OE1	2.29	0.53
1:B:412:VAL:HG11	1:B:423:ILE:HD11	1.90	0.53
2:C:133:ILE:CG2	2:C:138:PRO:HB3	2.39	0.53
2:C:248:CYS:O	2:C:252:ILE:HG13	2.09	0.53
1:E:1003:ARG:HB3	1:E:1008:GLU:HG3	1.91	0.53
1:E:906:LEU:HD11	9:E:1097:ORN:HB2	1.91	0.53
1:K:783:GLN:HE22	1:K:1042:THR:HB	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:285:LYS:HG3	2:F:314:PHE:CZ	2.44	0.52
1:K:114:MET:HG2	1:K:117:ALA:O	2.08	0.52
1:H:265:ASN:ND2	11:H:1418:HOH:O	2.38	0.52
2:I:350:PHE:CD2	2:I:354:PRO:HD3	2.44	0.52
1:K:0:MET:CG	1:K:1:PRO:HD2	2.36	0.52
1:B:828:GLN:O	1:B:839:ILE:HB	2.09	0.52
1:E:342[B]:ARG:HG3	1:E:343:THR:HG23	1.91	0.52
1:H:490:GLN:O	1:H:494:LYS:HG2	2.09	0.52
2:I:270:LEU:HA	2:I:273:GLN:OE1	2.08	0.52
1:K:711:LEU:HB2	1:K:727:VAL:HG23	1.91	0.52
2:L:275:LEU:HD12	2:L:275:LEU:O	2.09	0.52
1:B:727:VAL:HG21	1:B:733:LEU:HD12	1.92	0.52
1:E:420:LEU:HD11	1:E:444:ALA:CB	2.37	0.52
1:H:27:TYR:CE1	1:H:312:LYS:HE3	2.45	0.52
1:B:1017:SER:O	1:B:1021:ALA:HB3	2.09	0.52
1:B:669:ASP:OD2	1:B:676:ARG:NH2	2.32	0.52
1:E:515:LEU:HD23	1:E:515:LEU:C	2.30	0.52
1:H:463:VAL:HG21	2:I:88:ILE:HG12	1.91	0.52
1:K:65:ILE:HG21	1:K:917:MET:HB3	1.92	0.52
2:L:371:ILE:HA	2:L:374:ILE:HD12	1.90	0.52
1:E:560:LYS:HE2	11:E:1755:HOH:O	2.10	0.52
1:B:639:VAL:HG21	1:B:650:ALA:HB2	1.90	0.52
2:F:300:VAL:HG22	2:F:328:THR:O	2.09	0.52
1:H:125:ALA:HB3	1:H:301:PRO:HG3	1.92	0.52
1:H:144:ARG:NH1	1:H:160:ASP:OD1	2.43	0.52
2:I:232:ASN:N	2:I:233:PRO:HD3	2.25	0.52
1:K:340:GLY:HA2	11:K:1453:HOH:O	2.09	0.52
1:K:715:PRO:HG3	1:K:723:ALA:O	2.09	0.52
2:L:192:PHE:O	2:L:215:ARG:N	2.39	0.52
2:F:258:PHE:O	2:F:261:THR:HB	2.09	0.52
1:H:712:VAL:HG12	1:H:712:VAL:O	2.10	0.52
1:H:801:SER:O	1:H:805:GLN:HG3	2.09	0.52
1:K:871:LYS:HD3	1:K:876:GLN:HG2	1.92	0.52
1:E:653:LEU:HD22	1:E:658:VAL:HG21	1.91	0.52
2:F:170:TRP:HB3	2:F:216:LEU:HB2	1.90	0.52
2:F:350:PHE:CD1	2:F:366:LEU:HD21	2.44	0.52
1:K:456:ASN:ND2	11:K:1374:HOH:O	2.30	0.52
1:B:82:PRO:O	1:B:112:VAL:HG22	2.10	0.52
1:H:952:ASP:HB3	1:H:1043:LEU:HD22	1.91	0.52
2:I:175:TRP:CZ2	2:I:177:LEU:HA	2.45	0.52
2:I:212:ARG:HB3	2:I:371:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:906:LEU:HD11	9:K:1097:ORN:HD3	1.91	0.51
1:K:738:GLN:NE2	1:K:739:THR:N	2.48	0.51
2:L:324:ASN:ND2	2:L:324:ASN:H	2.00	0.51
1:B:410:PRO:HG3	11:B:1886:HOH:O	2.10	0.51
1:E:783:GLN:HE22	1:E:1042:THR:HB	1.75	0.51
1:H:763:VAL:O	1:H:826:ASN:HA	2.10	0.51
2:I:324:ASN:N	2:I:324:ASN:OD1	2.31	0.51
2:L:345:LYS:HB3	2:L:346:PRO:CD	2.34	0.51
1:B:502:ALA:HB2	1:B:509:GLU:HA	1.91	0.51
2:I:71:GLU:O	2:I:203:ARG:HG3	2.10	0.51
1:H:675:GLU:HA	1:H:678:GLN:HG2	1.92	0.51
1:H:703:LYS:O	1:H:706:GLU:HB3	2.10	0.51
1:K:641:TYR:OH	1:K:864:ALA:HB3	2.11	0.51
1:K:733:LEU:HD22	1:K:737:PHE:CD2	2.45	0.51
1:B:622:LEU:O	1:B:626:LEU:HG	2.11	0.51
1:E:953:LYS:NZ	5:E:1082:PO4:O4	2.43	0.51
1:H:488:LEU:HD23	1:H:519:TYR:HD2	1.75	0.51
2:I:217:THR:HG22	2:I:217:THR:O	2.11	0.51
2:I:298:LYS:HE2	2:I:303:ASN:OD1	2.11	0.51
1:K:1003[B]:ARG:NH1	1:K:1008[B]:GLU:OE1	2.38	0.51
1:E:884:PRO:HG2	11:E:1969:HOH:O	2.09	0.51
1:H:999:HIS:HD2	1:H:1002:ASP:H	1.59	0.51
1:H:701:VAL:HG11	1:H:730:GLU:OE2	2.11	0.51
1:H:707:ILE:HG22	1:H:708:GLY:O	2.11	0.51
1:E:0:MET:HG2	11:E:1242:HOH:O	2.11	0.51
1:H:374:THR:HG23	1:H:376:GLN:H	1.76	0.51
2:I:337:LEU:HD11	2:I:339:GLY:O	2.11	0.51
1:K:1002:ASP:O	1:K:1006[A]:ASN:OD1	2.29	0.51
1:E:676:ARG:O	1:E:679:HIS:HB2	2.11	0.51
1:K:707:ILE:CG2	1:K:753:HIS:HB2	2.40	0.51
2:L:27:VAL:HG22	2:L:131:CYS:HB2	1.93	0.51
2:C:176:THR:O	2:C:180:GLY:N	2.39	0.51
1:E:484:ASN:ND2	6:E:1090:CL:CL	2.79	0.51
1:E:891:GLU:OE1	9:E:1097:ORN:NE	2.43	0.51
1:B:673:ASP:HB3	1:B:676:ARG:HG3	1.92	0.50
1:E:0:MET:O	1:E:328:GLY:O	2.29	0.50
1:E:146:GLY:HA3	1:E:157:VAL:HG13	1.93	0.50
2:I:156:MET:SD	2:I:158:LEU:HD21	2.51	0.50
2:I:225:ALA:HA	2:I:258:PHE:CZ	2.46	0.50
2:F:81:VAL:HG13	2:F:110:ILE:HG23	1.93	0.50
2:F:163:THR:OG1	2:F:164:THR:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:54:THR:CG2	2:I:118:LEU:HD23	2.38	0.50
2:L:246:ALA:HB3	2:L:247:PRO:HD3	1.93	0.50
1:B:382:GLU:OE2	1:B:603:GLU:OE2	2.29	0.50
1:B:678:GLN:O	1:B:682:GLU:OE1	2.29	0.50
2:C:205:ILE:HG13	2:C:355:GLU:CG	2.42	0.50
2:C:208:MET:SD	2:C:355:GLU:HA	2.51	0.50
1:E:511:GLU:O	1:E:515:LEU:HB2	2.11	0.50
1:H:31:GLN:HB3	1:H:320:LYS:HG2	1.93	0.50
1:E:31:GLN:HB3	1:E:320:LYS:HG2	1.93	0.50
1:E:622:LEU:O	1:E:626:LEU:HG	2.11	0.50
1:E:890:LYS:HE3	11:E:1962:HOH:O	2.10	0.50
1:E:956:VAL:HG22	1:E:956:VAL:O	2.11	0.50
1:K:2:LYS:HB2	1:K:41:TYR:OH	2.11	0.50
2:L:244:ASP:OD1	2:L:245:PRO:HD2	2.11	0.50
1:B:906:LEU:CD1	9:B:1095:ORN:HD3	2.37	0.50
1:B:804:ILE:CD1	1:B:836:VAL:HG23	2.42	0.50
1:E:1050:ALA:O	1:E:1053:LEU:HB2	2.12	0.50
2:F:121:LEU:CD1	2:F:125:LYS:HD2	2.42	0.50
2:F:6:LEU:O	2:F:132:ILE:HA	2.11	0.50
2:F:246:ALA:N	2:F:247:PRO:HD2	2.27	0.50
2:F:261:THR:HG22	2:F:262:ASP:N	2.27	0.50
1:H:352:ASP:OD2	2:I:116:ARG:HD2	2.11	0.50
2:I:208:MET:HG2	11:I:3149:HOH:O	2.10	0.50
1:B:808:MET:HG2	1:B:829:PHE:CD2	2.46	0.50
1:H:162:GLY:O	1:H:165:CYS:HB3	2.12	0.50
1:H:794:SER:OG	1:H:796:PRO:O	2.29	0.50
1:B:697:ILE:H	1:B:697:ILE:CD1	2.22	0.50
1:E:288:ASN:HB3	1:E:291:ASN:OD1	2.11	0.50
1:H:633:LYS:N	1:H:634:PRO:HD3	2.27	0.50
1:K:227:CYS:C	1:K:268:MET:HE1	2.32	0.50
1:K:621:THR:O	1:K:625:VAL:HG23	2.12	0.50
1:K:697:ILE:CD1	1:K:697:ILE:H	2.22	0.50
2:L:133:ILE:CD1	2:L:143:ALA:HB2	2.41	0.50
2:C:10:GLU:HB2	2:C:128:GLN:OE1	2.12	0.50
2:C:244:ASP:OD1	2:C:245:PRO:HD2	2.11	0.50
2:C:255:ILE:HA	2:C:258:PHE:CD2	2.47	0.50
2:F:32:PHE:O	2:F:291:HIS:HB2	2.12	0.50
1:H:562:MET:HE2	1:H:634:PRO:HG3	1.92	0.50
2:I:64:GLY:HA3	2:I:94:ASN:OD1	2.12	0.50
1:B:681:VAL:HG23	1:B:686:LEU:HB2	1.94	0.50
2:C:276:ALA:O	2:C:281:ALA:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:LEU:CD2	2:F:146:LYS:HD2	2.42	0.50
2:F:57:TYR:CE1	2:F:58:PRO:HD2	2.47	0.50
2:F:188:ASP:OD1	2:F:188:ASP:N	2.44	0.49
1:H:92:GLN:HB2	1:H:173:MET:HG2	1.93	0.49
2:I:48:TYR:HA	2:I:51:GLN:HE21	1.76	0.49
1:E:1020[B]:ARG:NH1	11:E:2427:HOH:O	2.45	0.49
1:E:725:GLU:HG3	1:E:726:ILE:N	2.26	0.49
2:F:48:TYR:CE2	2:F:311:ASN:ND2	2.80	0.49
1:H:901:GLY:O	1:H:1026:ARG:NH2	2.45	0.49
1:K:312:LYS:HE2	1:K:607:THR:O	2.12	0.49
1:B:725:GLU:OE2	1:B:735:ARG:NH2	2.45	0.49
2:F:261:THR:CG2	2:F:263:ILE:HG13	2.42	0.49
2:I:12:GLY:HA2	2:I:144:LEU:HD13	1.94	0.49
1:B:678:GLN:HG3	1:B:688:GLN:HE22	1.78	0.49
1:B:697:ILE:HD12	1:B:697:ILE:N	2.25	0.49
1:E:348:GLU:O	2:F:294:ASN:HB2	2.12	0.49
1:E:749:VAL:HG12	1:E:749:VAL:O	2.13	0.49
2:F:142:LEU:HD23	2:F:146:LYS:HD2	1.93	0.49
1:H:424:ARG:HD3	11:H:1536:HOH:O	2.12	0.49
2:I:85:LEU:HD12	2:I:86:PRO:HD2	1.94	0.49
1:K:420:LEU:HD22	1:K:446:LEU:HD11	1.93	0.49
2:C:25:SER:HA	2:C:132:ILE:O	2.12	0.49
2:C:228:VAL:HG11	2:C:258:PHE:CZ	2.47	0.49
1:E:137:LYS:HE3	1:E:273:GLU:OE2	2.13	0.49
1:K:0:MET:O	1:K:328:GLY:O	2.29	0.49
1:K:673:ASP:CG	1:K:676:ARG:HG3	2.33	0.49
1:K:815:LEU:HD11	1:K:838:LEU:HD21	1.94	0.49
2:C:364:ALA:N	2:C:365:PRO:HD2	2.28	0.49
1:E:132:ASP:HB2	11:E:1380:HOH:O	2.12	0.49
1:E:77:ILE:O	1:E:81:ARG:N	2.42	0.49
2:F:295:HIS:CE1	2:F:333:PHE:CD2	3.00	0.49
1:B:63:THR:O	1:B:1064:VAL:HG23	2.13	0.49
1:E:526:LYS:HD2	2:F:116:ARG:HD3	1.94	0.49
2:F:261:THR:HG22	2:F:263:ILE:H	1.77	0.49
2:I:222:GLN:HA	2:I:250:TYR:CD2	2.48	0.49
1:K:234:GLU:HB2	1:K:252:ALA:HA	1.95	0.49
2:C:277:LEU:HD21	2:C:283:THR:HG23	1.95	0.49
2:C:341:HIS:CD2	2:C:348:PHE:CB	2.96	0.49
2:F:133:ILE:CG2	2:F:138:PRO:HB3	2.43	0.49
1:H:709:TYR:HA	1:H:710:PRO:C	2.32	0.49
2:I:272:HIS:HB2	2:I:349:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:12:GLY:HA2	2:L:144:LEU:HD13	1.95	0.49
1:E:754:PHE:CD1	8:E:1096:ADP:C2	3.01	0.49
1:K:574:GLY:HA3	11:K:1836:HOH:O	2.13	0.49
2:L:158:LEU:O	2:L:161:GLU:HB2	2.12	0.49
2:C:29:GLU:OE2	2:C:285:LYS:NZ	2.32	0.48
2:C:39:TYR:CZ	2:C:61:GLY:HA2	2.48	0.48
1:E:218:GLU:OE2	1:E:282:ASN:HB2	2.13	0.48
2:F:44:THR:HG21	2:F:70:GLU:HB3	1.95	0.48
1:H:425:ARG:HD3	1:H:425:ARG:C	2.33	0.48
1:H:827:VAL:HG22	1:H:841:VAL:HG22	1.95	0.48
2:C:300:VAL:HG22	2:C:328:THR:O	2.13	0.48
1:E:166:ILE:N	1:E:166:ILE:HD12	2.28	0.48
1:H:439:ALA:O	1:H:443:ARG:HG3	2.13	0.48
1:H:559:GLU:OE1	1:H:635:LYS:HD2	2.12	0.48
1:H:727:VAL:HG11	1:H:733:LEU:HA	1.94	0.48
1:K:644:GLN:NE2	1:K:648:LYS:HZ3	2.11	0.48
2:L:318:GLU:O	2:L:321:LEU:HB2	2.13	0.48
1:H:697:ILE:N	1:H:697:ILE:HD12	2.28	0.48
1:K:297:ILE:HG13	11:K:1381:HOH:O	2.14	0.48
1:B:949:ARG:HG3	1:B:1015:THR:OG1	2.14	0.48
1:B:270:VAL:HG12	1:B:299:MET:HE3	1.95	0.48
1:B:35:ALA:HB1	1:B:324:LYS:HE3	1.95	0.48
2:C:32:PHE:HA	2:C:54:THR:O	2.13	0.48
2:F:261:THR:HG22	2:F:263:ILE:HG13	1.95	0.48
1:H:587:ALA:O	1:H:590:GLU:HB2	2.12	0.48
1:K:694:VAL:HG21	1:K:700:ALA:CA	2.43	0.48
1:B:940:LYS:HB3	1:B:966[A]:GLN:OE1	2.13	0.48
1:E:872:SER:O	1:E:876:GLN:HG3	2.14	0.48
1:H:484:ASN:OD1	1:H:487:PHE:N	2.37	0.48
2:I:170:TRP:HB3	2:I:216:LEU:HB2	1.95	0.48
1:K:558:ARG:HG3	1:K:558:ARG:HH11	1.78	0.48
1:B:804:ILE:HD12	1:B:836:VAL:CG2	2.44	0.48
1:E:633:LYS:N	1:E:634:PRO:HD3	2.29	0.48
2:I:234:ASP:OD1	2:I:378:ARG:HD2	2.14	0.48
2:L:212:ARG:NH1	2:L:212:ARG:HG3	2.29	0.48
1:B:0:MET:HB3	1:B:1:PRO:HD3	1.95	0.48
1:E:708:GLY:O	1:E:753:HIS:ND1	2.39	0.48
2:F:324:ASN:HD22	2:F:324:ASN:N	1.97	0.48
2:F:266:PHE:HB2	2:F:370:PHE:CD1	2.49	0.48
2:F:34:THR:HA	2:F:56:THR:OG1	2.14	0.48
1:K:382:GLU:OE2	1:K:603:GLU:OE2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:670:ARG:NH2	1:K:818:GLU:OE2	2.32	0.48
1:B:813:GLN:NE2	11:B:1673:HOH:O	2.47	0.48
1:E:196:ASP:OD2	1:E:1036:LYS:NZ	2.42	0.48
1:E:218:GLU:OE2	1:E:282:ASN:ND2	2.36	0.48
1:E:824:LEU:HG	1:E:864:ALA:HB2	1.96	0.48
1:H:1036:LYS:HE2	11:H:1338:HOH:O	2.13	0.48
1:H:713:VAL:CG2	1:H:727:VAL:HG21	2.44	0.48
2:I:295:HIS:HE1	2:I:331:SER:OG	1.97	0.48
1:K:644:GLN:NE2	1:K:648:LYS:NZ	2.61	0.48
2:L:226:GLU:O	2:L:230:LYS:HG3	2.13	0.48
2:L:248:CYS:O	2:L:251:ALA:HB3	2.14	0.48
2:C:321:LEU:HD12	2:C:321:LEU:HA	1.68	0.48
1:E:674:ARG:HG2	1:E:750:LEU:HD11	1.94	0.48
2:F:163:THR:HG21	2:F:221:ALA:HB3	1.95	0.48
1:H:1019:ARG:HA	1:H:1019:ARG:HD2	1.51	0.48
1:H:382:GLU:OE2	1:H:603:GLU:OE2	2.32	0.48
1:H:675:GLU:HA	1:H:678:GLN:CG	2.43	0.48
2:I:291:HIS:HD2	2:I:311:ASN:OD1	1.97	0.48
1:K:713:VAL:HG11	1:K:736:TYR:HE2	1.77	0.48
2:L:246:ALA:N	2:L:247:PRO:HD2	2.29	0.48
1:B:547:GLU:OE2	2:C:114:ASP:HA	2.14	0.48
2:C:376:GLN:O	2:C:379:LYS:HB2	2.14	0.48
2:C:48:TYR:HA	2:C:51:GLN:HE21	1.79	0.48
1:E:1020[B]:ARG:NH1	1:E:1020[B]:ARG:HG2	2.15	0.48
1:E:819:LEU:O	1:E:820:GLN:HB2	2.14	0.48
2:F:212:ARG:HB3	2:F:371:ILE:CD1	2.44	0.48
1:H:171:PHE:HB3	1:H:199:PRO:HG2	1.95	0.48
1:H:8:SER:OG	1:H:83:ASP:N	2.45	0.48
1:K:806:ASP:OD1	1:K:809:ARG:NH1	2.47	0.48
1:B:702:GLU:CA	1:B:705:LYS:HD2	2.28	0.47
1:E:487:PHE:O	1:E:491:LEU:HG	2.14	0.47
2:I:295:HIS:HE1	2:I:331:SER:CB	2.27	0.47
2:L:50:ARG:HB3	2:L:50:ARG:HE	1.36	0.47
1:B:699:MET:O	1:B:703:LYS:HB2	2.13	0.47
1:B:839:ILE:O	1:B:840:GLU:HB3	2.14	0.47
1:B:943:ARG:HD3	1:B:971:ASP:OD1	2.15	0.47
2:C:265:VAL:O	2:C:347:ALA:HA	2.14	0.47
1:E:129[A]:ARG:HG3	1:E:147:ILE:HG13	1.96	0.47
1:E:480:ILE:HG22	11:E:1714:HOH:O	2.14	0.47
1:E:971:ASP:HA	1:E:988:ARG:O	2.14	0.47
2:L:25:SER:HA	2:L:132:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:290:HIS:HB2	2:C:312:HIS:NE2	2.30	0.47
1:E:1020[B]:ARG:HH21	1:E:1023:GLU:HG3	1.76	0.47
2:F:163:THR:HB	2:F:198:ASP:O	2.14	0.47
2:I:318:GLU:HA	2:I:321:LEU:HD13	1.97	0.47
2:F:46:PRO:HG2	2:F:200:GLY:O	2.15	0.47
2:F:226:GLU:OE2	2:F:257:LYS:HE3	2.14	0.47
1:K:0:MET:HG3	1:K:1:PRO:CD	2.38	0.47
1:K:374:THR:OG1	1:K:375:THR:N	2.47	0.47
1:K:829:PHE:CE1	1:K:838:LEU:HD13	2.50	0.47
2:L:208:MET:SD	2:L:355:GLU:HA	2.54	0.47
1:E:674:ARG:HD2	1:E:674:ARG:N	2.23	0.47
2:F:40:GLN:HA	2:F:43:LEU:HD12	1.96	0.47
1:H:343:THR:HB	1:H:344:PRO:HD2	1.97	0.47
1:H:578:ASP:OD2	1:H:604:THR:HB	2.14	0.47
2:I:150:PHE:CD1	2:I:151:PRO:HD2	2.49	0.47
2:I:156:MET:HG2	2:I:158:LEU:HG	1.97	0.47
2:I:190:LEU:CB	2:I:215:ARG:HB3	2.45	0.47
1:K:990:VAL:HG23	1:K:1003[A]:ARG:CZ	2.45	0.47
2:L:195:VAL:HG13	2:L:219:VAL:CG1	2.44	0.47
1:H:353:TYR:OH	1:H:528:VAL:HG13	2.14	0.47
1:H:685:LYS:O	1:H:686:LEU:HD23	2.15	0.47
2:C:190:LEU:HD11	2:C:210:VAL:HG13	1.97	0.47
1:E:587:ALA:HB2	1:E:862:LYS:HG2	1.96	0.47
1:K:27:TYR:CE1	1:K:312:LYS:HE3	2.50	0.47
1:K:288:ASN:OD1	1:K:289:PRO:HD2	2.15	0.47
2:C:322:PRO:HB2	2:C:324:ASN:HD22	1.79	0.47
1:E:645:THR:CB	1:E:646:PRO:HD3	2.44	0.47
1:E:670:ARG:HD3	11:E:1800:HOH:O	2.15	0.47
1:H:725:GLU:HG2	1:H:726:ILE:H	1.80	0.47
1:H:952:ASP:CB	1:H:1043:LEU:HD22	2.45	0.47
2:C:225:ALA:HB2	2:C:254:ALA:HA	1.97	0.47
1:E:478:VAL:HB	1:E:482:GLY:HA3	1.96	0.47
1:E:317:PRO:HG3	1:E:609:TYR:OH	2.15	0.47
1:E:645:THR:HB	1:E:646:PRO:CD	2.43	0.47
2:F:39:TYR:CZ	2:F:61:GLY:HA2	2.50	0.47
1:H:714:ARG:HB2	1:H:750:LEU:HB2	1.96	0.47
1:B:221:ARG:CZ	1:B:272:ARG:HG2	2.45	0.47
1:B:343:THR:HB	11:B:1452:HOH:O	2.15	0.47
1:B:712:VAL:HG12	1:B:712:VAL:O	2.14	0.47
1:E:904:PRO:HB2	1:E:1039:TYR:HH	1.77	0.47
1:E:993:VAL:HG22	1:E:999:HIS:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:588:LEU:HD23	1:H:588:LEU:HA	1.75	0.47
1:H:901:GLY:HA2	1:H:1030:ARG:NH1	2.29	0.47
1:K:990:VAL:CG2	1:K:1003[A]:ARG:HD2	2.45	0.47
1:K:346:SER:O	2:L:296:PRO:HB3	2.15	0.47
1:B:805:GLN:HA	1:B:808:MET:HE2	1.96	0.47
1:B:986:ASN:ND2	11:B:1770:HOH:O	2.37	0.47
2:C:348:PHE:CE1	2:C:370:PHE:HB2	2.50	0.47
1:E:524:VAL:HG22	1:E:547:GLU:H	1.80	0.47
2:F:277:LEU:HD23	2:F:281:ALA:O	2.15	0.47
2:F:55:LEU:HA	2:F:55:LEU:HD23	1.76	0.47
1:H:1025:SER:HB3	7:H:1090:GLN:HB3	1.97	0.47
1:H:234:GLU:HB2	1:H:252:ALA:HA	1.97	0.47
1:H:258:LYS:NZ	11:H:1416:HOH:O	2.48	0.47
1:K:480:ILE:HG13	1:K:480:ILE:O	2.15	0.47
1:B:808:MET:HG2	1:B:829:PHE:CE2	2.50	0.46
1:B:935:ASN:HB2	11:B:1138:HOH:O	2.14	0.46
2:C:290:HIS:HB3	2:C:310:GLN:HB3	1.97	0.46
1:E:691:ASN:HA	1:E:751:LEU:O	2.14	0.46
2:F:350:PHE:HB2	2:F:366:LEU:HD23	1.97	0.46
2:F:374:ILE:O	2:F:378:ARG:HG3	2.14	0.46
1:H:478:VAL:HG23	1:H:482:GLY:HA3	1.93	0.46
2:I:338:GLN:NE2	11:I:3165:HOH:O	2.43	0.46
2:L:50:ARG:HD3	11:L:4826:HOH:O	2.14	0.46
1:B:508:ARG:HH12	1:B:510:ALA:HB3	1.80	0.46
1:E:478:VAL:HG23	1:E:479:GLY:N	2.29	0.46
1:E:58:GLU:HB3	11:E:1312:HOH:O	2.14	0.46
1:E:713:VAL:HG23	1:E:727:VAL:HG23	1.96	0.46
2:F:38:GLY:HA3	2:F:358:PRO:HB3	1.96	0.46
1:H:480:ILE:CD1	1:H:507:VAL:HG21	2.44	0.46
1:H:665:PRO:O	1:H:668:ILE:HB	2.16	0.46
1:H:725:GLU:HG2	1:H:726:ILE:N	2.30	0.46
2:I:121:LEU:O	2:I:121:LEU:HD12	2.15	0.46
2:I:249:ASP:O	2:I:253:THR:HG23	2.15	0.46
2:I:370:PHE:O	2:I:374:ILE:HD12	2.15	0.46
1:K:236:PHE:CE1	1:K:457:ILE:HD13	2.50	0.46
2:L:201:ALA:HB2	2:L:239:SER:HB2	1.98	0.46
2:L:212:ARG:HH11	2:L:212:ARG:HG3	1.79	0.46
2:L:341:HIS:CD2	2:L:348:PHE:HB3	2.51	0.46
2:L:45:ASP:HB2	11:L:4256:HOH:O	2.15	0.46
1:B:44:ILE:HG23	1:B:62:ALA:HB3	1.97	0.46
1:E:222:ASP:CG	1:E:226:ASN:HB2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:GLU:O	1:H:157:VAL:HG23	2.15	0.46
2:I:298:LYS:HB2	2:I:332:LEU:HD21	1.98	0.46
2:I:57:TYR:CE1	2:I:58:PRO:HD2	2.49	0.46
2:L:212:ARG:HB3	2:L:371:ILE:CD1	2.45	0.46
1:B:725:GLU:CG	1:B:726:ILE:N	2.79	0.46
2:C:350:PHE:CG	2:C:366:LEU:CD2	2.98	0.46
1:H:157:VAL:HG11	1:H:205:ILE:HB	1.97	0.46
1:H:3:ARG:HD3	1:H:6:ILE:HD12	1.97	0.46
1:H:749:VAL:HG12	1:H:749:VAL:O	2.14	0.46
1:H:795:LEU:HD23	1:H:795:LEU:C	2.35	0.46
2:I:15:PHE:HD1	6:I:384:CL:CL	2.35	0.46
2:C:175:TRP:CD1	2:C:180:GLY:HA2	2.51	0.46
1:E:84:ALA:HA	1:E:113:THR:O	2.16	0.46
2:F:158:LEU:HA	2:F:158:LEU:HD23	1.81	0.46
1:H:163:PHE:HB3	1:H:164:PRO:HA	1.96	0.46
1:H:668:ILE:HA	1:H:843:PRO:HG2	1.97	0.46
1:B:727:VAL:HG13	1:B:732:ASP:HB3	1.98	0.46
1:E:856:THR:O	1:E:1071:ILE:HD12	2.15	0.46
1:E:44:ILE:HA	1:E:62:ALA:O	2.16	0.46
2:F:246:ALA:HB3	2:F:247:PRO:CD	2.40	0.46
2:F:350:PHE:CG	2:F:366:LEU:CD2	2.98	0.46
1:H:767:CYS:HB2	1:H:772:VAL:HG22	1.97	0.46
1:K:16:PRO:HG3	1:K:916:VAL:CG1	2.46	0.46
1:K:5:ASP:N	1:K:5:ASP:OD1	2.49	0.46
1:B:709:TYR:HA	1:B:710:PRO:C	2.36	0.46
1:B:714:ARG:HB2	1:B:750:LEU:CB	2.45	0.46
2:C:246:ALA:C	2:C:248:CYS:H	2.18	0.46
1:E:127:ASP:HB3	1:E:130:ARG:HB2	1.97	0.46
1:H:281:SER:OG	1:H:301:PRO:HA	2.16	0.46
1:K:412:VAL:HG21	1:K:423:ILE:HD11	1.96	0.46
1:K:990:VAL:HG21	1:K:1003[A]:ARG:HD2	1.98	0.46
1:K:990:VAL:HG22	1:K:991:ASN:N	2.31	0.46
2:L:156:MET:HA	11:L:4680:HOH:O	2.14	0.46
2:L:350:PHE:CD2	2:L:354:PRO:HD3	2.49	0.46
1:B:671:ALA:CB	1:B:843:PRO:HG3	2.46	0.46
1:B:8:SER:HB3	1:B:42:ARG:HB3	1.97	0.46
2:C:286:MET:CE	2:C:312:HIS:ND1	2.78	0.46
1:E:701:VAL:CG1	1:E:705:LYS:HE3	2.33	0.46
1:E:711:LEU:O	1:E:726:ILE:HA	2.16	0.46
2:F:133:ILE:CD1	2:F:143:ALA:HB2	2.46	0.46
2:I:364:ALA:N	2:I:365:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:692:ALA:CB	1:K:707:ILE:HD11	2.46	0.46
1:B:666:ASP:CG	1:B:676:ARG:HH22	2.19	0.46
1:B:758:ALA:O	1:B:783:GLN:HB2	2.16	0.46
1:E:151:MET:HG3	1:E:155:LEU:HD11	1.98	0.46
1:E:466:GLU:O	1:E:470:ARG:HG2	2.15	0.46
1:H:804:ILE:HD13	1:H:804:ILE:HA	1.82	0.46
1:H:945:LEU:C	1:H:946:LEU:HD12	2.36	0.46
2:I:237:PHE:HZ	2:I:268:ILE:HD12	1.81	0.46
1:K:239:MET:HE3	8:K:1095:ADP:C4	2.51	0.46
2:L:46:PRO:HA	2:L:76:HIS:CG	2.50	0.46
1:E:492:LYS:HA	1:E:492:LYS:HD2	1.57	0.46
1:E:525:TYR:CE1	1:E:544:SER:HB3	2.51	0.46
1:E:730:GLU:OE2	1:E:734:ARG:NH1	2.47	0.46
2:F:335:GLY:HA2	11:F:2170:HOH:O	2.16	0.46
1:H:706:GLU:O	1:H:706:GLU:HG3	2.16	0.46
1:K:0:MET:HG2	1:K:1:PRO:N	2.30	0.46
1:K:26:ASP:OD1	1:K:52:THR:HB	2.16	0.46
1:B:980:LEU:HD12	1:B:987:PRO:HG3	1.98	0.45
1:E:66:GLU:HB3	1:E:67:PRO:HD2	1.97	0.45
2:F:324:ASN:HA	2:F:343:THR:OG1	2.15	0.45
1:H:815:LEU:HD13	1:H:841:VAL:HG21	1.98	0.45
1:K:362:ASN:OD1	1:K:380:VAL:HG21	2.16	0.45
1:K:74:ARG:NH1	1:K:74:ARG:HG2	2.20	0.45
2:L:185:LYS:HD3	2:L:190:LEU:HD21	1.98	0.45
1:B:105:GLY:HA2	11:B:1230:HOH:O	2.14	0.45
1:B:478:VAL:HB	1:B:482:GLY:HA3	1.99	0.45
1:B:949:ARG:H	1:B:949:ARG:HG3	1.28	0.45
2:F:364:ALA:N	2:F:365:PRO:CD	2.79	0.45
1:K:990:VAL:CB	1:K:1003[A]:ARG:NH1	2.76	0.45
2:L:232:ASN:N	2:L:233:PRO:CD	2.79	0.45
2:L:245:PRO:HB3	2:L:270:LEU:CD1	2.46	0.45
2:L:74:GLN:HG3	2:L:76:HIS:NE2	2.31	0.45
2:C:191:PRO:HD2	2:C:213:GLY:O	2.16	0.45
2:F:232:ASN:N	2:F:233:PRO:CD	2.80	0.45
1:K:697:ILE:O	1:K:701:VAL:HG23	2.16	0.45
1:K:736:TYR:O	1:K:738:GLN:N	2.49	0.45
1:K:74:ARG:CG	1:K:74:ARG:HH11	2.24	0.45
2:L:324:ASN:ND2	2:L:324:ASN:N	2.61	0.45
1:B:173:MET:HB2	5:B:1078:PO4:O1	2.15	0.45
1:B:138:ILE:HG21	1:B:273:GLU:HB2	1.98	0.45
1:E:1020[B]:ARG:NH2	1:E:1023:GLU:CG	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:GLU:HB2	11:E:2347:HOH:O	2.15	0.45
1:E:342[B]:ARG:NH1	1:E:536:ALA:HB3	2.24	0.45
1:E:954[B]:GLU:HG2	1:E:955:ARG:N	2.32	0.45
2:I:267:GLY:HA3	2:I:271:GLY:O	2.17	0.45
1:K:1035:TYR:HA	11:K:1859:HOH:O	2.15	0.45
1:K:264:ARG:O	1:K:268:MET:HG3	2.17	0.45
1:K:502:ALA:HB1	1:K:507:VAL:O	2.16	0.45
1:E:725:GLU:CG	1:E:726:ILE:N	2.79	0.45
1:E:966[B]:GLN:HG2	11:E:2075:HOH:O	2.15	0.45
2:F:197:TYR:CB	2:F:199:PHE:CZ	3.00	0.45
1:H:410:PRO:HG3	11:H:1895:HOH:O	2.17	0.45
2:I:269:CYS:O	2:I:272:HIS:HB3	2.16	0.45
2:I:300:VAL:HG23	2:I:301:GLU:N	2.31	0.45
1:K:157:VAL:HG12	1:K:205:ILE:CG2	2.47	0.45
1:K:686:LEU:HD22	1:K:811:GLN:HG2	1.98	0.45
2:C:232:ASN:N	2:C:233:PRO:CD	2.79	0.45
1:H:1027:VAL:O	1:H:1031:SER:HB2	2.16	0.45
1:H:475:VAL:HG13	1:H:483:LEU:HD21	1.97	0.45
2:I:285:LYS:HG3	2:I:314:PHE:CZ	2.50	0.45
1:B:762:ASP:O	1:B:778:MET:HE3	2.17	0.45
1:E:945:LEU:HB3	1:E:1012:ILE:HG12	1.99	0.45
1:E:1027:VAL:CG1	1:E:1028:ILE:N	2.80	0.45
1:E:157:VAL:HG11	1:E:205:ILE:HB	1.98	0.45
1:H:0:MET:HB2	11:H:1825:HOH:O	2.16	0.45
2:I:218:ILE:CD1	2:I:218:ILE:N	2.80	0.45
2:I:295:HIS:HE1	2:I:331:SER:HB2	1.81	0.45
1:E:515:LEU:CD2	1:E:519:TYR:CE2	2.98	0.45
1:E:684:LEU:HD12	1:E:815:LEU:HD23	1.99	0.45
1:E:738:GLN:C	1:E:740:ALA:H	2.20	0.45
1:H:492:LYS:HA	1:H:492:LYS:HD2	1.59	0.45
1:H:966:GLN:HB2	11:H:1768:HOH:O	2.16	0.45
2:I:223:THR:CG2	2:I:224:SER:N	2.80	0.45
1:K:144:ARG:NH2	1:K:160:ASP:OD1	2.46	0.45
1:K:582:VAL:O	1:K:586:LEU:HG	2.17	0.45
1:K:780:HIS:CE1	1:K:788:SER:CB	3.00	0.45
1:B:73:VAL:O	1:B:76:ILE:N	2.50	0.45
1:H:964:LEU:HD23	1:H:968:PHE:O	2.16	0.45
2:I:139:ASP:OD2	2:I:142:LEU:HB2	2.17	0.45
2:I:197:TYR:CB	2:I:199:PHE:CZ	2.98	0.45
1:K:805:GLN:O	1:K:809:ARG:HG3	2.17	0.45
1:B:733:LEU:HG	1:B:737:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:478:VAL:CG2	1:E:479:GLY:N	2.79	0.45
2:F:284:VAL:HG12	2:F:285:LYS:N	2.31	0.45
2:F:321:LEU:HA	2:F:321:LEU:HD12	1.79	0.45
1:H:701:VAL:HG13	1:H:730:GLU:CG	2.43	0.45
2:L:50:ARG:HG3	2:L:158:LEU:HD13	1.99	0.45
1:B:100:GLU:OE1	1:B:103:ARG:NE	2.38	0.44
1:E:6:ILE:HD13	1:E:6:ILE:HG21	1.67	0.44
2:F:365:PRO:HA	11:F:2276:HOH:O	2.16	0.44
1:H:733:LEU:O	1:H:737:PHE:HB2	2.17	0.44
1:H:819:LEU:O	1:H:820:GLN:HB2	2.17	0.44
2:I:272:HIS:HA	2:I:349:SER:HB2	1.99	0.44
1:K:901:GLY:O	1:K:1026:ARG:NH2	2.50	0.44
1:B:125:ALA:HB3	1:B:301:PRO:HG3	1.99	0.44
1:E:1003:ARG:CB	1:E:1008:GLU:HG3	2.46	0.44
1:E:1000:ILE:HG21	1:E:1028:ILE:HG12	1.99	0.44
2:F:41:GLU:HG3	2:F:69:ASP:O	2.17	0.44
1:H:890:LYS:NZ	11:H:1673:HOH:O	2.50	0.44
2:I:32:PHE:O	2:I:291:HIS:HB2	2.17	0.44
2:I:67:ASP:O	2:I:70:GLU:HB2	2.16	0.44
1:K:830:ALA:HB2	1:K:839:ILE:HD11	1.99	0.44
1:K:862:LYS:HE2	11:K:1622:HOH:O	2.17	0.44
1:K:533:ALA:HB2	2:L:116:ARG:NH1	2.31	0.44
1:B:702:GLU:HA	1:B:702:GLU:OE1	2.18	0.44
1:B:733:LEU:HG	1:B:737:PHE:HD2	1.81	0.44
1:B:804:ILE:HG22	1:B:805:GLN:N	2.32	0.44
1:H:697:ILE:O	1:H:700:ALA:HB3	2.17	0.44
1:K:966:GLN:HG3	1:K:966:GLN:O	2.17	0.44
2:L:363:ALA:C	2:L:365:PRO:HD2	2.37	0.44
1:B:221:ARG:NH2	1:B:272:ARG:HG2	2.32	0.44
2:I:26:ALA:O	2:I:131:CYS:HA	2.16	0.44
2:I:284:VAL:O	2:I:315:ALA:N	2.43	0.44
2:I:279:SER:CB	2:I:325:LEU:HD11	2.48	0.44
1:K:702:GLU:HA	1:K:702:GLU:OE1	2.17	0.44
2:L:273:GLN:HE21	2:L:351:GLN:HE22	1.65	0.44
1:B:290:LYS:NZ	11:B:1364:HOH:O	2.50	0.44
1:H:480:ILE:HD12	1:H:507:VAL:CG2	2.45	0.44
1:K:711:LEU:O	1:K:726:ILE:HA	2.16	0.44
2:L:39:TYR:CZ	2:L:61:GLY:HA2	2.52	0.44
1:B:513:ARG:HD3	11:B:1566:HOH:O	2.17	0.44
1:B:726:ILE:CD1	1:B:754:PHE:CD1	3.00	0.44
2:C:318:GLU:O	2:C:321:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:LEU:O	1:E:158:ALA:HB3	2.17	0.44
2:F:52:ILE:O	2:F:52:ILE:HG22	2.18	0.44
1:H:264:ARG:CZ	2:I:360:PRO:HB3	2.48	0.44
2:I:208:MET:O	2:I:211:ASP:HB2	2.18	0.44
1:K:947:SER:O	1:K:1014:ASN:HA	2.16	0.44
1:K:378:LYS:HE2	11:K:1329:HOH:O	2.17	0.44
1:K:691:ASN:HD22	1:K:691:ASN:N	2.14	0.44
2:L:238:LEU:O	2:L:271:GLY:HA3	2.17	0.44
1:B:697:ILE:O	1:B:700:ALA:HB3	2.17	0.44
1:H:990:VAL:CG2	1:H:1003:ARG:NH1	2.80	0.44
2:I:181:LEU:HD23	2:I:181:LEU:HA	1.80	0.44
2:I:190:LEU:HD13	2:I:215:ARG:HA	1.99	0.44
2:I:208:MET:SD	2:I:355:GLU:HA	2.58	0.44
1:K:44:ILE:HA	1:K:62:ALA:O	2.18	0.44
1:K:972:ALA:O	1:K:990:VAL:HG12	2.17	0.44
1:B:988:ARG:HB2	1:K:986:ASN:HD21	1.83	0.44
2:C:222:GLN:HG3	2:C:250:TYR:CE2	2.52	0.44
2:C:345:LYS:HG3	2:C:346:PRO:HD2	2.00	0.44
1:E:599:ASN:O	1:E:617:PHE:HA	2.17	0.44
1:E:694:VAL:HG21	1:E:700:ALA:CB	2.47	0.44
1:E:986:ASN:ND2	11:E:2050:HOH:O	2.43	0.44
1:E:990:VAL:HG22	1:E:991:ASN:N	2.33	0.44
2:F:83:ARG:O	2:F:112:ASP:HA	2.18	0.44
1:H:104:GLN:NE2	1:H:104:GLN:HA	2.33	0.44
1:H:126:GLU:HB2	1:H:171:PHE:CZ	2.52	0.44
1:K:928:ALA:HB2	1:K:1052:ALA:HB1	2.00	0.44
1:K:990:VAL:HB	1:K:1003[A]:ARG:HH11	1.78	0.44
2:L:176:THR:HG1	2:L:179:GLY:H	1.65	0.44
1:B:352:ASP:OD2	2:C:116:ARG:HD2	2.18	0.44
2:C:193:HIS:N	2:C:234:ASP:OD2	2.45	0.44
2:C:332:LEU:HA	2:C:332:LEU:HD12	1.41	0.44
1:E:953:LYS:O	1:E:956:VAL:HG12	2.18	0.44
2:F:246:ALA:N	2:F:247:PRO:CD	2.80	0.44
1:H:330:THR:O	1:H:333:GLU:HB2	2.18	0.44
1:H:768:ASP:OD1	1:H:770:GLU:HB2	2.18	0.44
2:I:327:VAL:HG22	2:I:337:LEU:HD13	2.00	0.44
1:K:0:MET:HB3	1:K:223:LYS:NZ	2.32	0.44
2:L:144:LEU:O	2:L:148:ARG:HG3	2.18	0.44
1:E:224:ASN:ND2	1:E:330:THR:HG21	2.33	0.43
2:F:345:LYS:HA	2:F:345:LYS:HD3	1.68	0.43
1:H:714:ARG:HH11	1:H:714:ARG:HD2	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:237:PHE:CZ	2:I:268:ILE:HD12	2.52	0.43
2:I:295:HIS:CE1	2:I:331:SER:HB2	2.53	0.43
2:I:341:HIS:ND1	2:I:342:ARG:N	2.66	0.43
2:I:345:LYS:HB3	2:I:346:PRO:HD2	2.00	0.43
1:K:158:ALA:O	1:K:162:GLY:N	2.49	0.43
1:K:697:ILE:HD12	1:K:697:ILE:N	2.27	0.43
1:K:70:TRP:CE2	1:K:71:GLU:HG3	2.53	0.43
2:C:272:HIS:HA	2:C:349:SER:HB2	2.00	0.43
1:E:857:GLY:HA2	1:E:1068:HIS:CE1	2.53	0.43
1:E:966[B]:GLN:HG3	1:E:1053:LEU:CD1	2.43	0.43
1:H:193:ARG:NH2	11:H:1318:HOH:O	2.39	0.43
1:K:1053:LEU:HD23	1:K:1053:LEU:HA	1.71	0.43
1:K:810[B]:GLN:HB2	1:K:810[B]:GLN:HE21	1.31	0.43
2:L:6:LEU:CD2	2:L:7:LEU:N	2.81	0.43
2:C:286:MET:HB2	2:C:313:GLY:O	2.17	0.43
1:E:212:TRP:CZ3	1:E:295:ILE:HD12	2.54	0.43
2:I:204:ASN:ND2	2:I:355:GLU:O	2.48	0.43
2:C:163:THR:CB	2:C:221:ALA:HB2	2.49	0.43
1:E:75:LYS:HE3	1:E:1058:THR:O	2.18	0.43
1:E:636:GLY:HA2	1:E:659:PRO:O	2.18	0.43
1:E:81:ARG:HD3	11:E:2311:HOH:O	2.18	0.43
2:F:99:SER:O	2:F:103:LYS:HG3	2.18	0.43
1:H:1027:VAL:HG12	11:H:1778:HOH:O	2.18	0.43
1:K:707:ILE:HG23	1:K:753:HIS:HB2	2.00	0.43
1:B:695:THR:H	1:B:699:MET:CE	2.29	0.43
1:B:795:LEU:C	1:B:795:LEU:HD23	2.38	0.43
1:B:805:GLN:HA	1:B:808:MET:CE	2.49	0.43
1:E:480:ILE:HD11	1:E:515:LEU:HD12	2.00	0.43
1:H:124:LYS:HD3	1:H:274:ILE:HA	1.99	0.43
1:H:596:ILE:HA	1:H:614:ARG:O	2.17	0.43
1:H:783:GLN:N	1:H:783:GLN:NE2	2.46	0.43
1:B:727:VAL:HG11	1:B:733:LEU:HA	2.01	0.43
2:C:27:VAL:O	2:C:78:GLN:HG2	2.19	0.43
2:C:350:PHE:HB2	2:C:366:LEU:HD21	1.99	0.43
1:E:824:LEU:HG	1:E:864:ALA:CB	2.48	0.43
1:H:459:ARG:O	1:H:463:VAL:HG22	2.19	0.43
2:I:39:TYR:CZ	2:I:61:GLY:HA2	2.53	0.43
1:K:670:ARG:NH1	1:K:818:GLU:O	2.48	0.43
2:L:236:ILE:HB	2:L:265:VAL:HG22	2.01	0.43
1:E:388:ARG:NH2	1:E:547:GLU:OE2	2.43	0.43
1:H:58:GLU:HG2	1:H:58:GLU:H	0.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:163:THR:HB	2:L:221:ALA:HB2	2.01	0.43
1:B:1016:THR:CG2	1:B:1017:SER:N	2.81	0.43
1:B:360:ARG:CZ	1:B:570:ARG:HG2	2.49	0.43
2:C:298:LYS:NZ	2:C:303:ASN:OD1	2.33	0.43
1:E:288:ASN:OD1	1:E:289:PRO:HD2	2.19	0.43
1:E:943:ARG:HD3	1:E:971:ASP:OD1	2.19	0.43
1:H:525:TYR:CE2	1:H:544:SER:HB3	2.54	0.43
2:I:300:VAL:CG2	2:I:301:GLU:N	2.81	0.43
1:B:1039:TYR:O	9:B:1095:ORN:N	2.49	0.43
2:C:285:LYS:HG3	2:C:314:PHE:CD2	2.51	0.43
2:C:286:MET:HE1	2:C:312:HIS:ND1	2.33	0.43
2:C:290:HIS:HB2	2:C:312:HIS:CD2	2.54	0.43
2:F:293:GLY:HA2	2:F:309:ALA:HA	2.01	0.43
2:F:326:ARG:O	2:F:340:ILE:HA	2.19	0.43
1:K:526:LYS:HB2	1:K:543:TYR:CZ	2.54	0.43
1:K:945:LEU:HB3	1:K:1012:ILE:HG12	2.01	0.43
2:L:176:THR:OG1	2:L:179:GLY:N	2.46	0.43
1:B:862:LYS:O	1:B:866:ARG:HG3	2.19	0.43
1:H:966:GLN:HG2	1:H:1053:LEU:HD13	2.01	0.43
1:H:671:ALA:HB3	1:H:843:PRO:CG	2.48	0.43
1:H:946:LEU:N	1:H:946:LEU:CD1	2.80	0.43
1:B:1020:ARG:HA	1:B:1020:ARG:HD3	1.54	0.42
1:B:645:THR:HB	1:B:646:PRO:HD3	2.01	0.42
2:F:264:PRO:HB3	2:F:373:LEU:HB3	2.00	0.42
2:F:317:ASP:HB3	2:F:320:THR:HG23	2.01	0.42
1:H:466:GLU:O	1:H:470:ARG:HG2	2.19	0.42
1:H:804:ILE:HG22	1:H:805:GLN:N	2.33	0.42
1:H:824:LEU:HG	1:H:864:ALA:HB2	2.00	0.42
1:E:989:LEU:HD23	1:H:978:ILE:HG12	2.01	0.42
1:K:439:ALA:O	1:K:443:ARG:HG3	2.19	0.42
1:K:639:VAL:HG21	1:K:650:ALA:CB	2.49	0.42
2:L:135:GLY:O	2:L:138:PRO:HD3	2.19	0.42
1:B:906:LEU:HD11	9:B:1095:ORN:CD	2.41	0.42
1:E:22:ALA:HB1	1:E:23:CYS:H	1.56	0.42
1:E:850:PRO:O	1:E:853:SER:HB2	2.19	0.42
2:F:318:GLU:HB2	2:F:321:LEU:HD22	2.01	0.42
2:L:226:GLU:HA	2:L:229:LEU:HD12	2.01	0.42
2:L:364:ALA:N	2:L:365:PRO:CD	2.81	0.42
2:L:83:ARG:O	2:L:112:ASP:HA	2.19	0.42
1:B:299:MET:HG3	1:B:299:MET:O	2.18	0.42
1:B:478:VAL:CG2	1:B:482:GLY:HA3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:978:ILE:HG22	1:B:979:VAL:N	2.34	0.42
1:E:733:LEU:HD22	1:E:737:PHE:HD2	1.85	0.42
1:H:1013:ILE:O	1:H:1013:ILE:HG23	2.19	0.42
5:H:1082:PO4:O3	7:H:1090:GLN:HG2	2.18	0.42
1:H:151:MET:HE3	1:H:151:MET:HB2	1.88	0.42
1:H:165:CYS:C	1:H:166:ILE:HD12	2.39	0.42
1:H:824:LEU:HG	1:H:864:ALA:CB	2.49	0.42
1:K:517:ASP:HB2	11:K:1585:HOH:O	2.19	0.42
1:K:7:LYS:HB2	1:K:83:ASP:OD2	2.18	0.42
2:F:113:ILE:O	2:F:115:THR:N	2.53	0.42
1:H:213:LYS:O	1:H:286:ALA:HA	2.19	0.42
2:I:380:THR:HG22	2:I:380:THR:O	2.18	0.42
2:I:58:PRO:HA	2:I:83:ARG:HB3	2.00	0.42
2:L:7:LEU:HB3	2:L:15:PHE:HB2	2.01	0.42
2:C:295:HIS:CE1	2:C:333:PHE:HD2	2.37	0.42
2:C:48:TYR:HA	2:C:51:GLN:NE2	2.35	0.42
1:E:480:ILE:HG23	1:E:481:THR:N	2.34	0.42
1:E:531:CYS:O	1:E:532:ALA:HB3	2.18	0.42
2:F:370:PHE:O	2:F:374:ILE:HG13	2.19	0.42
10:H:1095:NET:H62	10:H:1095:NET:H72	1.76	0.42
1:H:805:GLN:HA	1:H:808:MET:CE	2.49	0.42
1:H:890:LYS:HG2	1:H:891:GLU:N	2.33	0.42
1:H:549:GLU:OE1	2:I:117:LYS:HA	2.19	0.42
2:I:332:LEU:HA	2:I:332:LEU:HD12	1.68	0.42
2:I:45:ASP:HB3	2:I:48:TYR:HD2	1.84	0.42
1:K:129:ARG:HB2	1:K:147:ILE:HD12	2.01	0.42
1:K:864:ALA:O	1:K:868:MET:HG3	2.19	0.42
2:L:322:PRO:CB	2:L:324:ASN:HD21	2.31	0.42
1:B:312:LYS:HE2	1:B:607:THR:O	2.20	0.42
1:E:901:GLY:HA2	1:E:1030:ARG:NH1	2.34	0.42
2:F:332:LEU:HA	2:F:332:LEU:HD12	1.64	0.42
2:F:351:GLN:HG3	2:F:351:GLN:O	2.20	0.42
2:F:78:GLN:NE2	2:F:78:GLN:HA	2.34	0.42
1:H:733:LEU:HD23	1:H:733:LEU:HA	1.84	0.42
2:I:45:ASP:HB3	2:I:48:TYR:CD2	2.54	0.42
1:K:134:ALA:HB1	1:K:273:GLU:CG	2.49	0.42
2:C:158:LEU:HA	2:C:158:LEU:HD23	1.90	0.42
2:C:198:ASP:O	2:C:221:ALA:HB2	2.19	0.42
2:C:261:THR:CG2	2:C:262:ASP:N	2.78	0.42
2:C:363:ALA:O	2:C:366:LEU:HB2	2.19	0.42
1:E:901:GLY:O	1:E:1026:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:ASN:ND2	11:E:1539:HOH:O	2.44	0.42
1:E:39:GLU:CG	1:E:324:LYS:HE2	2.50	0.42
1:E:58:GLU:OE1	1:E:58:GLU:N	2.37	0.42
1:E:738:GLN:HB3	1:E:739:THR:H	1.60	0.42
1:E:803:GLU:HB3	11:E:1972:HOH:O	2.18	0.42
2:F:269:CYS:HB2	11:F:2274:HOH:O	2.18	0.42
2:F:7:LEU:HB3	2:F:15:PHE:HB2	2.00	0.42
1:H:223:LYS:HE2	1:H:328:GLY:O	2.20	0.42
1:H:831:VAL:HA	1:H:835:GLU:O	2.19	0.42
2:I:214:CYS:HB2	2:I:216:LEU:HD21	2.02	0.42
2:I:222:GLN:H	2:I:222:GLN:HE21	1.66	0.42
1:K:31:GLN:OE1	1:K:319:ALA:HB3	2.19	0.42
1:K:990:VAL:HG23	1:K:1003[A]:ARG:NE	2.35	0.42
2:L:324:ASN:C	2:L:343:THR:HG23	2.40	0.42
1:B:408:PHE:O	1:B:443:ARG:NH2	2.49	0.42
1:E:1036:LYS:HE2	11:E:1447:HOH:O	2.19	0.42
2:F:249:ASP:OD1	2:F:249:ASP:N	2.50	0.42
2:F:28:GLY:HA3	2:F:50:ARG:O	2.20	0.42
1:H:410:PRO:HD3	1:H:500:ARG:NH2	2.35	0.42
1:H:512:ILE:O	1:H:515:LEU:HB3	2.20	0.42
2:I:20:ILE:HG13	2:I:109:ALA:HB3	2.01	0.42
2:I:121:LEU:C	2:I:121:LEU:HD12	2.38	0.42
1:K:150:THR:O	1:K:153:GLU:HB2	2.20	0.42
1:K:701:VAL:HG23	1:K:701:VAL:H	1.60	0.42
1:K:69:HIS:O	1:K:73:VAL:HG23	2.19	0.42
1:K:805:GLN:HA	1:K:808:MET:HE2	2.01	0.42
1:B:1050:ALA:HA	1:B:1053:LEU:HD12	2.02	0.42
1:B:348:GLU:O	2:C:294:ASN:HB2	2.20	0.42
2:C:163:THR:HB	2:C:221:ALA:HB2	2.01	0.42
2:C:199:PHE:O	2:C:241:GLY:HA3	2.20	0.42
1:E:815:LEU:HD11	1:E:838:LEU:HD11	2.01	0.42
1:E:884:PRO:HA	1:E:885:PRO:HD3	1.80	0.42
1:E:940:LYS:HE3	11:E:2085:HOH:O	2.19	0.42
2:F:170:TRP:C	2:F:171:THR:HG23	2.39	0.42
2:F:170:TRP:HD1	2:F:210:VAL:HG21	1.85	0.42
2:F:300:VAL:CG2	2:F:301:GLU:N	2.81	0.42
11:H:1657:HOH:O	2:I:112:ASP:HB3	2.19	0.42
2:I:350:PHE:HB2	2:I:366:LEU:HD23	2.01	0.42
2:I:55:LEU:HD13	2:I:60:ILE:HD12	2.02	0.42
1:K:1019:ARG:HA	1:K:1019:ARG:HD2	1.50	0.42
1:K:201:LYS:NZ	1:K:201:LYS:HB3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:490:GLN:HG2	1:K:490:GLN:O	2.20	0.42
1:K:802:GLN:HB2	1:K:802:GLN:HE21	1.56	0.42
2:L:139:ASP:HB3	2:L:142:LEU:HB3	2.02	0.42
1:B:946:LEU:HG	1:B:1013:ILE:CG2	2.49	0.42
2:C:210:VAL:HA	2:C:214:CYS:O	2.19	0.42
1:E:140:LEU:HA	1:E:140:LEU:HD23	1.85	0.42
1:E:980:LEU:HA	1:E:980:LEU:HD23	1.86	0.42
1:H:137:LYS:HE3	1:H:273:GLU:OE2	2.19	0.42
1:H:424:ARG:HG2	1:H:424:ARG:O	2.19	0.42
1:H:804:ILE:HG12	1:H:834:ASN:ND2	2.35	0.42
2:I:145:GLU:O	2:I:149:ALA:N	2.47	0.42
1:B:187:PHE:HZ	1:B:205:ILE:HD13	1.84	0.41
1:B:0:MET:H2	1:B:223:LYS:NZ	2.16	0.41
1:B:418[B]:GLU:OE1	1:B:421:THR:HB	2.19	0.41
1:B:969:GLU:O	1:B:970:LEU:HD23	2.20	0.41
1:E:1023:GLU:HG2	1:E:1023:GLU:H	1.67	0.41
1:E:703:LYS:HD2	1:E:703:LYS:HA	1.37	0.41
1:E:641:TYR:OH	1:E:864:ALA:HB3	2.19	0.41
2:F:13:THR:HG22	2:F:15:PHE:CE2	2.55	0.41
2:F:365:PRO:O	2:F:368[A]:ASP:HB2	2.20	0.41
1:H:297:ILE:HG13	11:H:1376:HOH:O	2.19	0.41
1:H:335[B]:MET:HB3	1:H:341:GLY:HA2	2.02	0.41
1:H:441:ALA:HB1	1:H:446:LEU:HD23	2.02	0.41
1:K:330:THR:OG1	1:K:333:GLU:HG3	2.20	0.41
1:K:65:ILE:CG2	1:K:917:MET:HB3	2.49	0.41
1:B:0:MET:HB3	1:B:1:PRO:CD	2.50	0.41
1:B:852:VAL:O	1:B:856:THR:HG23	2.19	0.41
2:C:325:LEU:HD23	2:C:342:ARG:HG2	2.02	0.41
1:E:733:LEU:HD23	1:E:733:LEU:HA	1.77	0.41
2:F:350:PHE:CG	2:F:366:LEU:HD21	2.55	0.41
2:F:9:LEU:O	2:F:12:GLY:N	2.50	0.41
1:H:894:LEU:HA	1:H:895:PRO:HD3	1.92	0.41
1:H:378:LYS:HB3	1:H:899:PHE:HE1	1.85	0.41
1:K:903:ASP:OD1	1:K:904:PRO:HD2	2.20	0.41
1:B:418[B]:GLU:HG2	1:H:421:THR:HG21	2.02	0.41
1:B:866:ARG:HH11	1:B:866:ARG:HD2	1.69	0.41
1:E:357:LYS:HE3	11:E:1555:HOH:O	2.20	0.41
1:E:410:PRO:HG2	11:E:1655:HOH:O	2.20	0.41
1:E:668:ILE:O	1:E:672:GLU:HG2	2.20	0.41
1:E:710:PRO:HG2	1:E:754:PHE:HD2	1.85	0.41
1:E:990:VAL:HB	1:E:1003:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:354:PRO:HB3	2:F:363:ALA:O	2.20	0.41
1:H:645:THR:CB	1:H:646:PRO:HD3	2.50	0.41
1:H:709:TYR:HB3	1:H:710:PRO:HA	2.01	0.41
2:I:298:LYS:HB2	2:I:332:LEU:HD11	2.02	0.41
1:K:733:LEU:HA	1:K:733:LEU:HD23	1.73	0.41
1:K:894:LEU:HA	1:K:895:PRO:HD3	1.75	0.41
1:B:234:GLU:HB2	1:B:252:ALA:HA	2.01	0.41
1:B:270:VAL:HG12	1:B:299:MET:CE	2.50	0.41
1:B:526:LYS:HB2	1:B:543:TYR:CZ	2.55	0.41
1:B:6:ILE:HD13	1:B:6:ILE:HG21	1.78	0.41
1:E:707:ILE:HG22	1:E:711:LEU:HD21	2.03	0.41
2:F:212:ARG:HB3	2:F:371:ILE:HD12	2.01	0.41
10:H:1095:NET:H31	10:H:1095:NET:H63	1.92	0.41
1:H:416:ASP:HB3	1:H:419:ALA:HB2	2.02	0.41
1:H:633:LYS:N	1:H:634:PRO:CD	2.83	0.41
1:H:75:LYS:HA	1:H:75:LYS:HD2	1.73	0.41
1:K:104:GLN:NE2	1:K:104:GLN:HA	2.36	0.41
1:K:213:LYS:O	1:K:286:ALA:HA	2.21	0.41
1:K:23:CYS:HB3	1:K:575:ILE:HD12	2.01	0.41
1:B:1027:VAL:O	1:B:1031:SER:HB2	2.20	0.41
2:C:150:PHE:HA	2:C:151:PRO:HD3	1.90	0.41
2:C:222:GLN:HA	2:C:250:TYR:HD2	1.86	0.41
2:C:344:ASP:N	2:C:344:ASP:OD1	2.46	0.41
2:C:355:GLU:O	2:C:356:ALA:HB3	2.20	0.41
1:E:16:PRO:HG3	1:E:916:VAL:HG13	2.03	0.41
2:F:142:LEU:O	2:F:145:GLU:HB3	2.21	0.41
2:F:251:ALA:O	2:F:255:ILE:HD12	2.20	0.41
2:I:366:LEU:HD12	2:I:366:LEU:N	2.35	0.41
1:K:105:GLY:HA2	11:K:1247:HOH:O	2.21	0.41
1:K:239:MET:HE3	1:K:239:MET:HB3	1.95	0.41
1:K:645:THR:HB	1:K:646:PRO:HD3	2.03	0.41
1:K:810[A]:GLN:HB3	1:K:814:LYS:NZ	2.35	0.41
1:B:991:ASN:HD21	1:K:974:HIS:HE2	1.66	0.41
1:B:0:MET:CB	1:B:1:PRO:CD	2.98	0.41
1:B:670:ARG:HG2	1:B:676:ARG:NH1	2.36	0.41
2:C:364:ALA:N	2:C:365:PRO:CD	2.83	0.41
2:C:93:ARG:HD3	2:C:93:ARG:HH11	1.72	0.41
1:E:324:LYS:NZ	11:E:2115:HOH:O	2.54	0.41
1:E:480:ILE:HD11	1:E:515:LEU:CD1	2.50	0.41
1:E:711:LEU:HD23	1:E:753:HIS:HA	2.01	0.41
2:F:206:LEU:HA	2:F:216:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:342:ARG:HH21	2:F:345:LYS:HG2	1.84	0.41
1:H:698:GLU:OE2	1:H:698:GLU:HA	2.15	0.41
2:I:123:ARG:O	2:I:287:LYS:HE2	2.20	0.41
2:I:332:LEU:N	2:I:332:LEU:CD1	2.82	0.41
2:L:255:ILE:CG2	2:L:278:ALA:CB	2.99	0.41
2:C:246:ALA:HB3	2:C:247:PRO:HD3	2.01	0.41
2:C:43:LEU:HD21	2:C:80:LEU:HD13	2.03	0.41
1:E:853:SER:HA	1:E:858:VAL:O	2.20	0.41
2:F:25:SER:OG	2:F:133:ILE:HG12	2.21	0.41
1:H:197:LEU:HA	1:H:197:LEU:HD12	1.75	0.41
1:H:228:ILE:HG21	1:H:228:ILE:HD13	1.76	0.41
1:H:502:ALA:HB2	1:H:509:GLU:HA	2.02	0.41
1:H:760:GLU:HG2	1:H:780:HIS:ND1	2.36	0.41
1:K:729:ASP:O	1:K:732:ASP:HB2	2.21	0.41
1:B:694:VAL:HG11	1:B:700:ALA:N	2.36	0.41
1:B:726:ILE:HD13	1:B:754:PHE:CD1	2.56	0.41
1:B:953:LYS:HA	1:B:956:VAL:CG1	2.49	0.41
1:B:961:ALA:O	1:B:965:LYS:HB2	2.21	0.41
2:C:373:LEU:HD23	2:C:373:LEU:HA	1.74	0.41
1:E:125:ALA:HB3	1:E:301:PRO:HG3	2.03	0.41
1:E:343:THR:HB	11:E:1586:HOH:O	2.21	0.41
1:E:804:ILE:HA	1:E:804:ILE:HD13	1.67	0.41
1:H:1:PRO:HB2	1:H:2:LYS:H	1.59	0.41
1:H:517[B]:ASP:OD1	1:H:522:HIS:HE1	2.04	0.41
1:H:810:GLN:HG3	11:H:1702:HOH:O	2.21	0.41
2:I:238:LEU:HB2	2:I:267:GLY:CA	2.51	0.41
1:K:562:MET:HE3	1:K:629:VAL:HG22	2.02	0.41
2:L:192:PHE:O	2:L:215:ARG:HG2	2.21	0.41
2:L:38:GLY:HA3	2:L:358:PRO:CB	2.50	0.41
1:B:630:ARG:HD3	11:B:1570:HOH:O	2.21	0.41
1:B:781:ILE:HD12	1:B:781:ILE:N	2.36	0.41
1:B:771:MET:HG3	1:B:873:LEU:HD12	2.02	0.41
2:C:30:VAL:HG22	2:C:52:ILE:HB	2.03	0.41
2:C:350:PHE:CG	2:C:366:LEU:HD21	2.56	0.41
1:E:749:VAL:HG12	1:E:751:LEU:HD13	2.03	0.41
2:F:217:THR:O	2:F:217:THR:HG22	2.19	0.41
2:F:334:ASP:OD1	2:F:336:THR:HG23	2.20	0.41
2:I:223:THR:HG22	2:I:224:SER:N	2.35	0.41
2:I:48:TYR:O	2:I:51:GLN:HB2	2.20	0.41
2:I:66:ASN:HA	2:I:95:THR:OG1	2.20	0.41
1:K:630:ARG:HD3	1:K:630:ARG:HH11	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:738:GLN:NE2	1:K:739:THR:CG2	2.84	0.41
1:B:117:ALA:HA	11:B:1239:HOH:O	2.20	0.41
1:B:762:ASP:HB3	1:B:778:MET:HE1	2.02	0.41
1:B:867:VAL:HA	1:B:871:LYS:O	2.21	0.41
2:C:172:GLN:O	2:C:207:ARG:HA	2.20	0.41
2:C:270:LEU:O	2:C:273:GLN:N	2.54	0.41
1:E:420:LEU:HA	1:E:420:LEU:HD12	1.81	0.41
1:E:586:LEU:HD23	1:E:589:ARG:NH2	2.36	0.41
1:H:10:LEU:HA	1:H:44:ILE:O	2.21	0.41
1:H:702:GLU:O	1:H:705:LYS:N	2.54	0.41
1:K:464:GLN:O	1:K:468:LEU:HG	2.20	0.41
1:B:335:MET:HB3	1:B:341:GLY:HA2	2.03	0.40
1:B:678:GLN:C	1:B:681:VAL:HG12	2.40	0.40
1:E:955:ARG:NH2	1:E:1044:ASN:OD1	2.47	0.40
1:E:158:ALA:HB2	1:E:187:PHE:CZ	2.56	0.40
1:E:470:ARG:HG2	1:E:470:ARG:H	1.70	0.40
1:H:515:LEU:HD12	1:H:515:LEU:HA	1.75	0.40
1:H:997:ARG:HG2	1:H:998:PRO:HA	2.02	0.40
2:I:246:ALA:N	2:I:247:PRO:CD	2.84	0.40
2:L:27:VAL:CG1	2:L:150:PHE:HB2	2.51	0.40
10:B:1096:NET:H31	10:B:1096:NET:H63	1.82	0.40
1:B:658:VAL:HG13	1:B:659:PRO:HD2	2.02	0.40
1:B:762:ASP:HB3	1:B:778:MET:CE	2.50	0.40
2:C:190:LEU:HD23	2:C:190:LEU:HA	1.93	0.40
2:C:212:ARG:NH1	2:C:212:ARG:CG	2.83	0.40
1:E:1071:ILE:HG22	1:E:1072:LYS:HD2	2.03	0.40
1:E:969:GLU:HG2	11:E:2042:HOH:O	2.21	0.40
2:F:259:LEU:O	2:F:345:LYS:HE3	2.21	0.40
2:I:23:THR:HG23	2:I:134:ALA:O	2.21	0.40
2:I:376:GLN:HB3	2:I:376:GLN:HE21	1.60	0.40
1:K:644:GLN:HE21	1:K:648:LYS:HZ3	1.67	0.40
1:K:673:ASP:O	1:K:677:PHE:HB3	2.22	0.40
1:K:780:HIS:CE1	1:K:788:SER:HB3	2.53	0.40
2:L:6:LEU:HD22	2:L:8:VAL:HG23	2.03	0.40
1:B:187:PHE:CZ	1:B:205:ILE:HD13	2.56	0.40
2:C:82:ILE:O	2:C:111:ALA:HA	2.20	0.40
1:E:1016:THR:HG21	1:E:1022:ILE:HA	2.04	0.40
1:E:707:ILE:CG2	1:E:711:LEU:CD2	2.99	0.40
2:F:261:THR:CG2	2:F:262:ASP:N	2.84	0.40
1:H:166:ILE:O	1:H:205:ILE:HA	2.20	0.40
1:H:766:ILE:HA	1:H:823:GLY:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:900:PRO:HD2	6:H:1085:CL:CL	2.59	0.40
2:I:215:ARG:CG	2:I:215:ARG:NH1	2.80	0.40
1:K:1001:GLN:HG3	11:K:1783:HOH:O	2.21	0.40
1:K:810[A]:GLN:HE21	1:K:814:LYS:HZ1	1.60	0.40
1:K:949:ARG:NH2	11:K:2034:HOH:O	2.30	0.40
2:L:218:ILE:N	2:L:218:ILE:CD1	2.81	0.40
1:B:955:ARG:HB3	1:B:1043:LEU:CD2	2.51	0.40
2:C:326:ARG:O	2:C:340:ILE:HA	2.21	0.40
1:E:164:PRO:HA	1:E:181:ALA:O	2.21	0.40
1:E:221:ARG:CZ	1:E:272:ARG:HG2	2.51	0.40
1:E:991:ASN:ND2	1:H:974:HIS:NE2	2.69	0.40
1:H:443:ARG:HD2	1:H:443:ARG:HH11	1.53	0.40
1:H:830:ALA:HB2	1:H:839:ILE:HD11	2.02	0.40
2:I:63:VAL:O	2:I:94:ASN:HB2	2.21	0.40
1:K:714:ARG:HB2	1:K:750:LEU:HB2	2.02	0.40
1:K:74:ARG:CG	1:K:74:ARG:NH1	2.82	0.40
1:B:369:ALA:HA	6:B:1086:CL:CL	2.58	0.40
1:B:694:VAL:HA	1:B:699:MET:HE3	2.03	0.40
1:B:734:ARG:O	1:B:738:GLN:N	2.40	0.40
2:C:152:GLY:O	2:C:156:MET:HE3	2.21	0.40
2:C:228:VAL:CG1	2:C:258:PHE:CE1	3.05	0.40
2:C:191:PRO:O	2:C:378:ARG:NH1	2.55	0.40
1:E:600:CYS:HA	1:E:617:PHE:CE1	2.56	0.40
1:E:684:LEU:HD23	1:E:684:LEU:HA	1.84	0.40
2:F:273:GLN:HE22	2:F:314:PHE:HB2	1.86	0.40
1:H:964:LEU:HA	1:H:964:LEU:HD23	1.91	0.40
1:H:981:GLY:HA2	1:H:985:ILE:O	2.22	0.40
1:K:137:LYS:HE3	1:K:273:GLU:OE2	2.22	0.40
1:K:819:LEU:O	1:K:820:GLN:HB2	2.22	0.40

All (1) 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)
11:B:2056:HOH:O	11:E:2344:HOH:O[4_455]	1.95	0.25

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	B	1059/1073 (99%)	1008 (95%)	48 (4%)	3 (0%)	43	43
1	E	1064/1073 (99%)	1008 (95%)	54 (5%)	2 (0%)	49	51
1	H	1057/1073 (98%)	1016 (96%)	38 (4%)	3 (0%)	43	43
1	K	1059/1073 (99%)	1012 (96%)	43 (4%)	4 (0%)	36	34
2	C	377/382 (99%)	356 (94%)	19 (5%)	2 (0%)	31	27
2	F	379/382 (99%)	359 (95%)	19 (5%)	1 (0%)	43	43
2	I	377/382 (99%)	354 (94%)	21 (6%)	2 (0%)	31	27
2	L	377/382 (99%)	362 (96%)	15 (4%)	0	100	100
All	All	5749/5820 (99%)	5475 (95%)	257 (4%)	17 (0%)	43	43

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	1	PRO
2	C	311	ASN
1	H	974	HIS
1	K	737	PHE
1	K	974	HIS
1	E	739	THR
1	K	1	PRO
1	B	974	HIS
1	E	1	PRO
2	F	346	PRO
2	I	239	SER
1	B	701	VAL
2	I	247	PRO
1	K	367	ALA
1	B	697	ILE
2	C	247	PRO
1	H	843	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	B	873/878 (99%)	805 (92%)	68 (8%)	14	10
1	E	878/878 (100%)	828 (94%)	50 (6%)	23	20
1	H	871/878 (99%)	813 (93%)	58 (7%)	18	15
1	K	872/878 (99%)	809 (93%)	63 (7%)	16	12
2	C	308/310 (99%)	277 (90%)	31 (10%)	8	5
2	F	309/310 (100%)	281 (91%)	28 (9%)	10	7
2	I	308/310 (99%)	275 (89%)	33 (11%)	7	4
2	L	308/310 (99%)	284 (92%)	24 (8%)	14	10
All	All	4727/4752 (100%)	4372 (92%)	355 (8%)	15	11

All (355) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	0	MET
1	B	2	LYS
1	B	54	MET
1	B	100	GLU
1	B	109	GLU
1	B	137	LYS
1	B	144	ARG
1	B	173	MET
1	B	184	ARG
1	B	185	GLU
1	B	223	LYS
1	B	235	ASN
1	B	277	GLU
1	B	282	ASN
1	B	296	VAL
1	B	312	LYS
1	B	325	LEU
1	B	362	ASN
1	B	383	VAL

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Mol	Chain	Res	Type
1	B	410	PRO
1	B	411	LYS
1	B	412	VAL
1	B	425	ARG
1	B	511	GLU
1	B	520[A]	ASP
1	B	520[B]	ASP
1	B	521	LEU
1	B	541	TYR
1	B	556	THR
1	B	559	GLU
1	B	570	ARG
1	B	651	ARG
1	B	674	ARG
1	B	685	LYS
1	B	687	LYS
1	B	688	GLN
1	B	698	GLU
1	B	707	ILE
1	B	734	ARG
1	B	750	LEU
1	B	752	ASP
1	B	762	ASP
1	B	770	GLU
1	B	783	GLN
1	B	799	THR
1	B	803	GLU
1	B	804	ILE
1	B	854	LYS
1	B	880	LYS
1	B	890	LYS
1	B	911[A]	ARG
1	B	911[B]	ARG
1	B	939	LYS
1	B	940	LYS
1	B	948	VAL
1	B	949	ARG
1	B	950	GLU
1	B	955	ARG
1	B	965	LYS
1	B	966[A]	GLN
1	B	966[B]	GLN

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Mol	Chain	Res	Type
1	B	1001	GLN
1	B	1017	SER
1	B	1019	ARG
1	B	1020	ARG
1	B	1060	LYS
1	B	1062	ILE
1	B	1072	LYS
2	C	2	ILE
2	C	18	ARG
2	C	74	GLN
2	C	87	LEU
2	C	104	ARG
2	C	106	ASN
2	C	154	ASN
2	C	160	LYS
2	C	166	GLU
2	C	169	SER
2	C	175	TRP
2	C	183	GLN
2	C	187	GLU
2	C	204	ASN
2	C	215	ARG
2	C	239	SER
2	C	252	ILE
2	C	259	LEU
2	C	285	LYS
2	C	306	MET
2	C	318	GLU
2	C	321	LEU
2	C	324	ASN
2	C	326	ARG
2	C	330	LYS
2	C	331	SER
2	C	332	LEU
2	C	357	SER
2	C	371	ILE
2	C	376	GLN
2	C	379	LYS
1	E	0	MET
1	E	173	MET
1	E	201	LYS
1	E	235	ASN

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Mol	Chain	Res	Type
1	E	274	ILE
1	E	298	GLU
1	E	312	LYS
1	E	324	LYS
1	E	332	ASP
1	E	362	ASN
1	E	413	SER
1	E	415	ASP
1	E	420	LEU
1	E	425	ARG
1	E	486	ASP
1	E	503	LYS
1	E	557	ASP
1	E	558	ARG
1	E	570	ARG
1	E	644	GLN
1	E	651	ARG
1	E	674	ARG
1	E	679	HIS
1	E	682	GLU
1	E	683	ARG
1	E	687	LYS
1	E	698	GLU
1	E	703	LYS
1	E	732	ASP
1	E	733	LEU
1	E	734	ARG
1	E	752	ASP
1	E	762	ASP
1	E	783	GLN
1	E	804	ILE
1	E	854	LYS
1	E	890	LYS
1	E	911	ARG
1	E	939	LYS
1	E	949	ARG
1	E	955	ARG
1	E	1017	SER
1	E	1019	ARG
1	E	1020[A]	ARG
1	E	1020[B]	ARG
1	E	1023	GLU

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Mol	Chain	Res	Type
1	E	1026	ARG
1	E	1060	LYS
1	E	1071	ILE
1	E	1072	LYS
2	F	18	ARG
2	F	25	SER
2	F	41	GLU
2	F	70	GLU
2	F	73	SER
2	F	106	ASN
2	F	131	CYS
2	F	136	ASP
2	F	154	ASN
2	F	161	GLU
2	F	174	SER
2	F	175	TRP
2	F	188	ASP
2	F	218	ILE
2	F	239	SER
2	F	252	ILE
2	F	257	LYS
2	F	260	GLU
2	F	269	CYS
2	F	301	GLU
2	F	306	MET
2	F	321	LEU
2	F	324	ASN
2	F	326	ARG
2	F	332	LEU
2	F	344	ASP
2	F	378	ARG
2	F	380	THR
1	H	0	MET
1	H	7	LYS
1	H	45	LEU
1	H	54	MET
1	H	89	MET
1	H	100	GLU
1	H	173	MET
1	H	235	ASN
1	H	274	ILE
1	H	277	GLU

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Mol	Chain	Res	Type
1	H	332	ASP
1	H	357	LYS
1	H	362	ASN
1	H	413	SER
1	H	421	THR
1	H	446	LEU
1	H	514	LYS
1	H	541	TYR
1	H	548	GLU
1	H	570	ARG
1	H	644	GLN
1	H	674	ARG
1	H	675	GLU
1	H	677	PHE
1	H	679	HIS
1	H	683	ARG
1	H	698	GLU
1	H	702	GLU
1	H	711	LEU
1	H	727	VAL
1	H	733	LEU
1	H	734	ARG
1	H	737	PHE
1	H	738	GLN
1	H	750	LEU
1	H	752	ASP
1	H	762	ASP
1	H	771	MET
1	H	783	GLN
1	H	802	GLN
1	H	804	ILE
1	H	834	ASN
1	H	840	GLU
1	H	854	LYS
1	H	871	LYS
1	H	890	LYS
1	H	894	LEU
1	H	911	ARG
1	H	939	LYS
1	H	949	ARG
1	H	955	ARG
1	H	1001	GLN

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Mol	Chain	Res	Type
1	H	1017	SER
1	H	1019	ARG
1	H	1020	ARG
1	H	1030	ARG
1	H	1060	LYS
1	H	1072	LYS
2	I	4	SER
2	I	6	LEU
2	I	18	ARG
2	I	35	SER
2	I	49	SER
2	I	50	ARG
2	I	73	SER
2	I	78	GLN
2	I	97	ASP
2	I	113	ILE
2	I	131	CYS
2	I	136	ASP
2	I	145	GLU
2	I	166	GLU
2	I	186	LYS
2	I	188	ASP
2	I	215	ARG
2	I	218	ILE
2	I	222	GLN
2	I	257	LYS
2	I	262	ASP
2	I	263	ILE
2	I	284	VAL
2	I	301	GLU
2	I	306	MET
2	I	318	GLU
2	I	330	LYS
2	I	331	SER
2	I	332	LEU
2	I	333	PHE
2	I	340	ILE
2	I	379	LYS
2	I	380	THR
1	K	2	LYS
1	K	45	LEU
1	K	54	MET

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Mol	Chain	Res	Type
1	K	102	GLU
1	K	136	LYS
1	K	147	ILE
1	K	173	MET
1	K	184	ARG
1	K	201	LYS
1	K	235	ASN
1	K	274	ILE
1	K	282	ASN
1	K	312	LYS
1	K	316	PHE
1	K	362	ASN
1	K	364	GLU
1	K	413	SER
1	K	421	THR
1	K	427	LEU
1	K	480	ILE
1	K	481	THR
1	K	521	LEU
1	K	541	TYR
1	K	558	ARG
1	K	570	ARG
1	K	651	ARG
1	K	672	GLU
1	K	678	GLN
1	K	682	GLU
1	K	683	ARG
1	K	691	ASN
1	K	694	VAL
1	K	698	GLU
1	K	706	GLU
1	K	732	ASP
1	K	733	LEU
1	K	737	PHE
1	K	738	GLN
1	K	752	ASP
1	K	762	ASP
1	K	783	GLN
1	K	804	ILE
1	K	810[A]	GLN
1	K	810[B]	GLN
1	K	813	GLN

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Mol	Chain	Res	Type
1	K	838	LEU
1	K	854	LYS
1	K	890	LYS
1	K	911	ARG
1	K	939	LYS
1	K	949	ARG
1	K	950	GLU
1	K	955	ARG
1	K	997	ARG
1	K	1000	ILE
1	K	1001	GLN
1	K	1013	ILE
1	K	1017	SER
1	K	1019	ARG
1	K	1020	ARG
1	K	1026	ARG
1	K	1060	LYS
1	K	1072	LYS
2	L	4	SER
2	L	6	LEU
2	L	25	SER
2	L	50	ARG
2	L	136	ASP
2	L	153	LEU
2	L	169	SER
2	L	175	TRP
2	L	188	ASP
2	L	190	LEU
2	L	218	ILE
2	L	222	GLN
2	L	226	GLU
2	L	239	SER
2	L	257	LYS
2	L	321	LEU
2	L	324	ASN
2	L	326	ARG
2	L	332	LEU
2	L	357	SER
2	L	372	GLU
2	L	375	GLU
2	L	376	GLN
2	L	379	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	104	GLN
1	B	265	ASN
1	B	678	GLN
1	B	688	GLN
1	B	783	GLN
1	B	802	GLN
1	B	811	GLN
1	B	813	GLN
1	B	834	ASN
1	B	935	ASN
1	B	941	HIS
1	B	986	ASN
1	B	991	ASN
1	B	999	HIS
1	B	1001	GLN
1	B	1034	GLN
1	B	1054	ASN
1	B	1070	GLN
2	C	51	GLN
2	C	74	GLN
2	C	154	ASN
2	C	204	ASN
2	C	291	HIS
2	C	324	ASN
2	C	329	HIS
1	E	224	ASN
1	E	265	ASN
1	E	456	ASN
1	E	678	GLN
1	E	783	GLN
1	E	802	GLN
1	E	813	GLN
1	E	834	ASN
1	E	935	ASN
1	E	941	HIS
1	E	986	ASN
1	E	991	ASN
1	E	999	HIS
1	E	1034	GLN
1	E	1070	GLN
2	F	78	GLN

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Mol	Chain	Res	Type
2	F	154	ASN
2	F	324	ASN
2	F	351	GLN
1	H	104	GLN
1	H	265	ASN
1	H	688	GLN
1	H	738	GLN
1	H	783	GLN
1	H	802	GLN
1	H	811	GLN
1	H	813	GLN
1	H	834	ASN
1	H	935	ASN
1	H	986	ASN
1	H	991	ASN
1	H	999	HIS
1	H	1001	GLN
1	H	1034	GLN
1	H	1054	ASN
1	H	1070	GLN
2	I	105	HIS
2	I	154	ASN
2	I	222	GLN
2	I	295	HIS
2	I	376	GLN
1	K	104	GLN
1	K	265	ASN
1	K	456	ASN
1	K	644	GLN
1	K	678	GLN
1	K	688	GLN
1	K	738	GLN
1	K	783	GLN
1	K	802	GLN
1	K	941	HIS
1	K	966	GLN
1	K	986	ASN
1	K	991	ASN
1	K	999	HIS
1	K	1001	GLN
1	K	1034	GLN
1	K	1054	ASN

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Mol	Chain	Res	Type
1	K	1070	GLN
2	L	183	GLN
2	L	324	ASN
2	L	351	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 107 ligands modelled in this entry, 74 are monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PO4	B	1078	3,4	4,4,4	1.97	2 (50%)	6,6,6	0.93	0
5	PO4	B	1082	-	4,4,4	2.35	2 (50%)	6,6,6	0.83	0
8	ADP	B	1093	3	24,29,29	1.22	2 (8%)	25,45,45	1.32	2 (8%)
8	ADP	B	1094	3	24,29,29	1.34	2 (8%)	25,45,45	1.28	3 (12%)
9	ORN	B	1095	-	4,8,8	0.83	0	3,9,9	0.69	0
10	NET	B	1096	-	8,8,8	0.65	0	10,10,10	0.68	0
5	PO4	E	1078	3,4	4,4,4	2.15	2 (50%)	6,6,6	0.81	0
5	PO4	E	1082	-	4,4,4	2.10	2 (50%)	6,6,6	1.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	ADP	E	1095	3	24,29,29	1.27	2 (8%)	25,45,45	1.15	2 (8%)
8	ADP	E	1096	3	24,29,29	1.42	5 (20%)	25,45,45	1.18	3 (12%)
9	ORN	E	1097	-	4,8,8	0.49	0	3,9,9	1.73	1 (33%)
10	NET	E	1098	-	8,8,8	0.74	0	10,10,10	0.40	0
5	PO4	H	1078	3,4	4,4,4	2.18	3 (75%)	6,6,6	0.61	0
5	PO4	H	1082	-	4,4,4	1.95	1 (25%)	6,6,6	0.98	0
8	ADP	H	1092	3	24,29,29	1.11	2 (8%)	25,45,45	1.44	1 (4%)
8	ADP	H	1093	3	24,29,29	1.38	4 (16%)	25,45,45	1.35	5 (20%)
9	ORN	H	1094	-	4,8,8	0.49	0	3,9,9	0.83	0
10	NET	H	1095	-	8,8,8	0.69	0	10,10,10	0.59	0
5	PO4	K	1078	3,4	4,4,4	1.93	2 (50%)	6,6,6	1.30	1 (16%)
5	PO4	K	1082	-	4,4,4	1.96	1 (25%)	6,6,6	0.65	0
5	PO4	K	1092	-	4,4,4	0.53	0	6,6,6	1.33	1 (16%)
8	ADP	K	1095	3	24,29,29	1.21	4 (16%)	25,45,45	1.26	2 (8%)
8	ADP	K	1096	3	24,29,29	1.39	4 (16%)	25,45,45	1.22	1 (4%)
9	ORN	K	1097	-	4,8,8	0.67	0	3,9,9	0.44	0
10	NET	K	1098	-	8,8,8	0.58	0	10,10,10	0.88	1 (10%)

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
8	ADP	B	1093	3	-	1/12/32/32	0/3/3/3
8	ADP	B	1094	3	-	4/12/32/32	0/3/3/3
9	ORN	B	1095	-	-	4/4/8/8	-
10	NET	B	1096	-	-	0/12/12/12	-
8	ADP	E	1095	3	-	1/12/32/32	0/3/3/3
8	ADP	E	1096	3	-	1/12/32/32	0/3/3/3
9	ORN	E	1097	-	-	3/4/8/8	-
10	NET	E	1098	-	-	1/12/12/12	-
8	ADP	H	1092	3	-	1/12/32/32	0/3/3/3
8	ADP	H	1093	3	-	1/12/32/32	0/3/3/3
9	ORN	H	1094	-	-	4/4/8/8	-
10	NET	H	1095	-	-	2/12/12/12	-
8	ADP	K	1095	3	-	1/12/32/32	0/3/3/3
8	ADP	K	1096	3	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ORN	K	1097	-	-	4/4/8/8	-
10	NET	K	1098	-	-	0/12/12/12	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1094	ADP	PB-O3A	3.94	1.66	1.60
8	K	1096	ADP	PB-O3A	3.74	1.65	1.60
8	E	1095	ADP	PB-O3A	3.63	1.65	1.60
5	B	1082	PO4	P-O4	-3.51	1.44	1.54
5	E	1078	PO4	P-O4	-3.44	1.44	1.54
8	E	1096	ADP	O3'-C3'	3.39	1.51	1.43
8	H	1093	ADP	PB-O3A	3.27	1.65	1.60
8	E	1096	ADP	PB-O3A	3.23	1.64	1.60
8	K	1095	ADP	PB-O3A	3.14	1.64	1.60
8	K	1096	ADP	C2-N1	3.11	1.39	1.33
5	H	1082	PO4	P-O4	-2.95	1.45	1.54
8	H	1093	ADP	O4'-C1'	-2.92	1.37	1.41
5	K	1082	PO4	P-O4	-2.90	1.45	1.54
8	E	1096	ADP	O2'-C2'	2.80	1.49	1.43
8	K	1096	ADP	O2'-C2'	2.61	1.49	1.43
5	H	1078	PO4	P-O2	-2.58	1.46	1.54
5	E	1082	PO4	P-O2	-2.55	1.46	1.54
5	E	1082	PO4	P-O4	-2.50	1.47	1.54
5	H	1078	PO4	P-O4	-2.50	1.47	1.54
8	B	1093	ADP	O3'-C3'	2.49	1.48	1.43
5	B	1078	PO4	P-O2	-2.45	1.47	1.54
8	H	1092	ADP	PB-O3A	2.43	1.63	1.60
8	H	1093	ADP	O2'-C2'	2.39	1.48	1.43
8	K	1095	ADP	O3'-C3'	2.37	1.48	1.43
5	K	1078	PO4	P-O2	-2.36	1.47	1.54
5	B	1078	PO4	P-O4	-2.34	1.47	1.54
5	K	1078	PO4	P-O3	-2.34	1.47	1.54
8	E	1096	ADP	C2-N1	2.30	1.38	1.33
5	B	1082	PO4	P-O2	-2.25	1.47	1.54
8	H	1093	ADP	O3'-C3'	2.20	1.48	1.43
8	B	1094	ADP	C2-N1	2.19	1.38	1.33
8	E	1095	ADP	O3'-C3'	2.16	1.48	1.43
8	K	1096	ADP	O4'-C1'	-2.16	1.38	1.41
8	K	1095	ADP	C2-N1	2.14	1.38	1.33
8	E	1096	ADP	O4'-C1'	-2.13	1.38	1.41
8	B	1093	ADP	O2'-C2'	2.11	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1092	ADP	O2'-C2'	2.09	1.47	1.43
8	K	1095	ADP	O4'-C1'	-2.09	1.38	1.41
5	H	1078	PO4	P-O3	-2.08	1.48	1.54
5	E	1078	PO4	P-O2	-2.01	1.48	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1092	ADP	C5-C6-N6	5.12	128.42	120.38
8	K	1096	ADP	C5-C6-N6	4.46	127.38	120.38
8	B	1094	ADP	C5-C6-N6	4.22	127.01	120.38
8	K	1095	ADP	C5-C6-N6	3.49	125.87	120.38
8	B	1093	ADP	C4'-O4'-C1'	3.08	113.04	109.83
8	E	1095	ADP	C5-C6-N6	3.08	125.22	120.38
8	H	1093	ADP	O3'-C3'-C2'	2.97	121.45	111.80
8	E	1096	ADP	C5-C6-N1	-2.75	113.85	120.31
8	H	1093	ADP	O2'-C2'-C3'	2.71	120.58	111.80
9	E	1097	ORN	CG-CB-CA	2.61	122.45	113.36
8	H	1093	ADP	C4-C5-N7	2.60	112.11	109.40
8	B	1093	ADP	C4-C5-N7	2.60	112.11	109.40
8	E	1096	ADP	C5-C6-N6	2.47	124.26	120.38
5	K	1092	PO4	O4-P-O3	2.32	115.45	107.99
8	E	1096	ADP	C2'-C3'-C4'	-2.32	98.16	102.60
8	H	1093	ADP	C5-C6-N6	2.29	123.98	120.38
8	B	1094	ADP	C5-C6-N1	-2.28	114.95	120.31
5	K	1078	PO4	O3-P-O1	-2.22	102.78	110.88
8	K	1095	ADP	O3'-C3'-C2'	2.12	118.66	111.80
8	H	1093	ADP	C5-C6-N1	-2.10	115.36	120.31
8	E	1095	ADP	O2'-C2'-C3'	2.05	118.44	111.80
8	B	1094	ADP	C2'-C3'-C4'	-2.01	98.75	102.60
10	K	1098	NET	C6-C5-N1	-2.01	105.23	114.56

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	H	1094	ORN	N-CA-CB-CG
9	H	1094	ORN	C-CA-CB-CG
9	E	1097	ORN	N-CA-CB-CG
9	E	1097	ORN	C-CA-CB-CG
9	K	1097	ORN	N-CA-CB-CG
9	K	1097	ORN	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
9	B	1095	ORN	N-CA-CB-CG
9	B	1095	ORN	C-CA-CB-CG
9	B	1095	ORN	CA-CB-CG-CD
9	H	1094	ORN	CA-CB-CG-CD
9	E	1097	ORN	NE-CD-CG-CB
10	H	1095	NET	C8-C7-N1-C1
8	B	1094	ADP	PA-O3A-PB-O1B
8	K	1096	ADP	PA-O3A-PB-O1B
9	H	1094	ORN	NE-CD-CG-CB
9	B	1095	ORN	NE-CD-CG-CB
8	H	1093	ADP	C5'-O5'-PA-O3A
8	B	1093	ADP	PB-O3A-PA-O1A
8	H	1092	ADP	PB-O3A-PA-O1A
8	E	1095	ADP	PB-O3A-PA-O1A
8	K	1096	ADP	PB-O3A-PA-O2A
8	K	1095	ADP	PB-O3A-PA-O1A
9	K	1097	ORN	CA-CB-CG-CD
10	H	1095	NET	C8-C7-N1-C5
8	B	1094	ADP	PB-O3A-PA-O2A
8	B	1094	ADP	PA-O3A-PB-O3B
8	K	1096	ADP	PA-O3A-PB-O3B
9	K	1097	ORN	NE-CD-CG-CB
8	B	1094	ADP	PB-O3A-PA-O1A
8	E	1096	ADP	PB-O3A-PA-O2A
8	K	1096	ADP	PB-O3A-PA-O1A
10	E	1098	NET	C8-C7-N1-C3

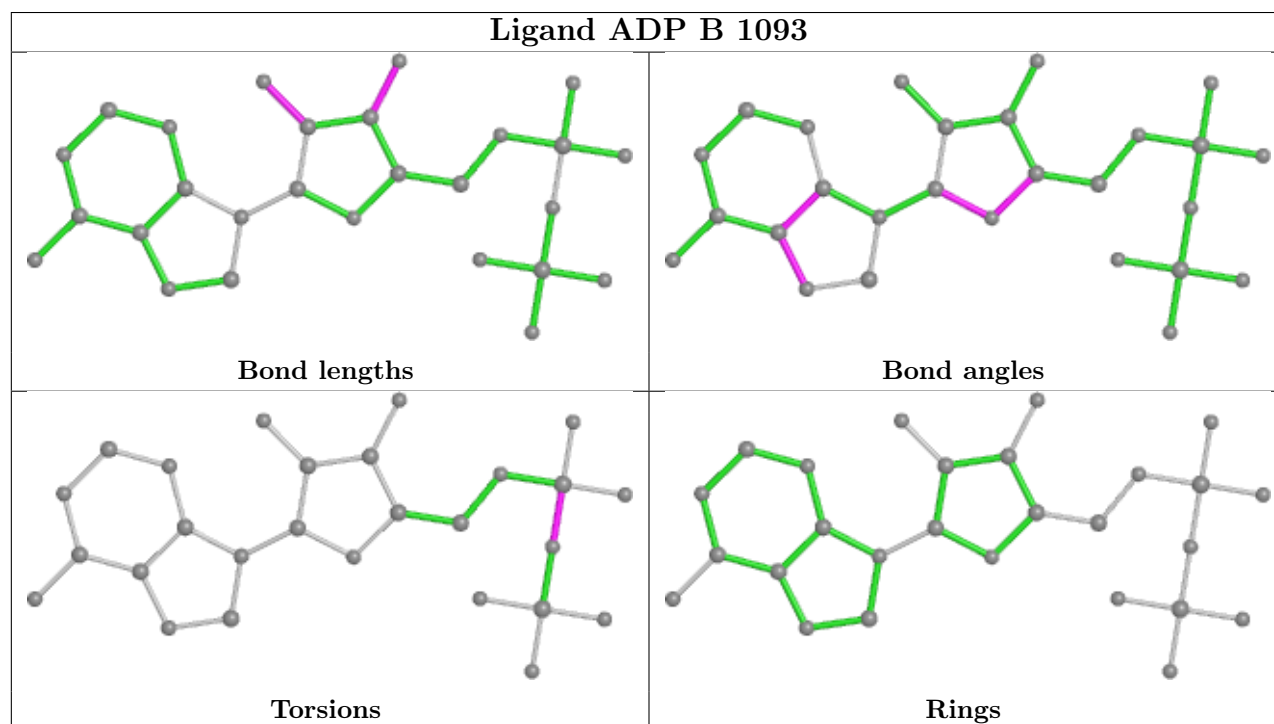
There are no ring outliers.

7 monomers are involved in 13 short contacts:

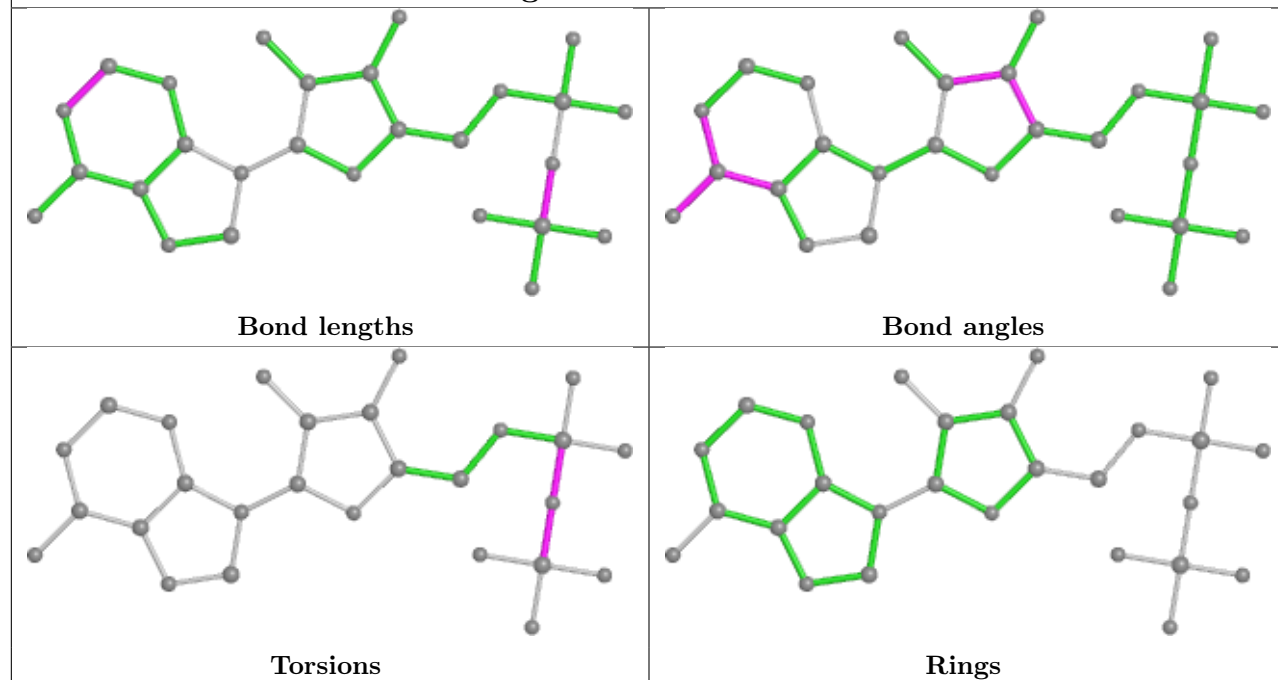
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1095	ORN	4	0
10	B	1096	NET	1	0
8	E	1096	ADP	1	0
9	E	1097	ORN	3	0
10	H	1095	NET	2	0
8	K	1095	ADP	1	0
9	K	1097	ORN	1	0

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

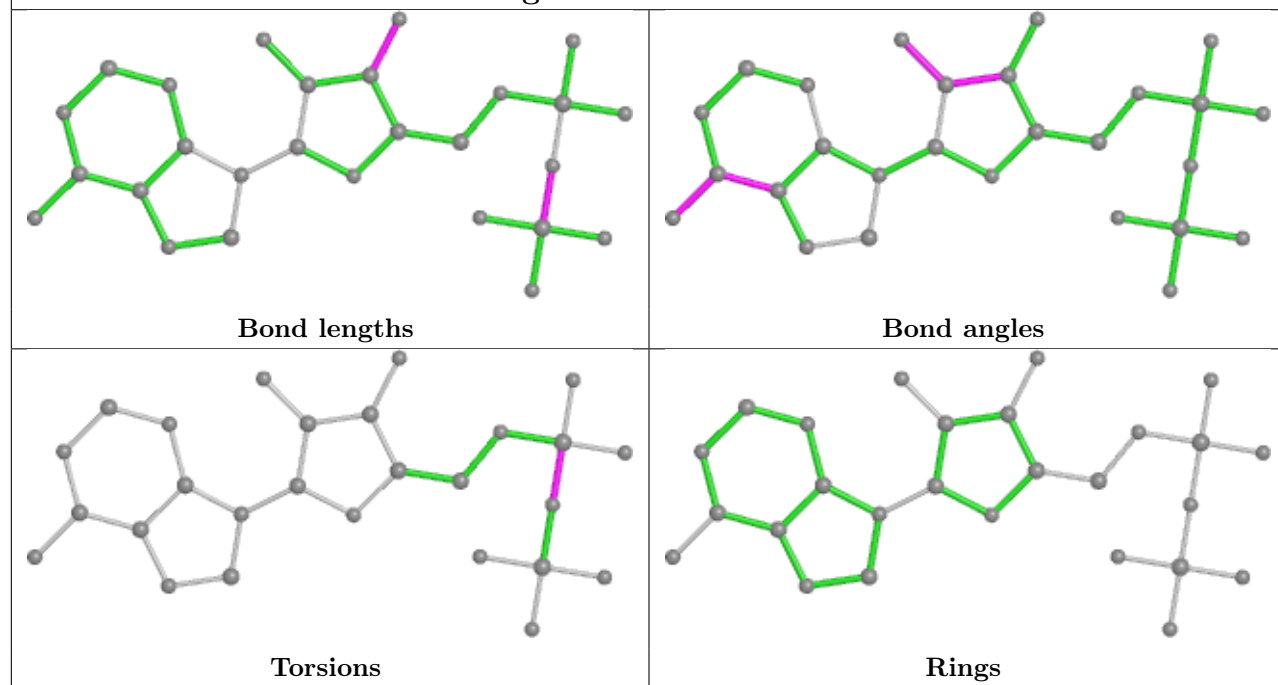
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



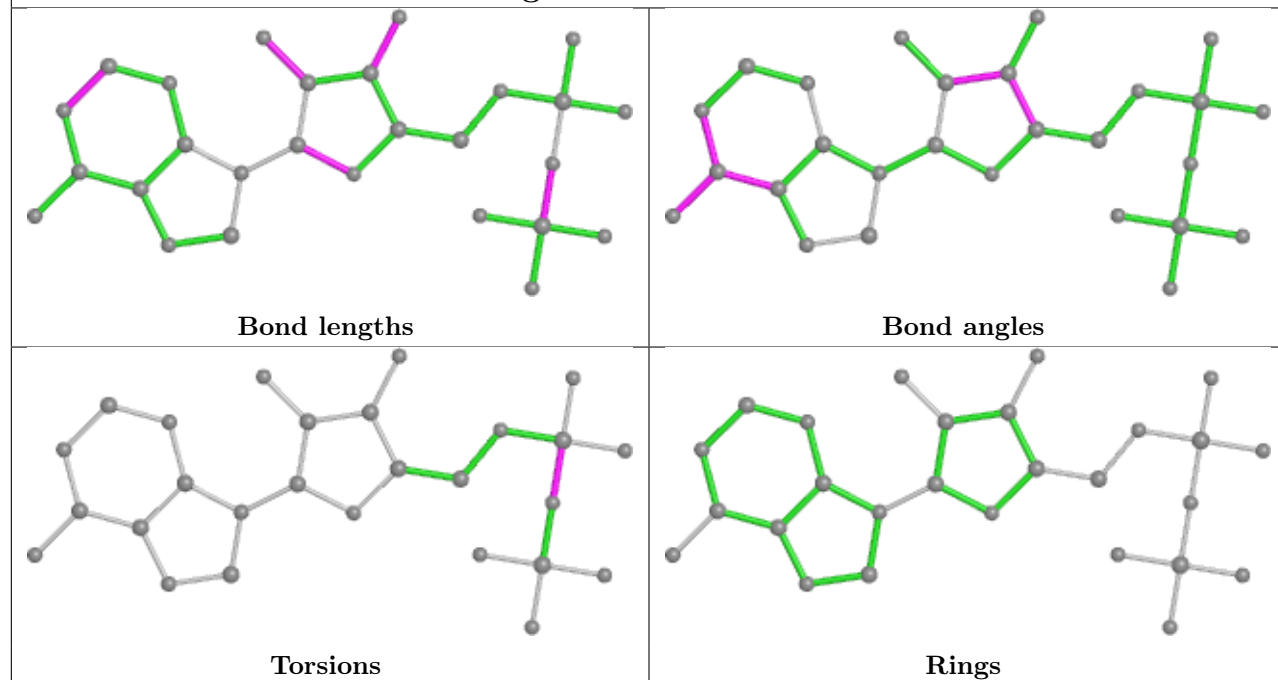
Ligand ADP B 1094



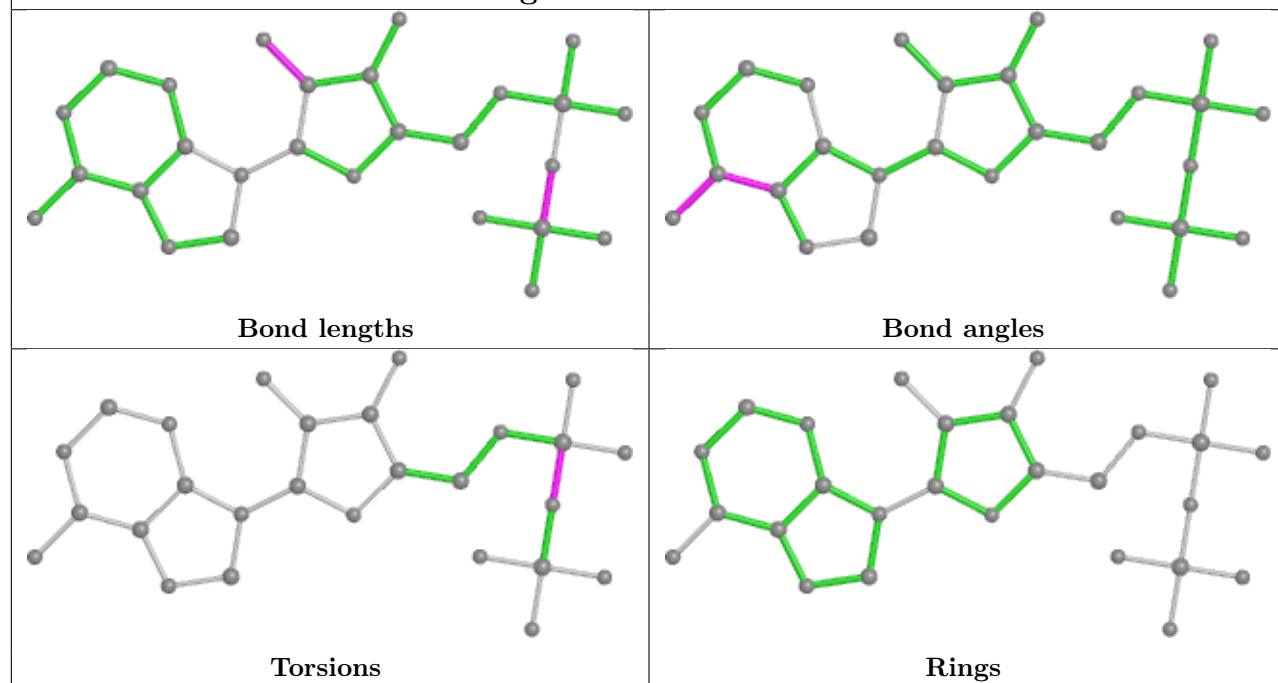
Ligand ADP E 1095



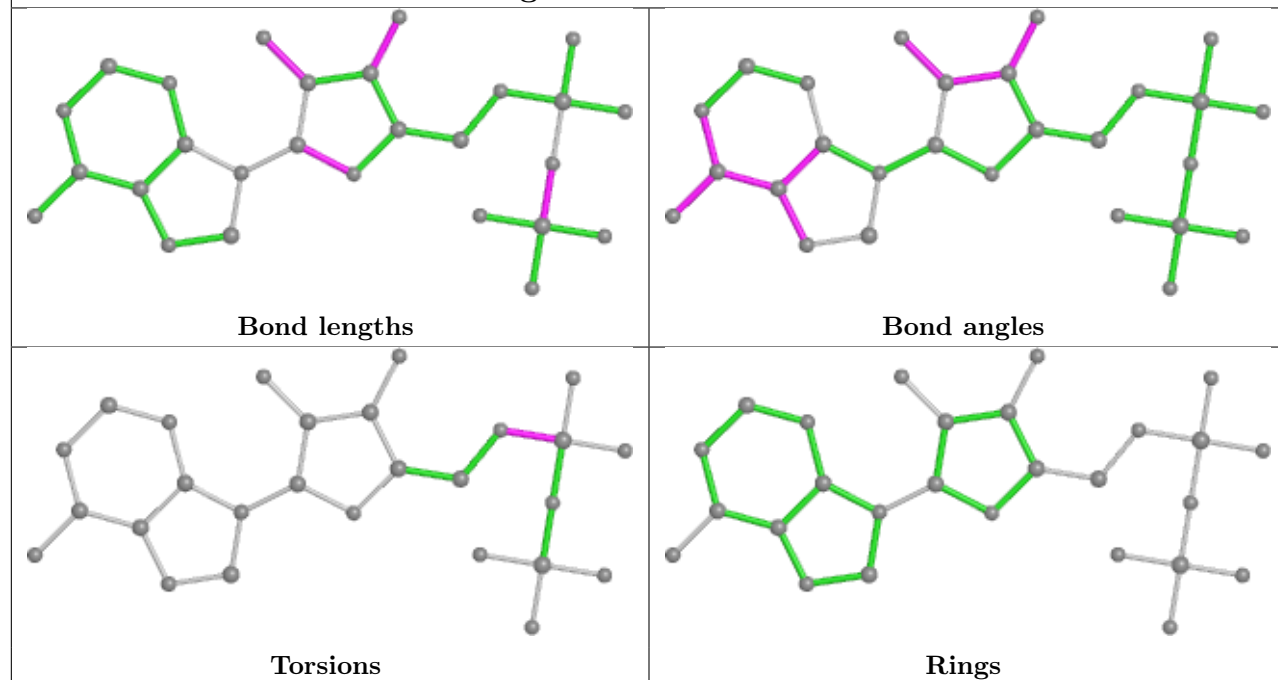
Ligand ADP E 1096



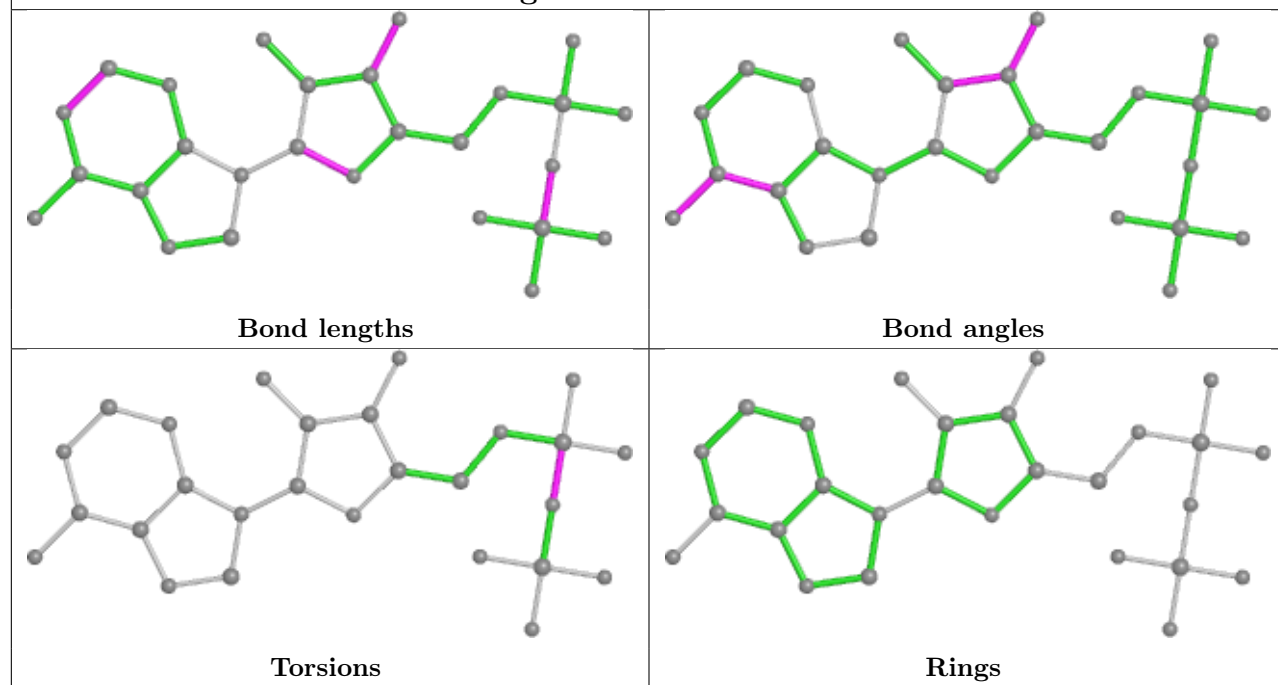
Ligand ADP H 1092

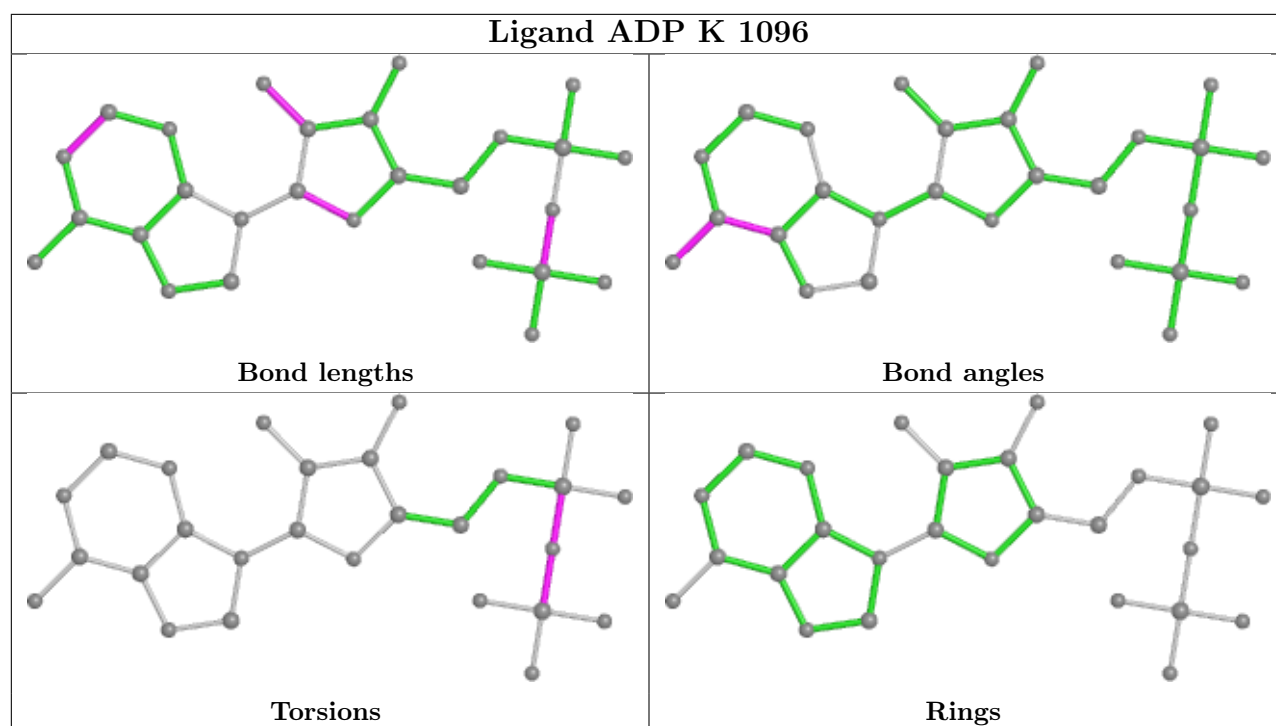


Ligand ADP H 1093



Ligand ADP K 1095





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.