



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:49 AM UTC

PDB ID : 1JDB / pdb_00001jdb
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

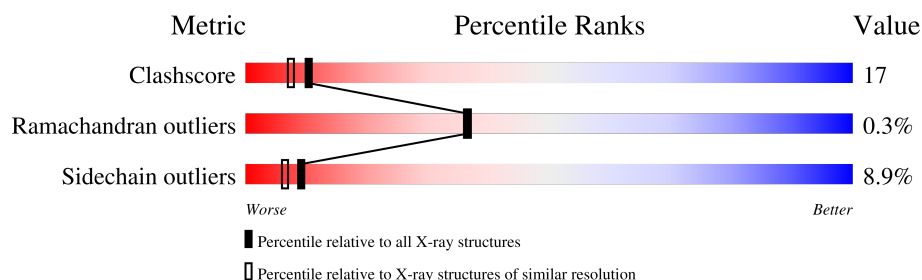
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	1073	64% 28% 6% .
1	E	1073	64% 28% 6% .
1	H	1073	62% 29% 6% ..
1	K	1073	67% 27% 5% ..
2	C	382	51% 39% 9% ..
2	F	382	42% 47% 9% ..
2	I	382	47% 41% 11% ..
2	L	382	58% 35% 5% ..

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	E	1082	-	-	X	-
5	PO4	H	1082	-	-	X	-
5	PO4	K	1082	-	-	X	-
7	GLN	B	1091	-	X	-	-

2 Entry composition [i](#)

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

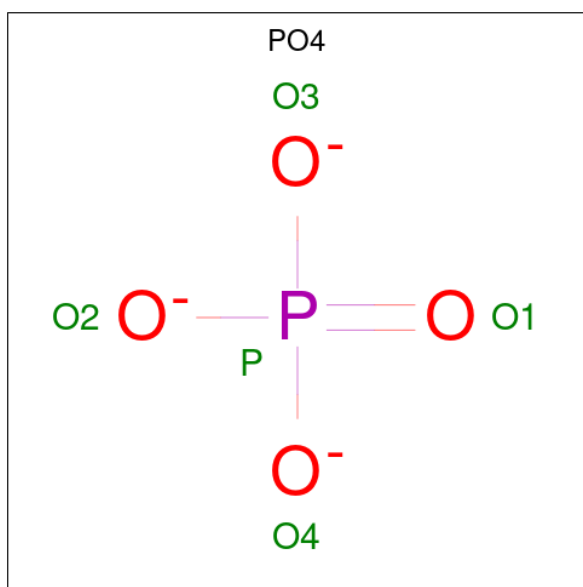
- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 5 is PHOSPHATE ION (CCD ID: 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 (CCD ID: CL) (formula: Cl).

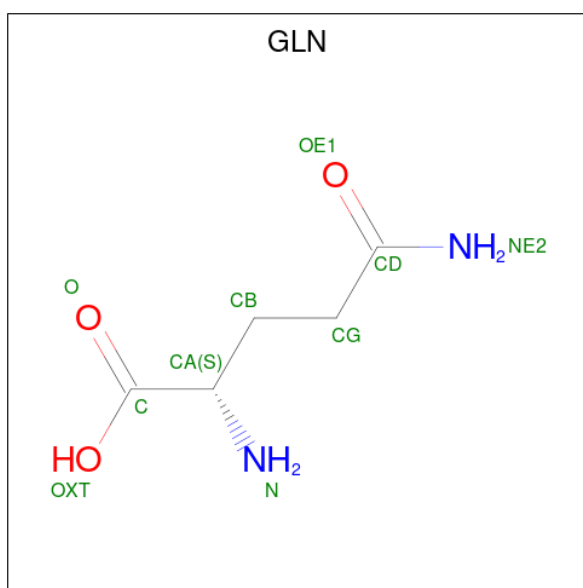
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	6	Total	Cl	0	0
			6	6		
6	C	1	Total	Cl	0	0
			1	1		
6	E	7	Total	Cl	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Cl	0	0
			1	1		
6	H	6	Total	Cl	0	0
			6	6		
6	I	1	Total	Cl	0	0
			1	1		
6	K	6	Total	Cl	0	0
			6	6		
6	L	1	Total	Cl	0	0
			1	1		

- Molecule 7 is GLUTAMINE (CCD ID: GLN) (formula: $C_5H_{10}N_2O_3$).



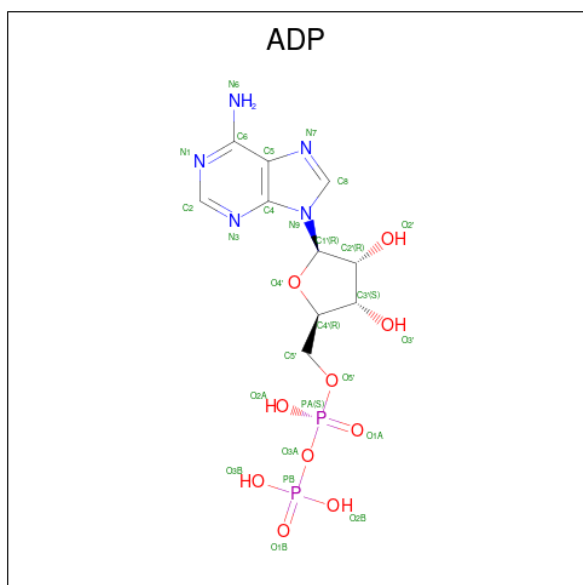
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			10	5	2	3		
7	B	1	Total	C	N	O	0	0
			10	5	2	3		
7	E	1	Total	C	N	O	0	0
			10	5	2	3		
7	E	1	Total	C	N	O	0	0
			10	5	2	3		
7	H	1	Total	C	N	O	0	0
			10	5	2	3		
7	H	1	Total	C	N	O	0	0
			10	5	2	3		

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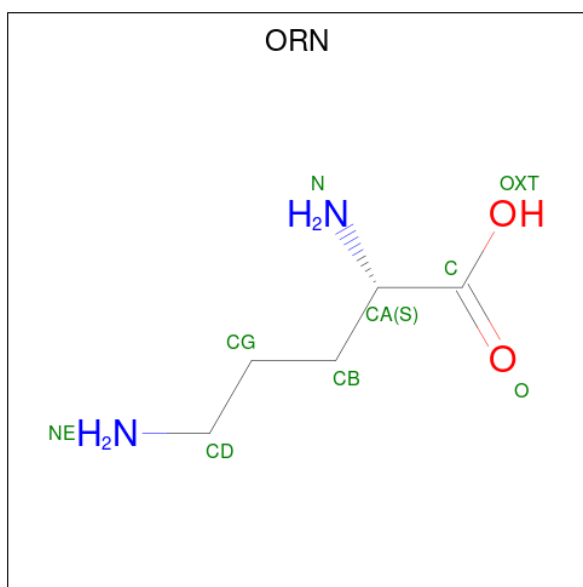
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	K	1	Total	C	N	O	0	0
			10	5	2	3		
7	K	1	Total	C	N	O	0	0
			10	5	2	3		

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



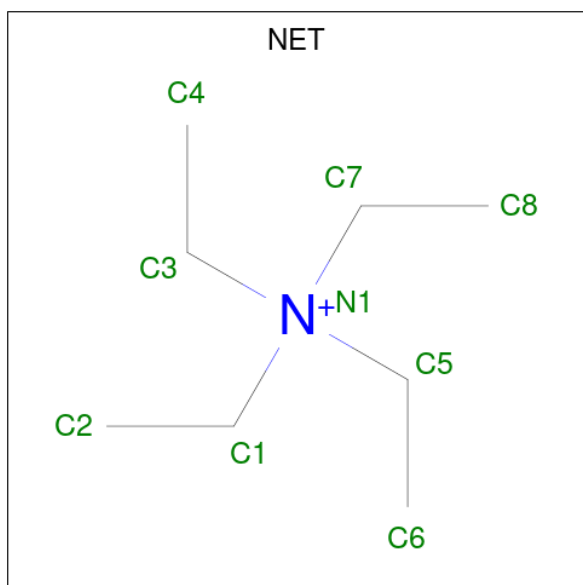
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	K	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 (CCD ID: ORN) (formula: $C_5H_{12}N_2O_2$).



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

- Molecule 10 is TETRAETHYLAMMONIUM ION (CCD ID: NET) (formula: C₈H₂₀N).



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

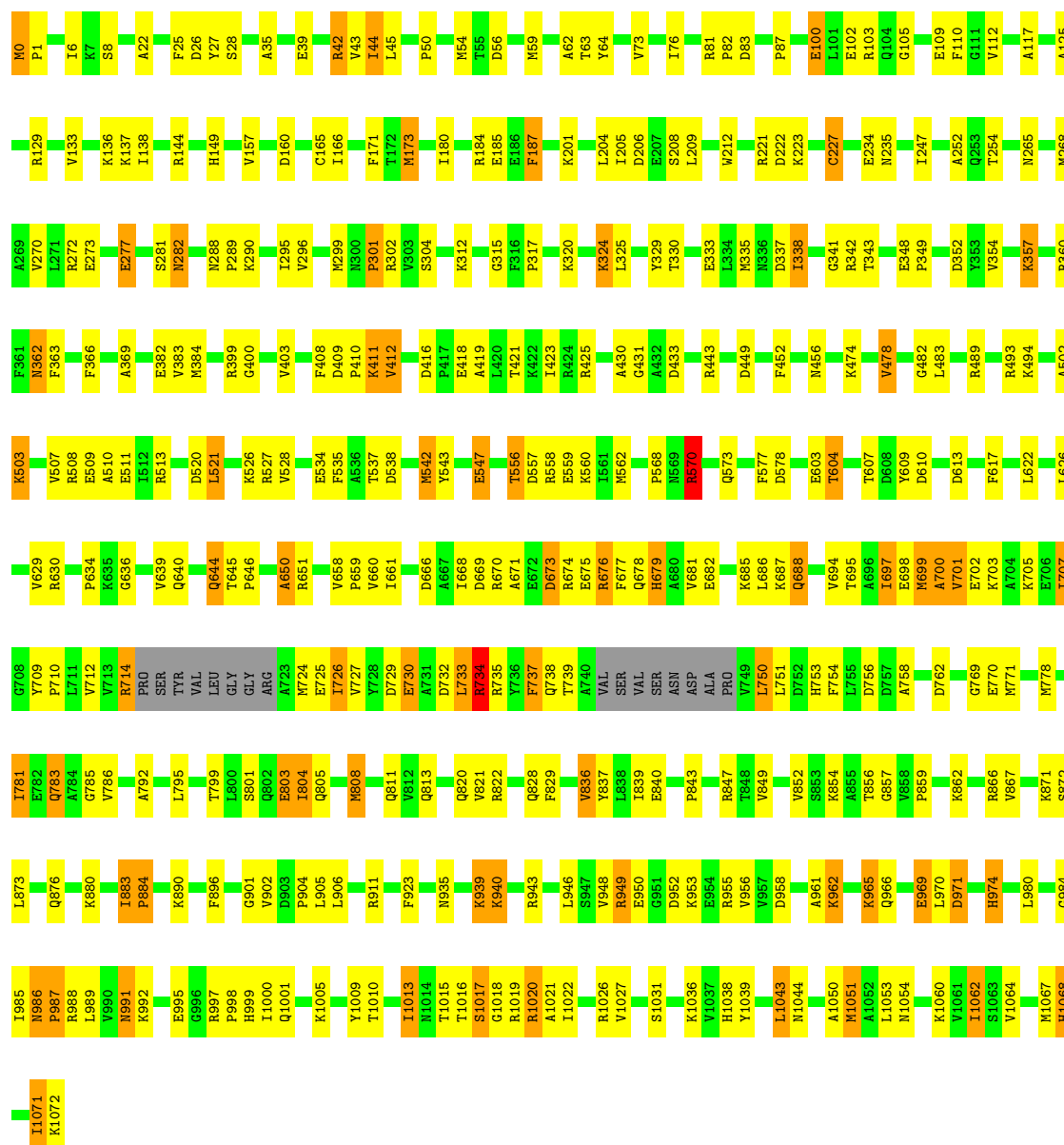
3 Residue-property plots

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

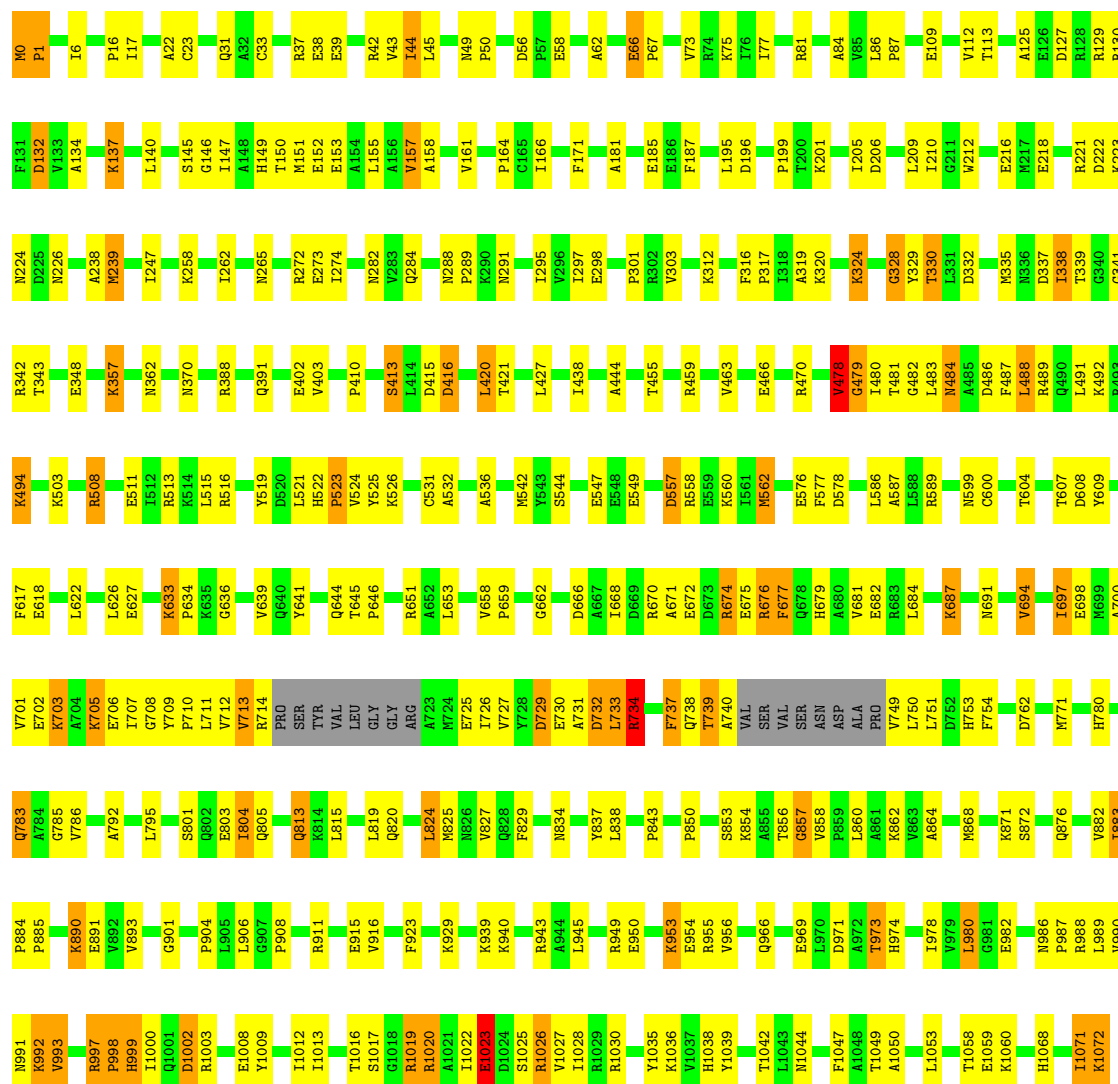
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE

Chain B: 



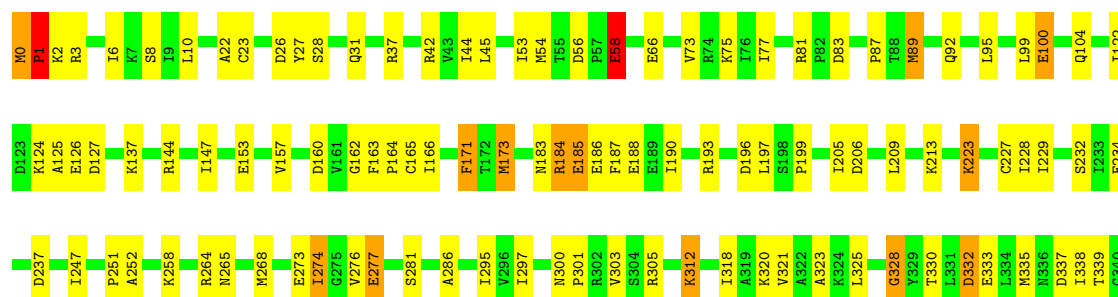
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE

Chain E: 



• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE

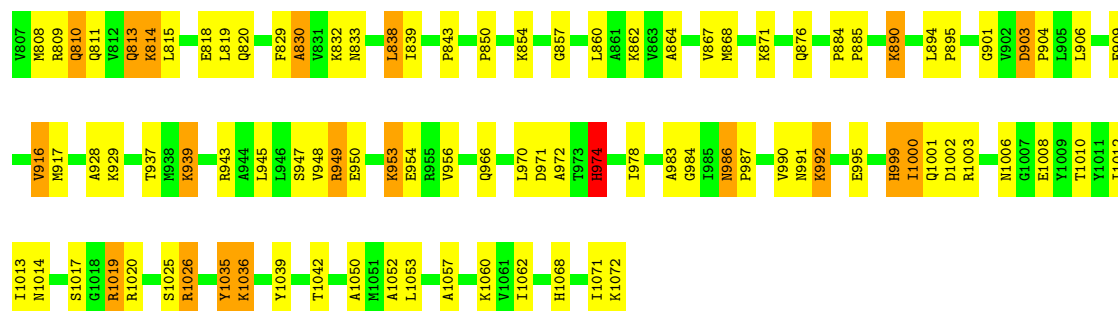
Chain H: 





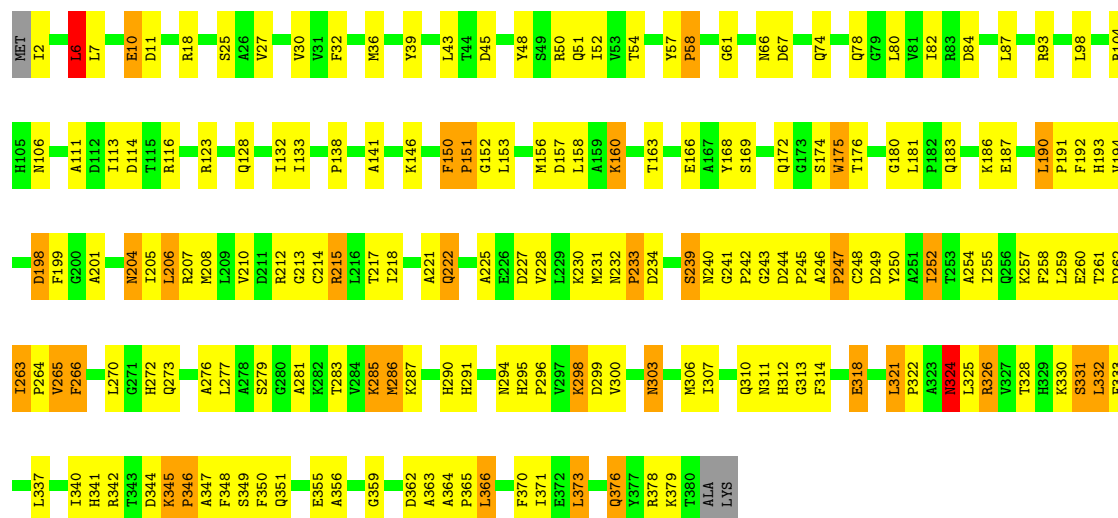
Response	Percentage
Yes, the U.S. is a democracy	67%
No, the U.S. is not a democracy	27%
Don't know	5%





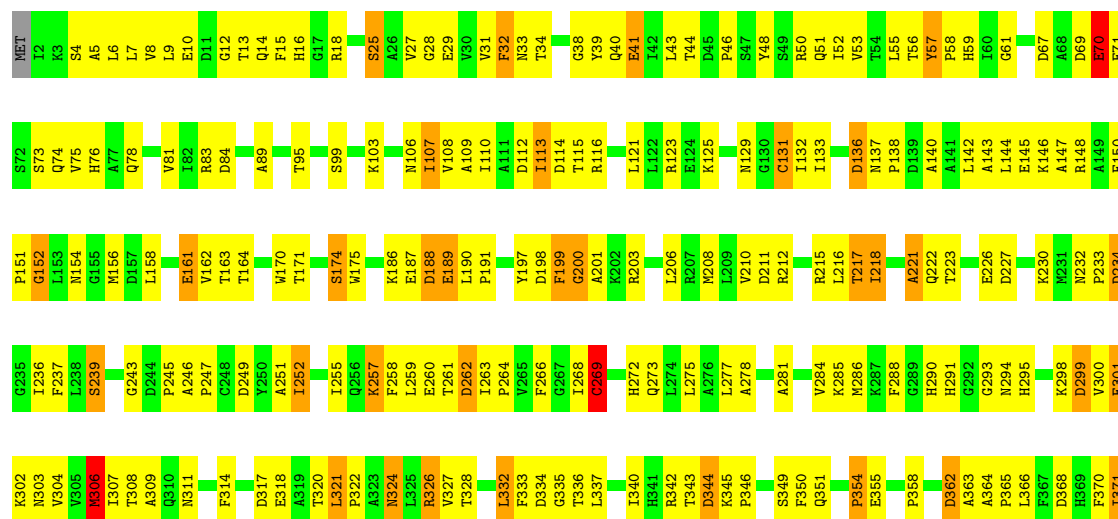
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE

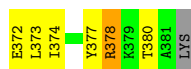
Chain C: 51% 39% 9% ..



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE

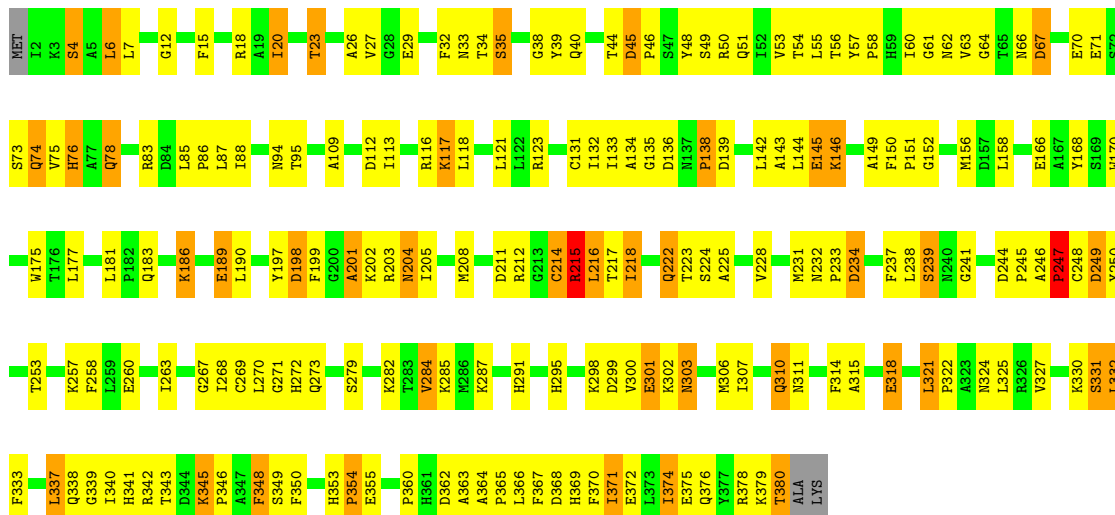
Chain F: 42% 47% 9% ..





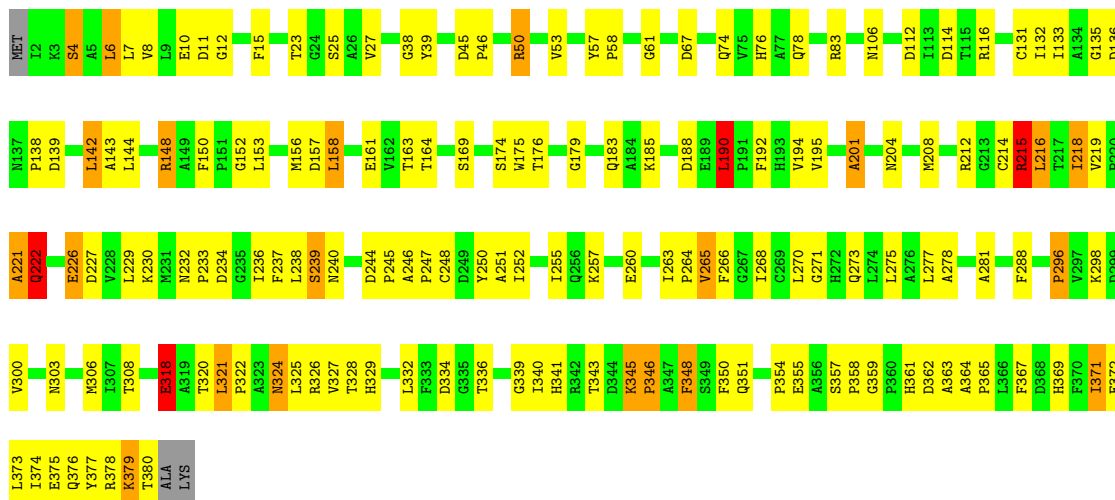
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE

Chain I: 47% 41% 11% ..



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE

Chain L: 58% 35% 5% ..



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: CL, PO4, K, ADP, ORN, NET, MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	1.08	1/8353 (0.0%)	1.81	146/11292 (1.3%)
1	E	1.09	0/8401	1.77	108/11352 (1.0%)
1	H	1.09	2/8329 (0.0%)	1.77	120/11259 (1.1%)
1	K	1.13	1/8349 (0.0%)	1.80	123/11289 (1.1%)
2	C	1.02	0/2957	1.81	49/4016 (1.2%)
2	F	1.00	0/2970	1.80	51/4034 (1.3%)
2	I	1.01	0/2957	1.78	41/4016 (1.0%)
2	L	1.06	0/2957	1.86	58/4016 (1.4%)
All	All	1.08	4/45273 (0.0%)	1.79	696/61274 (1.1%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	849	VAL	CA-CB	-5.92	1.51	1.54
1	H	66	GLU	N-CA	-5.35	1.42	1.46
1	B	673	ASP	CG-OD1	5.12	1.35	1.25
1	K	724	MET	CA-C	-5.10	1.46	1.52

All (696) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	697	ILE	N-CA-C	11.27	121.95	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	184	ARG	N-CA-C	10.82	125.58	112.38
2	L	380	THR	N-CA-CB	-10.55	93.56	111.50
1	H	557	ASP	CB-CA-C	-10.33	93.64	110.79
1	E	737	PHE	CA-CB-CG	-10.30	103.50	113.80
1	B	1068	HIS	CA-CB-CG	-10.14	103.66	113.80
1	B	1038	HIS	CA-CB-CG	-10.00	103.80	113.80
1	H	756	ASP	CA-CB-CG	9.76	122.36	112.60
2	F	53	VAL	N-CA-C	9.69	121.63	108.84
1	K	562	MET	CG-SD-CE	-9.68	79.60	100.90
1	H	184	ARG	CA-C-N	9.49	136.55	120.71
1	H	184	ARG	C-N-CA	9.49	136.55	120.71
1	H	352	ASP	CA-CB-CG	9.45	122.05	112.60
1	K	87	PRO	CB-CA-C	-9.38	99.60	109.92
1	E	604	THR	N-CA-C	9.17	123.88	110.59
1	K	337	ASP	CA-CB-CG	9.09	121.69	112.60
1	H	186	GLU	N-CA-C	-9.07	101.35	111.14
1	E	247	ILE	N-CA-C	-9.06	96.89	109.21
1	B	557	ASP	CA-CB-CG	8.86	121.46	112.60
1	B	737	PHE	CA-CB-CG	-8.86	104.94	113.80
2	L	260	GLU	N-CA-C	-8.79	102.71	113.97
1	E	829	PHE	CA-CB-CG	8.77	122.57	113.80
1	B	87	PRO	CB-CA-C	-8.70	100.26	110.00
2	L	379	LYS	N-CA-C	-8.69	100.82	111.33
2	L	327	VAL	CB-CA-C	-8.64	101.93	111.35
1	B	22	ALA	N-CA-C	8.62	121.44	109.29
1	B	558	ARG	N-CA-C	8.54	121.98	109.69
1	K	416	ASP	CA-CB-CG	8.50	121.10	112.60
1	K	706	GLU	CB-CA-C	8.47	125.25	110.85
1	K	658	VAL	N-CA-C	8.44	117.22	108.95
1	B	556	THR	CA-C-N	8.40	131.89	120.38
1	B	556	THR	C-N-CA	8.40	131.89	120.38
1	E	676	ARG	CA-C-O	8.39	129.70	120.63
1	B	337	ASP	CA-CB-CG	8.38	120.98	112.60
1	H	318	ILE	N-CA-C	8.36	119.14	110.36
1	K	617	PHE	CA-CB-CG	-8.32	105.48	113.80
2	C	260	GLU	N-CA-C	-8.31	103.28	113.50
1	E	792	ALA	N-CA-C	-8.20	97.29	110.32
1	B	1051	MET	CB-CA-C	-8.19	98.02	110.88
1	H	1038	HIS	CA-CB-CG	-8.15	105.65	113.80
2	F	84	ASP	CA-CB-CG	8.12	120.72	112.60
1	K	337	ASP	N-CA-C	8.11	119.74	111.07
2	I	4	SER	N-CA-C	8.08	121.34	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1000	ILE	CB-CA-C	-8.07	101.25	112.14
2	I	198	ASP	CA-CB-CG	7.96	120.56	112.60
1	H	247	ILE	N-CA-C	-7.95	97.13	108.58
1	H	999	HIS	CA-CB-CG	-7.92	105.88	113.80
1	E	484	ASN	CA-CB-CG	7.89	120.49	112.60
2	I	303	ASN	CA-CB-CG	-7.88	104.72	112.60
1	H	673	ASP	CA-C-N	7.86	132.61	120.82
1	H	673	ASP	C-N-CA	7.86	132.61	120.82
1	E	338	ILE	N-CA-C	7.86	123.04	112.04
1	K	984	GLY	CA-C-N	-7.84	113.47	123.19
1	K	984	GLY	C-N-CA	-7.84	113.47	123.19
1	H	185[A]	GLU	O-C-N	7.83	131.64	122.17
1	H	185[B]	GLU	O-C-N	7.83	131.64	122.17
1	H	87	PRO	CB-CA-C	-7.82	101.31	109.92
1	E	56	ASP	CA-C-N	7.79	128.20	119.32
1	E	56	ASP	C-N-CA	7.79	128.20	119.32
1	H	611	THR	N-CA-C	7.79	120.66	111.71
1	E	992	LYS	N-CA-C	-7.78	100.26	110.53
1	H	737	PHE	CA-CB-CG	-7.77	106.03	113.80
1	H	22	ALA	N-CA-C	7.77	120.24	109.29
1	K	792	ALA	N-CA-C	-7.77	100.06	110.55
1	E	416	ASP	CB-CA-C	7.75	121.90	109.51
1	H	337	ASP	CA-CB-CG	7.72	120.32	112.60
1	B	640	GLN	N-CA-C	7.70	122.67	113.28
1	E	455	THR	N-CA-C	7.70	122.98	112.90
2	I	345	LYS	O-C-N	7.67	127.87	121.35
1	K	562	MET	CB-CA-C	-7.67	96.59	109.48
1	K	37	ARG	CA-C-N	7.67	130.55	120.28
1	K	37	ARG	C-N-CA	7.67	130.55	120.28
1	K	22	ALA	N-CA-C	7.55	119.94	109.29
1	E	697	ILE	CB-CA-C	-7.55	102.22	111.88
1	E	1047	PHE	CA-CB-CG	-7.53	106.27	113.80
2	F	191	PRO	N-CA-C	7.53	124.00	113.53
1	H	558	ARG	N-CA-C	7.51	121.58	110.46
1	B	206	ASP	CA-CB-CG	7.50	120.10	112.60
1	B	785	GLY	N-CA-C	-7.50	105.56	114.48
1	H	184	ARG	N-CA-CB	-7.46	97.64	110.32
1	B	180	ILE	CA-C-N	-7.46	112.71	123.00
1	B	180	ILE	C-N-CA	-7.46	112.71	123.00
1	E	786	VAL	N-CA-C	-7.46	96.99	107.80
1	H	604	THR	N-CA-C	7.45	121.55	110.52
1	E	303	VAL	N-CA-C	-7.42	101.96	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	998	PRO	N-CA-CB	7.41	110.75	102.60
2	F	269	CYS	CB-CA-C	7.38	125.11	110.42
2	L	190	LEU	CA-C-N	7.38	127.24	119.05
2	L	190	LEU	C-N-CA	7.38	127.24	119.05
2	I	215	ARG	N-CA-C	-7.38	97.66	109.76
2	F	70	GLU	N-CA-CB	7.34	122.39	110.43
1	B	277	GLU	N-CA-CB	7.30	120.96	110.88
1	E	618	GLU	O-C-N	7.30	126.38	121.71
1	K	986	ASN	CA-CB-CG	7.28	119.88	112.60
1	B	604	THR	N-CA-C	7.27	121.22	110.46
1	E	893	VAL	N-CA-CB	7.27	121.44	111.41
2	C	45	ASP	CA-CB-CG	7.25	119.85	112.60
2	C	6	LEU	N-CA-CB	-7.24	98.05	111.52
1	H	556	THR	N-CA-CB	-7.22	100.13	110.81
2	L	201	ALA	N-CA-C	7.17	120.63	110.23
2	F	190	LEU	CA-C-N	7.16	126.99	119.05
2	F	190	LEU	C-N-CA	7.16	126.99	119.05
2	I	53	VAL	N-CA-C	7.15	119.13	108.54
1	H	362	ASN	CA-CB-CG	7.14	119.74	112.60
1	K	786	VAL	N-CA-C	-7.14	96.81	107.37
1	E	666	ASP	CA-CB-CG	-7.12	105.48	112.60
1	K	455	THR	N-CA-C	7.10	122.24	113.50
2	L	157	ASP	CA-CB-CG	7.09	119.69	112.60
1	H	714	ARG	CA-C-O	-7.08	108.77	120.80
1	B	577	PHE	CA-CB-CG	-7.07	106.73	113.80
1	E	883	ILE	N-CA-CB	7.04	121.06	111.21
1	B	282	ASN	CA-CB-CG	7.00	119.61	112.60
2	L	361	HIS	CA-CB-CG	-7.00	106.80	113.80
1	B	733	LEU	N-CA-C	7.00	118.55	111.07
1	K	56	ASP	CA-C-N	6.97	127.27	119.32
1	K	56	ASP	C-N-CA	6.97	127.27	119.32
1	H	58	GLU	N-CA-CB	-6.96	98.71	110.41
1	H	879	THR	N-CA-CB	-6.96	101.74	111.00
1	B	542	MET	N-CA-C	6.93	120.80	109.85
1	K	338	ILE	N-CA-C	6.92	121.64	112.98
1	E	37	ARG	NE-CZ-NH1	6.92	128.42	121.50
2	L	359	GLY	CA-C-N	6.91	127.29	119.83
2	L	359	GLY	C-N-CA	6.91	127.29	119.83
1	H	849	VAL	N-CA-CB	6.89	115.14	110.52
1	B	962	LYS	CA-CB-CG	-6.88	100.33	114.10
2	F	136	ASP	CA-CB-CG	6.88	119.48	112.60
2	C	150	PHE	CA-C-N	6.87	126.83	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	150	PHE	C-N-CA	6.87	126.83	119.28
1	B	1068	HIS	N-CA-CB	-6.86	100.03	110.12
1	B	209	LEU	N-CA-C	-6.85	102.21	111.87
2	L	348	PHE	CA-CB-CG	6.85	120.65	113.80
1	H	786	VAL	N-CA-CB	6.84	118.80	111.00
1	B	411	LYS	N-CA-CB	-6.84	101.50	110.59
1	K	542	MET	N-CA-C	6.84	120.65	109.85
1	K	421	THR	CB-CA-C	6.82	122.45	110.85
1	B	338	ILE	N-CA-C	6.82	121.50	112.98
1	B	969	GLU	N-CA-C	-6.81	100.44	110.52
1	K	209	LEU	N-CA-C	-6.81	103.04	112.30
1	H	556	THR	CA-C-N	6.80	129.39	120.28
1	H	556	THR	C-N-CA	6.80	129.39	120.28
1	K	860	LEU	N-CA-C	6.80	119.55	111.33
2	L	215	ARG	N-CA-CB	6.79	120.31	110.06
1	B	992	LYS	N-CA-C	-6.78	101.39	110.55
2	I	45	ASP	CA-CB-CG	6.77	119.37	112.60
2	I	67	ASP	N-CA-C	6.76	118.31	111.07
1	E	993	VAL	N-CA-C	6.75	117.50	110.62
1	H	421	THR	CB-CA-C	6.73	122.30	110.85
1	B	556	THR	CA-C-O	6.73	126.84	119.24
1	H	81	ARG	CB-CA-C	-6.72	105.16	111.00
1	K	916	VAL	N-CA-CB	6.70	121.90	112.52
1	B	557	ASP	N-CA-CB	-6.69	100.02	110.06
1	H	300	ASN	CA-CB-CG	-6.68	105.92	112.60
2	I	234	ASP	N-CA-C	-6.68	104.95	113.23
1	B	999	HIS	CA-CB-CG	-6.68	107.12	113.80
2	I	74	GLN	CB-CA-C	-6.68	97.09	111.11
1	H	557	ASP	N-CA-C	6.65	118.53	111.28
2	L	379	LYS	CA-C-N	-6.64	109.75	121.70
2	L	379	LYS	C-N-CA	-6.64	109.75	121.70
2	F	237	PHE	CA-CB-CG	-6.61	107.19	113.80
1	K	553	ASN	CB-CA-C	-6.60	106.51	111.20
2	I	310	GLN	N-CA-C	6.60	119.21	108.26
1	K	503	LYS	CB-CA-C	-6.59	99.85	110.79
1	K	247	ILE	N-CA-C	-6.59	100.20	108.89
1	B	836	VAL	N-CA-C	6.57	117.98	107.73
1	K	337	ASP	CA-C-N	-6.57	111.03	121.34
1	K	337	ASP	C-N-CA	-6.57	111.03	121.34
1	H	338	ILE	N-CA-C	6.56	121.23	112.04
1	H	501	LEU	N-CA-C	-6.55	104.22	111.36
1	H	455	THR	N-CA-C	6.54	121.47	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	349	PRO	N-CA-CB	6.54	109.04	103.35
2	I	362	ASP	N-CA-C	6.54	119.23	111.71
2	I	20	ILE	CA-C-O	6.53	124.55	119.46
1	E	780	HIS	CA-CB-CG	6.52	120.32	113.80
1	K	753	HIS	CA-CB-CG	-6.51	107.29	113.80
1	H	654	GLU	N-CA-C	-6.51	104.11	111.14
1	E	542	MET	N-CA-C	6.49	120.11	109.85
1	B	449	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	171	PHE	N-CA-C	6.48	120.48	112.58
1	K	587	ALA	N-CA-C	6.48	118.00	111.07
1	H	677	PHE	CA-CB-CG	6.48	120.28	113.80
1	B	997	ARG	CB-CA-C	6.47	118.89	108.87
2	C	190	LEU	CB-CA-C	6.46	119.84	109.51
2	L	204	ASN	N-CA-C	6.45	118.31	111.28
1	K	1000	ILE	N-CA-CB	-6.45	103.36	110.51
1	H	323	ALA	N-CA-C	-6.44	104.18	111.07
1	K	304	SER	N-CA-C	6.43	116.73	108.24
2	F	362	ASP	N-CA-C	6.43	118.29	111.28
1	B	650	ALA	N-CA-C	6.43	118.83	111.11
2	F	108	VAL	N-CA-C	-6.43	101.29	109.58
2	L	142	LEU	N-CA-CB	-6.42	100.65	110.16
1	E	337	ASP	CB-CA-C	-6.42	100.18	110.84
1	B	849	VAL	CA-C-O	6.42	123.59	118.71
1	B	644	GLN	N-CA-C	6.42	117.94	111.07
1	E	239	MET	CA-C-N	-6.41	115.91	123.08
1	E	239	MET	C-N-CA	-6.41	115.91	123.08
1	H	408	PHE	CA-CB-CG	-6.40	107.40	113.80
2	C	263	ILE	N-CA-CB	6.40	116.58	109.99
2	C	303	ASN	CA-CB-CG	-6.38	106.22	112.60
1	K	995	GLU	N-CA-C	6.38	117.90	111.07
2	C	307	ILE	CA-C-N	-6.38	111.87	122.21
2	C	307	ILE	C-N-CA	-6.38	111.87	122.21
1	K	19	ILE	CA-C-N	-6.38	113.55	122.86
1	K	19	ILE	C-N-CA	-6.38	113.55	122.86
1	K	604	THR	N-CA-C	6.37	119.83	110.59
2	L	345	LYS	O-C-N	6.36	126.73	121.32
2	L	379	LYS	CA-C-O	6.36	127.50	120.63
2	F	223	THR	CA-CB-CG2	6.36	121.30	110.50
1	E	513	ARG	NE-CZ-NH1	6.34	127.84	121.50
1	B	859	PRO	N-CA-CB	6.34	106.96	102.65
2	C	36	MET	N-CA-CB	6.34	120.92	110.39
1	K	686	LEU	N-CA-CB	6.34	120.72	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	4	SER	N-CA-C	6.33	118.88	110.53
2	F	95	THR	N-CA-CB	6.32	119.33	110.98
2	F	89	ALA	N-CA-C	-6.31	99.41	109.76
1	E	1038	HIS	CA-CB-CG	-6.31	107.49	113.80
2	L	320	THR	CA-CB-OG1	6.29	119.04	109.60
1	E	557	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	661	ILE	CA-CB-CG2	-6.28	99.83	110.50
2	L	214	CYS	CB-CA-C	-6.28	100.56	110.79
1	H	953	LYS	N-CA-C	6.26	118.63	111.11
1	B	613	ASP	N-CA-C	-6.26	104.38	111.14
2	L	378	ARG	CB-CA-C	-6.26	98.65	110.67
1	H	328	GLY	N-CA-C	6.26	123.66	115.40
1	K	1071	ILE	CB-CA-C	6.25	121.78	111.59
2	L	240	ASN	N-CA-C	-6.25	101.53	110.59
1	B	337	ASP	N-CA-C	6.25	118.61	111.11
1	B	56	ASP	CA-C-N	6.24	126.44	119.32
1	B	56	ASP	C-N-CA	6.24	126.44	119.32
1	E	209	LEU	N-CA-C	-6.24	103.81	112.30
1	B	25	PHE	CA-CB-CG	-6.24	107.56	113.80
1	B	315	GLY	N-CA-C	-6.24	107.10	115.21
1	B	987	PRO	CB-CA-C	-6.24	101.99	110.60
1	K	300	ASN	CA-C-N	6.24	127.64	119.84
1	K	300	ASN	C-N-CA	6.24	127.64	119.84
1	K	970	LEU	N-CA-C	6.23	119.86	109.95
2	I	62	ASN	CA-CB-CG	6.23	118.83	112.60
1	K	578	ASP	CA-CB-CG	-6.23	106.37	112.60
1	B	573	GLN	CA-C-N	6.21	128.42	122.27
1	B	573	GLN	C-N-CA	6.21	128.42	122.27
2	C	331	SER	N-CA-CB	6.21	119.58	109.95
1	E	608	ASP	N-CA-C	-6.21	99.15	109.46
1	H	206	ASP	CA-CB-CG	6.21	118.81	112.60
1	B	660	VAL	CA-C-N	-6.21	115.63	122.27
1	B	660	VAL	C-N-CA	-6.21	115.63	122.27
1	K	635	LYS	N-CA-C	-6.20	104.42	112.23
1	E	479	GLY	CA-C-N	6.17	128.46	120.56
1	E	479	GLY	C-N-CA	6.17	128.46	120.56
1	B	528	VAL	N-CA-C	-6.17	100.74	108.89
2	I	189	GLU	N-CA-C	-6.17	104.82	112.90
1	H	26	ASP	CA-CB-CG	6.17	118.77	112.60
1	K	171	PHE	N-CA-C	6.16	120.74	113.23
2	F	162	VAL	CB-CA-C	-6.16	104.61	110.70
1	E	675	GLU	N-CA-CB	6.15	118.93	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	661	ILE	CA-C-O	-6.15	116.82	121.68
1	E	785	GLY	N-CA-C	-6.15	107.17	114.48
1	B	998	PRO	N-CA-CB	6.14	109.36	102.60
2	L	10	GLU	CB-CA-C	-6.14	98.19	110.42
1	B	136	LYS	CA-C-O	6.14	127.06	120.55
2	C	204	ASN	N-CA-C	6.14	117.97	111.28
1	K	618	GLU	N-CA-CB	-6.13	100.14	111.18
2	C	240	ASN	N-CA-C	-6.12	101.90	110.35
1	K	611	THR	N-CA-C	6.09	118.89	111.82
1	E	195	LEU	CA-C-O	6.08	127.00	120.55
1	K	337	ASP	CB-CA-C	-6.08	101.33	110.88
1	K	604	THR	O-C-N	6.07	129.78	122.68
1	B	483	LEU	N-CA-CB	6.06	117.93	110.53
1	K	885	PRO	CB-CA-C	-6.06	102.45	110.27
1	E	488	LEU	N-CA-C	-6.04	104.77	111.36
2	C	151	PRO	CB-CA-C	-6.04	102.79	112.21
1	H	26	ASP	N-CA-C	-6.03	104.27	111.69
2	I	204	ASN	N-CA-CB	6.03	118.99	110.12
2	C	266	PHE	CA-C-N	-6.03	116.97	121.61
2	C	266	PHE	C-N-CA	-6.03	116.97	121.61
1	K	987	PRO	CB-CA-C	-6.03	101.83	110.75
1	H	58	GLU	CA-CB-CG	-6.01	102.08	114.10
1	B	43	VAL	N-CA-C	6.01	116.51	107.80
1	E	149	HIS	CA-CB-CG	-5.99	107.81	113.80
1	K	295	ILE	O-C-N	-5.99	116.79	123.26
1	H	991	ASN	CB-CA-C	-5.99	99.66	109.53
2	I	75	VAL	N-CA-C	-5.99	98.51	107.37
2	F	221	ALA	N-CA-C	5.98	118.59	111.71
1	K	26	ASP	CA-CB-CG	5.97	118.57	112.60
1	H	542	MET	N-CA-C	5.96	119.28	109.85
1	H	171	PHE	N-CA-C	5.96	119.85	112.58
1	B	570	ARG	CD-NE-CZ	-5.96	116.06	124.40
1	E	370	ASN	N-CA-C	-5.96	100.83	109.59
1	H	701	VAL	O-C-N	5.96	127.89	121.94
1	E	112	VAL	N-CA-CB	5.94	118.16	111.21
1	E	297	ILE	N-CA-C	5.94	116.97	111.45
1	B	995	GLU	CA-C-N	-5.93	114.12	121.83
1	B	995	GLU	C-N-CA	-5.93	114.12	121.83
1	H	56	ASP	CA-C-N	5.93	126.08	119.32
1	H	56	ASP	C-N-CA	5.93	126.08	119.32
1	B	362	ASN	CA-CB-CG	5.93	118.53	112.60
2	C	359	GLY	O-C-N	5.92	127.69	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	378	ARG	O-C-N	5.92	129.55	122.27
2	I	354	PRO	N-CA-CB	5.92	109.19	103.51
2	C	243	GLY	CA-C-N	5.91	128.59	120.67
2	C	243	GLY	C-N-CA	5.91	128.59	120.67
2	L	378	ARG	CA-C-N	5.91	128.48	120.38
2	L	378	ARG	C-N-CA	5.91	128.48	120.38
1	E	145	SER	N-CA-C	5.91	115.90	108.45
1	K	903	ASP	CA-C-O	5.91	123.13	119.29
1	B	883	ILE	CB-CA-C	5.90	117.97	111.18
2	C	346	PRO	N-CA-CB	5.90	106.38	102.25
1	K	1035	TYR	CA-CB-CG	-5.90	103.28	113.90
1	H	89	MET	CA-CB-CG	5.89	125.89	114.10
1	K	830	ALA	N-CA-CB	5.88	120.56	110.68
2	L	183	GLN	CA-C-N	-5.88	111.71	120.94
2	L	183	GLN	C-N-CA	-5.88	111.71	120.94
1	B	560	LYS	N-CA-C	5.87	119.39	109.76
1	K	943	ARG	NE-CZ-NH1	5.87	127.37	121.50
2	C	373	LEU	O-C-N	5.86	128.33	122.12
1	K	608	ASP	N-CA-C	-5.86	99.69	109.24
2	I	76	HIS	CA-CB-CG	-5.85	107.95	113.80
1	H	528	VAL	N-CA-C	-5.84	101.26	109.21
2	I	367	PHE	N-CA-C	-5.84	105.04	111.82
2	C	307	ILE	CB-CA-C	5.84	118.16	110.91
1	B	699	MET	N-CA-C	-5.84	104.88	112.23
1	B	1010	THR	N-CA-C	-5.83	106.14	113.72
2	F	33	ASN	CB-CA-C	5.83	120.25	109.70
2	C	58	PRO	N-CA-C	5.83	122.43	113.75
1	K	999	HIS	CA-CB-CG	-5.83	107.97	113.80
1	K	570	ARG	CB-CA-C	-5.82	97.87	111.09
2	I	307	ILE	CB-CA-C	5.82	118.71	111.15
1	K	328	GLY	N-CA-C	5.81	121.61	114.69
1	E	316	PHE	CA-CB-CG	5.81	119.61	113.80
2	F	59	HIS	CA-CB-CG	-5.81	107.99	113.80
1	K	225	ASP	CA-C-N	-5.80	112.63	120.87
1	K	225	ASP	C-N-CA	-5.80	112.63	120.87
1	B	187	PHE	CA-CB-CG	5.80	119.60	113.80
1	K	25	PHE	CA-CB-CG	-5.80	108.00	113.80
1	B	160	ASP	CA-CB-CG	5.80	118.40	112.60
2	I	337	LEU	CB-CA-C	5.79	119.32	109.53
1	B	26	ASP	N-CA-C	-5.79	104.57	111.69
2	L	234	ASP	N-CA-C	-5.79	104.94	112.23
1	E	438	ILE	N-CA-C	-5.79	104.87	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	947	SER	CA-C-N	-5.79	114.73	122.77
1	H	947	SER	C-N-CA	-5.79	114.73	122.77
2	C	351	GLN	N-CA-C	5.78	117.66	111.36
1	H	653	LEU	O-C-N	5.78	128.74	122.15
1	E	362	ASN	CA-CB-CG	5.77	118.37	112.60
1	K	415	ASP	CA-CB-CG	-5.77	106.83	112.60
1	K	26	ASP	N-CA-C	-5.76	104.60	111.69
2	L	339	GLY	O-C-N	5.76	127.65	123.27
1	K	763	VAL	N-CA-CB	5.76	119.65	111.82
1	B	403	VAL	N-CA-C	-5.75	106.70	112.17
1	E	578	ASP	CA-CB-CG	-5.75	106.85	112.60
1	K	705	LYS	N-CA-C	-5.75	105.02	111.28
1	B	991	ASN	CB-CA-C	-5.74	99.70	109.51
1	E	328	GLY	N-CA-C	5.73	121.59	114.37
2	F	201	ALA	N-CA-C	5.73	117.69	110.24
1	B	503	LYS	CB-CA-C	-5.73	101.88	110.88
1	B	939	LYS	CA-C-O	-5.73	114.92	121.68
1	B	1000	ILE	N-CA-CB	-5.73	103.31	110.47
1	B	227	CYS	N-CA-C	5.72	117.72	108.34
1	H	624	ASP	CA-CB-CG	-5.71	106.89	112.60
1	K	419	ALA	N-CA-C	5.70	118.23	111.33
1	B	984	GLY	CA-C-N	-5.70	116.12	123.19
1	B	984	GLY	C-N-CA	-5.70	116.12	123.19
2	C	362	ASP	CA-CB-CG	5.70	118.30	112.60
1	K	953	LYS	N-CA-C	5.69	117.94	111.11
1	E	44	ILE	CA-C-N	-5.69	111.78	121.85
1	E	44	ILE	C-N-CA	-5.69	111.78	121.85
2	L	222	GLN	OE1-CD-NE2	5.68	128.28	122.60
2	I	214	CYS	CB-CA-C	-5.68	99.94	109.48
2	C	296	PRO	CB-CA-C	-5.68	104.47	111.11
1	K	369	ALA	N-CA-CB	-5.67	102.25	110.36
1	K	703	LYS	N-CA-C	-5.67	105.09	111.28
1	H	809	ARG	CB-CA-C	-5.67	101.37	110.79
1	K	676	ARG	CA-C-O	5.67	126.43	120.42
2	C	206	LEU	O-C-N	5.66	127.90	122.07
2	C	174	SER	N-CA-C	5.66	118.48	110.50
2	F	5	ALA	N-CA-CB	5.66	120.33	111.56
2	I	38	GLY	N-CA-C	5.65	123.68	115.32
1	B	433	ASP	CA-CB-CG	-5.65	106.95	112.60
2	C	10	GLU	CB-CA-C	-5.64	99.52	110.46
1	H	568	PRO	CB-CA-C	-5.63	104.02	111.23
2	L	216	LEU	N-CA-C	5.63	118.57	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	43	VAL	N-CA-C	5.63	115.96	107.75
1	B	734	ARG	O-C-N	5.62	127.86	122.07
1	H	229	ILE	N-CA-CB	5.62	118.75	111.67
1	E	997	ARG	N-CA-C	5.62	118.69	110.10
2	F	308	THR	N-CA-C	5.62	118.22	109.52
1	H	209	LEU	N-CA-C	-5.61	104.67	112.30
1	B	110	PHE	N-CA-C	5.58	120.08	112.88
1	H	342	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	K	229	ILE	N-CA-CB	5.58	118.39	111.41
1	B	83	ASP	CA-CB-CG	-5.57	107.03	112.60
1	H	917	MET	N-CA-CB	5.56	120.51	110.83
1	E	1059	GLU	N-CA-C	5.56	117.03	110.97
2	C	141	ALA	CA-C-O	5.56	126.31	120.42
1	H	305	ARG	CA-C-N	5.56	128.18	120.29
1	H	305	ARG	C-N-CA	5.56	128.18	120.29
2	C	67	ASP	N-CA-C	5.55	118.26	111.82
1	K	867	VAL	CB-CA-C	-5.55	104.75	112.02
1	B	558	ARG	CA-C-N	5.55	129.80	122.42
1	B	558	ARG	C-N-CA	5.55	129.80	122.42
1	E	824	LEU	N-CA-C	5.55	118.04	110.55
1	H	866	ARG	NE-CZ-NH2	-5.55	114.21	119.20
2	F	288	PHE	CA-CB-CG	5.55	119.35	113.80
1	K	640	GLN	N-CA-C	5.55	120.04	113.16
2	L	237	PHE	N-CA-C	5.54	118.00	109.07
2	L	346	PRO	N-CA-CB	5.54	106.13	102.25
2	L	288	PHE	CB-CA-C	5.54	116.31	109.16
1	H	992	LYS	N-CA-C	-5.54	103.60	110.41
1	B	302	ARG	CB-CA-C	-5.53	100.83	111.78
1	H	1051	MET	CB-CA-C	-5.53	101.61	110.79
1	K	50	PRO	CB-CA-C	-5.53	102.70	111.04
1	E	49	ASN	CA-C-N	5.52	125.14	119.56
1	E	49	ASN	C-N-CA	5.52	125.14	119.56
1	K	727	VAL	N-CA-C	-5.52	100.47	108.87
1	K	948	VAL	N-CA-CB	-5.52	105.48	112.60
1	B	247	ILE	N-CA-C	-5.52	101.70	109.21
1	H	911	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	B	1071	ILE	N-CA-CB	-5.52	104.70	110.72
2	L	4	SER	N-CA-C	5.52	118.28	110.50
1	B	849	VAL	N-CA-CB	5.51	114.22	110.52
1	K	301	PRO	CB-CA-C	-5.51	102.46	111.56
1	B	102	GLU	O-C-N	5.51	127.98	122.03
1	E	1023	GLU	CB-CA-C	-5.51	100.09	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	523	PRO	CB-CA-C	-5.50	103.74	110.95
2	C	373	LEU	CA-C-N	5.50	127.49	120.56
2	C	373	LEU	C-N-CA	5.50	127.49	120.56
1	E	677	PHE	CA-CB-CG	-5.50	108.30	113.80
1	H	237	ASP	CA-CB-CG	-5.50	107.10	112.60
2	L	190	LEU	CA-C-O	5.50	124.65	119.59
2	F	354	PRO	N-CA-CB	5.50	109.32	103.39
2	C	84	ASP	N-CA-C	5.49	118.41	108.69
2	L	227	ASP	CA-CB-CG	5.49	118.09	112.60
1	E	132	ASP	CA-CB-CG	5.49	118.09	112.60
1	H	757	ASP	CB-CA-C	5.48	119.67	111.89
1	H	954	GLU	N-CA-CB	-5.48	102.13	110.07
1	E	980	LEU	N-CA-C	-5.48	105.21	111.07
1	H	639	VAL	CA-C-O	5.48	124.16	118.96
1	B	985	ILE	O-C-N	5.47	128.93	123.18
1	B	847	ARG	CD-NE-CZ	-5.47	116.74	124.40
2	F	239	SER	N-CA-C	5.47	117.58	110.53
1	B	304	SER	N-CA-C	5.47	115.34	108.45
2	I	247	PRO	CA-C-N	-5.46	113.96	122.05
2	I	247	PRO	C-N-CA	-5.46	113.96	122.05
1	B	324	LYS	CA-CB-CG	-5.46	103.18	114.10
1	K	556	THR	N-CA-CB	-5.46	103.09	110.95
2	C	242	PRO	N-CA-C	5.45	118.86	111.22
2	F	262	ASP	CA-CB-CG	5.45	118.05	112.60
1	H	223	LYS	N-CA-CB	5.45	119.59	110.32
1	K	88	THR	N-CA-C	5.45	120.04	113.17
2	C	362	ASP	N-CA-C	5.45	118.72	111.75
1	H	342	ARG	CG-CD-NE	-5.45	100.01	112.00
1	H	364	GLU	CA-C-O	5.45	126.08	119.49
1	H	452	PHE	CA-CB-CG	-5.45	108.35	113.80
2	I	249	ASP	CA-CB-CG	5.45	118.05	112.60
1	K	556	THR	O-C-N	5.45	128.17	122.23
2	F	304	VAL	CB-CA-C	5.45	119.00	111.38
2	C	198	ASP	CA-CB-CG	5.44	118.04	112.60
2	L	362	ASP	N-CA-C	5.44	117.92	111.33
2	I	216	LEU	N-CA-C	5.44	118.44	109.85
2	L	265	VAL	N-CA-C	5.44	116.11	108.17
2	I	23	THR	N-CA-CB	5.44	118.27	110.06
1	K	731	ALA	CA-C-N	5.44	128.01	120.29
1	K	731	ALA	C-N-CA	5.44	128.01	120.29
1	H	446	LEU	N-CA-C	-5.43	102.44	110.48
1	B	1071	ILE	N-CA-C	5.43	116.40	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	372	GLU	N-CA-C	-5.43	105.05	110.97
2	L	308	THR	N-CA-C	5.43	118.12	109.81
2	F	299	ASP	CA-CB-CG	5.43	118.03	112.60
1	E	705	LYS	CA-C-N	5.43	128.01	120.63
1	E	705	LYS	C-N-CA	5.43	128.01	120.63
1	K	19	ILE	N-CA-CB	5.43	116.84	110.82
1	K	81	ARG	CB-CA-C	-5.43	106.28	111.00
1	B	884	PRO	N-CA-CB	5.41	108.33	103.08
2	L	377	TYR	CA-C-O	-5.41	115.11	120.90
1	H	711	LEU	N-CA-CB	-5.41	102.14	111.55
1	E	87	PRO	CB-CA-C	-5.41	102.64	111.56
2	F	41	GLU	N-CA-C	-5.41	105.55	111.82
1	E	576	GLU	CA-C-O	5.40	126.20	120.10
2	F	84	ASP	N-CA-C	5.40	118.20	108.48
1	K	164	PRO	N-CA-CB	5.40	108.54	102.60
1	H	342	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	H	686	LEU	N-CA-CB	5.39	120.31	111.08
1	E	1009	TYR	N-CA-C	5.39	118.52	109.95
1	H	781	ILE	N-CA-C	-5.39	105.84	110.74
2	I	201	ALA	N-CA-C	5.39	118.09	110.50
1	E	639	VAL	N-CA-CB	-5.38	105.12	112.28
1	H	991	ASN	OD1-CG-ND2	5.38	127.98	122.60
1	B	50	PRO	CB-CA-C	-5.38	103.83	111.68
1	B	971	ASP	CB-CA-C	-5.38	98.73	109.33
1	H	792	ALA	N-CA-C	-5.38	102.52	110.48
1	E	86	LEU	CA-C-O	5.37	123.87	119.36
1	K	362	ASN	CA-CB-CG	5.36	117.96	112.60
1	K	421	THR	CA-C-N	5.36	127.91	120.29
1	K	421	THR	C-N-CA	5.36	127.91	120.29
1	B	730	GLU	CG-CD-OE2	5.36	130.73	118.40
1	E	73	VAL	O-C-N	5.36	127.16	121.91
1	K	531	CYS	N-CA-C	5.36	118.96	111.56
1	B	133	VAL	O-C-N	5.36	127.35	121.83
1	B	1000	ILE	N-CA-C	5.36	116.73	110.62
1	B	431	GLY	N-CA-C	-5.36	103.17	112.06
1	K	693	THR	N-CA-CB	5.35	119.15	110.42
1	E	973	THR	N-CA-C	-5.35	102.60	110.52
1	H	624	ASP	N-CA-C	5.35	116.79	111.07
1	B	781	ILE	N-CA-C	-5.34	105.39	110.42
1	B	357	LYS	CB-CG-CD	-5.34	99.02	111.30
1	B	1013	ILE	N-CA-CB	5.34	118.63	111.90
2	C	299	ASP	CA-CB-CG	5.34	117.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	330	THR	CB-CA-C	5.34	119.31	109.71
1	K	498	ASP	CB-CA-C	-5.33	101.94	110.79
1	K	713	VAL	N-CA-C	5.33	115.46	107.51
1	E	734	ARG	O-C-N	5.33	127.56	122.07
1	B	400	GLY	CA-C-N	5.33	129.12	120.60
1	B	400	GLY	C-N-CA	5.33	129.12	120.60
2	I	117	LYS	CA-C-O	5.33	126.60	120.90
1	B	905	LEU	N-CA-CB	-5.32	101.57	110.83
1	E	238	ALA	N-CA-C	5.32	117.70	110.35
1	B	64	TYR	N-CA-C	5.32	117.30	108.20
2	C	345	LYS	O-C-N	5.32	125.69	121.55
2	I	204	ASN	N-CA-C	5.32	117.07	111.28
1	E	478	VAL	N-CA-C	5.31	116.04	110.62
1	H	807	VAL	CB-CA-C	-5.31	105.07	112.02
2	F	306	MET	N-CA-CB	5.31	120.61	111.00
1	B	201	LYS	N-CA-CB	-5.31	103.85	111.70
1	B	792	ALA	N-CA-C	-5.30	102.63	110.48
1	E	908	PRO	N-CA-CB	5.30	108.40	103.41
2	I	372	GLU	CA-C-N	5.30	127.39	120.28
2	I	372	GLU	C-N-CA	5.30	127.39	120.28
2	C	181	LEU	N-CA-CB	5.30	117.17	110.23
1	E	403	VAL	N-CA-C	-5.30	106.26	111.77
1	H	696	ALA	N-CA-C	5.30	117.93	110.14
1	B	974	HIS	N-CA-C	5.30	122.08	110.80
2	I	353	HIS	CA-CB-CG	5.29	119.09	113.80
1	B	700	ALA	O-C-N	5.29	129.63	122.59
1	B	986	ASN	CA-CB-CG	5.29	117.89	112.60
1	E	33	CYS	N-CA-CB	5.28	117.67	110.01
1	B	884	PRO	CA-C-N	5.28	124.89	119.56
1	B	884	PRO	C-N-CA	5.28	124.89	119.56
2	F	199	PHE	CA-C-O	5.28	125.67	119.28
1	H	894	LEU	CA-C-N	5.28	126.31	120.45
1	H	894	LEU	C-N-CA	5.28	126.31	120.45
2	F	227	ASP	CA-CB-CG	5.27	117.87	112.60
1	E	38	GLU	CB-CG-CD	5.27	121.56	112.60
1	H	403	VAL	N-CA-C	-5.27	107.58	112.43
1	B	494	LYS	O-C-N	-5.27	115.10	122.37
1	B	430	ALA	CA-C-N	5.26	128.46	122.67
1	B	430	ALA	C-N-CA	5.26	128.46	122.67
2	C	286	MET	CG-SD-CE	-5.26	89.32	100.90
2	L	53	VAL	N-CA-C	5.26	116.28	108.23
1	E	109	GLU	CA-C-N	-5.26	114.23	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	109	GLU	C-N-CA	-5.26	114.23	122.65
1	E	402	GLU	CA-C-N	-5.25	114.26	122.56
1	E	402	GLU	C-N-CA	-5.25	114.26	122.56
2	L	296	PRO	CB-CA-C	-5.25	105.83	111.56
1	H	886	TYR	CA-C-N	-5.25	114.83	122.65
1	H	886	TYR	C-N-CA	-5.25	114.83	122.65
1	B	354	VAL	N-CA-CB	5.25	118.65	111.41
1	H	577	PHE	CA-CB-CG	-5.25	108.56	113.80
1	E	577	PHE	CA-CB-CG	-5.24	108.56	113.80
1	H	756	ASP	N-CA-CB	-5.24	102.32	110.29
1	E	860	LEU	N-CA-C	5.24	117.67	111.33
2	F	234	ASP	N-CA-C	-5.24	106.89	113.28
2	L	263	ILE	O-C-N	5.24	126.83	121.07
1	E	66	GLU	O-C-N	5.24	125.06	121.71
1	E	923	PHE	CA-CB-CG	-5.24	108.56	113.80
1	E	210	ILE	CA-C-N	-5.23	115.22	122.86
1	E	210	ILE	C-N-CA	-5.23	115.22	122.86
1	B	281	SER	O-C-N	-5.23	117.62	123.48
1	H	453	ASN	CA-CB-CG	-5.23	107.37	112.60
1	E	1035	TYR	CA-CB-CG	-5.23	104.49	113.90
2	F	200	GLY	CA-C-N	5.22	128.50	120.82
2	F	200	GLY	C-N-CA	5.22	128.50	120.82
1	K	619	PRO	N-CA-CB	5.22	107.96	103.31
2	L	158	LEU	N-CA-C	-5.22	107.29	113.97
2	F	59	HIS	CA-C-N	-5.22	116.72	123.19
2	F	59	HIS	C-N-CA	-5.22	116.72	123.19
1	B	958	ASP	CA-CB-CG	-5.21	107.39	112.60
1	H	23	CYS	N-CA-C	5.21	119.12	112.34
2	L	221	ALA	N-CA-C	5.21	117.64	111.33
2	L	174	SER	N-CA-C	5.21	118.19	110.48
1	E	206	ASP	CA-CB-CG	5.21	117.81	112.60
2	C	233	PRO	CB-CA-C	-5.21	105.16	111.46
1	B	254	THR	N-CA-C	5.21	118.94	112.59
1	B	157	VAL	N-CA-CB	5.21	116.64	110.55
1	K	406	THR	CA-C-O	5.20	125.32	119.18
1	H	190	ILE	N-CA-C	5.20	115.41	110.42
1	K	531	CYS	N-CA-CB	-5.20	104.00	111.54
2	C	264	PRO	N-CA-CB	5.19	108.12	103.19
1	H	1	PRO	CA-C-N	5.19	128.59	120.75
1	H	1	PRO	C-N-CA	5.19	128.59	120.75
1	K	253	GLN	CB-CA-C	-5.19	99.91	109.15
1	H	371	ASP	N-CA-C	5.19	119.30	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	67	ASP	CA-CB-CG	5.19	117.79	112.60
2	L	325	LEU	CA-C-N	-5.19	114.92	122.65
2	L	325	LEU	C-N-CA	-5.19	114.92	122.65
1	K	1036	LYS	CA-C-N	-5.19	115.49	122.91
1	K	1036	LYS	C-N-CA	-5.19	115.49	122.91
2	L	318	GLU	N-CA-C	5.18	118.76	112.23
1	E	857	GLY	CA-C-N	-5.18	118.86	122.59
1	E	857	GLY	C-N-CA	-5.18	118.86	122.59
1	H	443	ARG	CD-NE-CZ	-5.18	117.14	124.40
1	H	487	PHE	N-CA-CB	-5.18	102.48	110.20
2	I	146	LYS	CA-C-O	5.18	125.91	120.42
1	B	265	ASN	O-C-N	5.18	127.41	122.07
2	F	147	ALA	O-C-N	5.18	127.40	122.07
2	F	152	GLY	CA-C-O	-5.18	118.85	122.22
1	K	971	ASP	N-CA-CB	5.18	119.93	111.08
1	B	756	ASP	CA-CB-CG	5.18	117.78	112.60
1	H	618	GLU	N-CA-CB	-5.18	101.05	110.63
1	K	850	PRO	N-CA-CB	5.18	108.77	103.23
1	E	413	SER	CB-CA-C	-5.17	100.79	109.53
2	C	324	ASN	CA-CB-CG	5.17	117.77	112.60
1	E	50	PRO	CB-CA-C	-5.17	104.13	111.68
1	K	295	ILE	CA-C-N	-5.16	115.71	122.37
1	K	295	ILE	C-N-CA	-5.16	115.71	122.37
2	F	57	TYR	CA-CB-CG	-5.16	104.61	113.90
1	H	629	VAL	O-C-N	5.16	127.14	121.83
2	F	243	GLY	CA-C-N	5.15	127.81	120.49
2	F	243	GLY	C-N-CA	5.15	127.81	120.49
1	H	53	ILE	CA-C-O	5.15	126.03	120.47
1	B	208	SER	N-CA-C	5.15	117.94	109.76
1	B	568	PRO	CB-CA-C	-5.15	104.64	111.23
2	C	298	LYS	N-CA-C	5.15	117.63	109.24
2	I	74	GLN	N-CA-CB	-5.15	103.09	111.22
1	B	493	ARG	CD-NE-CZ	-5.14	117.20	124.40
1	B	1044	ASN	CA-CB-CG	-5.14	107.46	112.60
1	B	204	LEU	N-CA-C	-5.14	100.79	109.07
2	F	123	ARG	CA-C-N	5.14	127.43	120.44
2	F	123	ARG	C-N-CA	5.14	127.43	120.44
2	L	346	PRO	N-CA-C	-5.14	105.54	112.48
1	B	971	ASP	N-CA-CB	5.14	119.86	111.08
1	B	81	ARG	NE-CZ-NH2	-5.13	114.58	119.20
1	K	14	ALA	N-CA-C	5.13	119.59	113.23
1	K	25	PHE	N-CA-CB	5.13	118.44	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	820	GLN	CB-CA-C	-5.13	105.26	111.82
1	K	277	GLU	CB-CA-C	-5.13	100.45	109.07
1	B	786	VAL	N-CA-C	-5.12	100.37	107.80
1	B	187	PHE	N-CA-CB	5.12	117.43	110.01
1	H	774	ILE	N-CA-CB	5.12	116.83	111.00
1	E	697	ILE	N-CA-C	5.12	115.73	110.36
1	E	1002	ASP	CA-CB-CG	5.12	117.72	112.60
1	H	525	TYR	CB-CA-C	5.12	118.57	109.72
1	B	363	PHE	CA-C-O	5.11	125.93	120.20
2	C	98	LEU	N-CA-C	5.11	116.85	111.28
2	F	16	HIS	N-CA-C	5.11	116.63	108.41
2	I	260	GLU	N-CA-C	-5.11	106.88	113.01
1	E	37	ARG	CD-NE-CZ	5.10	131.54	124.40
1	B	28	SER	N-CA-C	5.10	116.53	111.07
1	E	915	GLU	N-CA-C	5.10	116.94	109.24
1	E	999	HIS	CA-CB-CG	-5.10	108.70	113.80
1	B	301	PRO	CA-C-O	-5.09	117.54	121.31
1	H	232	SER	N-CA-CB	5.09	118.99	110.85
1	H	517[A]	ASP	CA-CB-CG	5.09	117.69	112.60
1	H	517[B]	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	769	GLY	N-CA-C	-5.08	108.65	114.69
1	E	17	ILE	CB-CA-C	-5.08	103.32	111.59
1	K	754	PHE	CA-CB-CG	-5.08	108.72	113.80
1	K	983	ALA	N-CA-C	-5.08	106.78	113.17
1	B	673	ASP	CA-C-N	5.07	128.43	120.82
1	B	673	ASP	C-N-CA	5.07	128.43	120.82
1	E	494	LYS	N-CA-C	-5.07	106.78	113.17
1	K	650	ALA	N-CA-C	5.07	117.21	111.02
1	K	282	ASN	CA-CB-CG	5.07	117.67	112.60
1	K	416	ASP	CA-C-N	5.07	124.86	119.28
1	K	416	ASP	C-N-CA	5.07	124.86	119.28
1	B	923	PHE	CA-CB-CG	-5.07	108.73	113.80
1	E	729	ASP	CA-CB-CG	5.07	117.67	112.60
1	K	974	HIS	N-CA-C	5.07	121.59	110.80
1	H	339	THR	N-CA-C	-5.07	106.85	112.57
1	B	570	ARG	CB-CA-C	-5.06	99.61	111.09
1	K	784	ALA	N-CA-C	-5.06	102.90	110.23
2	F	109	ALA	CA-C-N	-5.05	115.92	122.94
2	F	109	ALA	C-N-CA	-5.05	115.92	122.94
1	H	99	LEU	N-CA-C	5.05	118.70	112.54
1	K	305	ARG	CD-NE-CZ	-5.04	117.34	124.40
1	B	222	ASP	N-CA-CB	5.04	118.22	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	PHE	CA-CB-CG	-5.04	108.76	113.80
2	C	265	VAL	N-CA-C	5.04	115.38	108.12
2	I	348	PHE	CA-CB-CG	5.04	118.84	113.80
2	L	148	ARG	NE-CZ-NH2	5.04	123.73	119.20
2	F	32	PHE	CB-CA-C	5.03	118.98	109.37
1	K	208	SER	N-CA-C	5.03	117.76	109.76
1	K	79	LYS	N-CA-C	5.03	118.56	112.23
2	L	204	ASN	N-CA-CB	5.03	117.51	110.12
1	E	403	VAL	CB-CA-C	-5.03	105.78	112.46
2	L	106	ASN	CA-CB-CG	-5.02	107.58	112.60
2	C	346	PRO	CB-CA-C	-5.02	106.31	112.89
1	H	337	ASP	N-CA-C	5.02	117.14	111.02
1	E	731	ALA	CA-C-N	5.02	127.50	120.28
1	E	731	ALA	C-N-CA	5.02	127.50	120.28
1	B	1009	TYR	N-CA-C	5.01	117.73	109.72
1	E	157	VAL	O-C-N	5.01	126.99	121.83
2	I	138	PRO	CA-C-N	5.01	129.08	122.42
2	I	138	PRO	C-N-CA	5.01	129.08	122.42
1	K	833	ASN	CB-CA-C	-5.01	104.62	111.73
2	L	11	ASP	CA-CB-CG	5.01	117.61	112.60
1	B	149	HIS	N-CA-C	-5.00	107.22	113.72
2	F	107	ILE	N-CA-C	5.00	115.89	108.23
1	H	183	ASN	O-C-N	-5.00	118.07	123.42

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	220	0
1	E	8223	0	8265	287	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	8179	0	8215	261	0
1	K	8201	0	8241	224	0
2	C	2895	0	2863	139	0
2	F	2904	0	2868	157	0
2	I	2895	0	2863	156	0
2	L	2895	0	2863	100	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	2	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
8	E	54	0	24	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	20	1
11	C	241	0	0	6	0
11	E	1022	0	0	31	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	1524	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 (1524) 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
2:I:228:VAL:HA	2:I:231:MET:HE3	1.35	1.09
1:K:562:MET:HE3	1:K:634:PRO:HG3	1.34	1.06
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
1:B:0:MET:H2	1:B:223:LYS:NZ	1.58	1.02
2:I:133:ILE:HD12	2:I:143:ALA:HB2	1.42	1.02
1:H:562:MET:HE3	1:H:634:PRO:HG3	1.39	1.00
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:NE2	1:H:783:GLN:H	1.60	0.97
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:HD12	1:E:697:ILE:H	1.27	0.95
2:C:261:THR:HG21	2:C:263:ILE:HG13	1.45	0.95
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:E:783:GLN:NE2	1.70	0.89
1:H:702:GLU:HA	1:H:705:LYS:HD2	1.53	0.89
1:B:562:MET:HE3	1:B:634:PRO:HG3	1.52	0.89
1:E:702:GLU:HA	1:E:705:LYS:HD2	1.51	0.89
1:B:0:MET:H2	1:B:223:LYS:HZ1	0.91	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
1:H:733:LEU:HD22	1:H:737:PHE:HD2	1.39	0.87
1:E:1020[B]:ARG:HG2	1:E:1020[B]:ARG:HH11	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:HG3	2:I:215:ARG:HH11	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:E:783:GLN:H	1:E:783:GLN:HE21	1.19	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:H	1:B:783:GLN:NE2	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
1:H:587:ALA:HB2	1:H:862:LYS:HG2	1.61	0.82
1:B:0:MET:N	1:B:223:LYS:HZ1	1.75	0.82
1:E:674:ARG:H	1:E:674:ARG:HD2	1.43	0.82
1:H:480:ILE:CD1	1:H:507:VAL:HG11	2.10	0.82
1:B:694:VAL:HA	1:B:699:MET:HE3	1.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:783:GLN:HE21	1:H:783:GLN:N	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
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:B:0:MET:N	1:B:223:LYS:NZ	2.28	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:31:GLN:OE1	1:E:319:ALA:HB3	1.84	0.77
1:E:1072:LYS:HE3	1:E:1072:LYS:HA	1.65	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
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:258:LYS:O	1:E:262:ILE:HG13	1.86	0.76
1:E:1072:LYS:HA	1:E:1072:LYS:CE	2.15	0.76
1:H:28[B]:SER:OG	1:H:303:VAL:HG21	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:K:783:GLN:HE21	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
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
2:C:286:MET:HE1	2:C:312:HIS:ND1	2.04	0.72
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
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:152:GLY:O	2:I:156:MET:HE3	1.89	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:674:ARG:H	1:E:674:ARG:CD	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:714:ARG:HG3	1:B:724:MET:HE2	1.73	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:152:GLY:O	2:L:156:MET:HE3	1.91	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:HD2	1:H:674:ARG:N	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:HD12	1:H:946:LEU:N	2.08	0.68
1:K:64:TYR:OH	1:K:79:LYS:HE2	1.93	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:HD12	1:B:697:ILE:H	1.58	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:L:208:MET:HE2	2:L:367:PHE:CE2	2.31	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:6:LEU:HD12	2:C:7:LEU:N	2.11	0.65
2:C:192:PHE:O	2:C:215:ARG:HG3	1.95	0.65
1:H:658:VAL:HG13	1:H:659:PRO:HD2	1.79	0.65
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:HD2	1:K:674:ARG:N	2.09	0.65
1:E:153:GLU:O	1:E:157:VAL:HG23	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:730:GLU:CD	1:B:734:ARG:HH21	2.05	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:OE1	1:H:100:GLU:HA	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
2:C:228:VAL:HA	2:C:231:MET:HE3	1.77	0.64
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:673:ASP:OD2	1:K:676:ARG:HG3	1.97	0.64
1:B:701:VAL:O	1:B:705:LYS:HG3	1.98	0.64
1:B:901:GLY:O	1:B:1026:ARG:NH2	2.30	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
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:HD13	2:L:218:ILE:N	2.12	0.64
1:K:738:GLN:HE21	1:K:738:GLN:C	2.06	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
1:K:783:GLN:H	1:K:783:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:709:TYR:HB3	1:E:710:PRO:HA	1.82	0.62
1:E:966[A]:GLN:HG2	1:E:1053:LEU:HD13	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:B:418[B]:GLU:CD	1:H:421:THR:HG21	2.24	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:480:ILE:HD12	1:H:507:VAL:HG11	1.79	0.61
1:H:857:GLY:HA2	1:H:1068:HIS:CE1	2.35	0.61
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:HD12	1:E:697:ILE:N	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:152:GLY:O	2:F:156:MET:HE3	2.00	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:E:783:GLN:HE21	1:E:783:GLN:N	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:762:ASP:HB3	1:B:778:MET:HE3	1.84	0.59
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
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
1:B:399:ARG:HD3	11:B:1493:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:MET:HE1	1:B:629:VAL:HG22	1.84	0.59
1:B:1018:GLY:O	1:B:1022:ILE:HG13	2.03	0.59
1:E:712:VAL:HG23	1:E:754:PHE:HB2	1.84	0.59
1:B:508:ARG:NH1	1:B:510:ALA:HB3	2.18	0.59
1:B:1062:ILE:HD13	1:B:1067:MET:HG3	1.84	0.59
2:F:67:ASP:O	2:F:70:GLU:HG3	2.03	0.59
2:F:295:HIS:CE1	2:F:333:PHE:HD2	2.21	0.59
2:I:350:PHE:HD2	2:I:354:PRO:HD3	1.65	0.59
1:K:691:ASN:N	1:K:691:ASN:ND2	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: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:H:163:PHE:HA	1:H:164:PRO:C	2.28	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:HH11	2:C:212:ARG:HG3	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
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
2:F:286:MET:HE1	2:F:290:HIS:CD2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:215:ARG:C	2:I:216:LEU:HD23	2.29	0.57
1:K:644:GLN:NE2	1:K:648:LYS:HZ3	2.02	0.57
2:F:31:VAL:HG11	2:F:51:GLN:OE1	2.05	0.57
2:F:158:LEU:O	2:F:161:GLU:HB2	2.04	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
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
2:F:186:LYS:N	2:F:189:GLU:OE1	2.30	0.57
1:H:274:ILE:HG22	1:H:276:VAL:HG23	1.87	0.57
1:H:999:HIS:CD2	1:H:1002:ASP:H	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:727:VAL:CG1	1:E:732:ASP:HB3	2.35	0.57
1:H:37:ARG:HG3	1:H:37:ARG:HH11	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:694:VAL:O	1:E:749:VAL:HB	2.05	0.56
1:E:725:GLU:HG3	1:E:726:ILE:H	1.70	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:515:LEU:C	1:E:515:LEU:HD23	2.30	0.56
1:E:727:VAL:HG12	1:E:732:ASP:HB3	1.87	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: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:40:GLN:HE21	2:I:70:GLU:HG3	1.71	0.56
2:I:238:LEU:HB2	2:I:267:GLY:HA2	1.86	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:27:TYR:CE1	1:B:312:LYS:HE3	2.41	0.56
1:B:212:TRP:CZ3	1:B:295:ILE:HD12	2.41	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:562:MET:HE3	1:H:634:PRO:CG	2.26	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:228:VAL:HA	2:C:231:MET:HE2	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:HD3	1:H:570:ARG:N	2.22	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
1:K:1025:SER:HB3	7:K:1093:GLN:HA	1.88	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: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:N	1:H:166:ILE:HD12	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
1:H:562:MET:HE1	1:H:629:VAL:HG22	1.90	0.54
2:I:238:LEU:O	2:I:271:GLY:HA3	2.07	0.54
1:K:673:ASP:CG	1:K:676:ARG:HG3	2.33	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
1:H:709:TYR:HA	1:H:710:PRO:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:286:MET:HE1	2:C:312:HIS:CE1	2.43	0.53
2:F:6:LEU:CD2	2:F:8:VAL:HG23	2.38	0.53
2:F:121:LEU:HD11	2:F:125:LYS:HD2	1.90	0.53
1:B:762:ASP:CB	1:B:778:MET:HE3	2.37	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
1:K:58:GLU:HG2	1:K:59:MET:HE2	1.90	0.53
2:L:277:LEU:HD23	2:L:281:ALA:O	2.08	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:29:GLU:OE2	2:F:285:LYS:NZ	2.31	0.53
2:F:150:PHE:CD1	2:F:151:PRO:HD2	2.43	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
1:H:425:ARG:HD3	1:H:425:ARG:C	2.33	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: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:B:1016:THR:HG22	1:B:1017:SER:N	2.22	0.53
2:I:208:MET:HE3	11:I:3149:HOH:O	2.09	0.53
1:K:227:CYS:SG	1:K:268:MET:HE2	2.48	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
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:OE1	2:I:355:GLU:N	2.36	0.53
1:E:677:PHE:O	1:E:681:VAL:HG23	2.09	0.53
1:E:992:LYS:NZ	5:E:1082:PO4:O1	2.30	0.53
1:H:560:LYS:HG2	1:H:594:GLU:OE1	2.09	0.53
2:L:355:GLU:OE1	2:L:355:GLU:N	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:906:LEU:HD11	9:E:1097:ORN:HB2	1.91	0.53
1:E:1003:ARG:HB3	1:E:1008:GLU:HG3	1.91	0.53
1:K:783:GLN:HE22	1:K:1042:THR:HB	1.74	0.53
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:669:ASP:OD2	1:B:676:ARG:NH2	2.32	0.52
1:B:1017:SER:O	1:B:1021:ALA:HB3	2.09	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:E:953:LYS:NZ	5:E:1082:PO4:O4	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:K:738:GLN:NE2	1:K:739:THR:N	2.48	0.51
1:K:906:LEU:HD11	9:K:1097:ORN:HD3	1.91	0.51
2:L:324:ASN:H	2:L:324:ASN:ND2	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:OD1	2:I:324:ASN:N	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:H:488:LEU:HD23	1:H:519:TYR:HD2	1.75	0.51
2:I:217:THR:O	2:I:217:THR:HG22	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:222:ASP:CG	1:E:226:ASN:HB2	2.36	0.51
1:E:239:MET:HE3	8:E:1095:ADP:C4	2.46	0.51
1:E:884:PRO:HG2	11:E:1969:HOH:O	2.09	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:H:999:HIS:HD2	1:H:1002:ASP:H	1.59	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
1:H:795:LEU:C	1:H:795:LEU:HD23	2.35	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
2:C:246:ALA:C	2:C:248:CYS:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:709:TYR:HA	1:B:710:PRO:C	2.36	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
1:B:666:ASP:CG	1:B:676:ARG:HH22	2.19	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
1:H:945:LEU:C	1:H:946:LEU:HD12	2.36	0.50
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:738:GLN:C	1:E:740:ALA:H	2.20	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:804:ILE:CD1	1:B:836:VAL:HG23	2.42	0.50
1:B:906:LEU:CD1	9:B:1095:ORN:HD3	2.37	0.50
1:E:1050:ALA:O	1:E:1053:LEU:HB2	2.12	0.50
2:F:6:LEU:O	2:F:132:ILE:HA	2.11	0.50
2:F:121:LEU:CD1	2:F:125:LYS:HD2	2.42	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:E:771[A]:MET:HE3	11:E:2284:HOH:O	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:621:THR:O	1:K:625:VAL:HG23	2.12	0.50
1:K:697:ILE:H	1:K:697:ILE:CD1	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
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:152:GLY:O	2:C:156:MET:HE3	2.11	0.50
2:C:276:ALA:O	2:C:281:ALA:HB3	2.12	0.50
2:F:57:TYR:CE1	2:F:58:PRO:HD2	2.47	0.50
2:F:142:LEU:CD2	2:F:146:LYS:HD2	2.42	0.50
1:K:644:GLN:HE21	1:K:648:LYS:HZ3	1.57	0.50
2:F:188:ASP:N	2:F:188:ASP:OD1	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:725:GLU:HG3	1:E:726:ILE:N	2.26	0.49
1:E:1020[B]:ARG:NH1	11:E:2427:HOH:O	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ILE:O	1:E:81:ARG:N	2.42	0.49
1:E:132:ASP:HB2	11:E:1380:HOH:O	2.12	0.49
2:F:295:HIS:CE1	2:F:333:PHE:CD2	3.00	0.49
2:L:363:ALA:C	2:L:365:PRO:HD2	2.37	0.49
1:B:63:THR:O	1:B:1064:VAL:HG23	2.13	0.49
1:B:795:LEU:HD23	1:B:795:LEU:C	2.38	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
2:I:272:HIS:HB2	2:I:349:SER:HB2	1.95	0.49
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: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: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
2:L:318:GLU:O	2:L:321:LEU:HB2	2.13	0.48
1:H:697:ILE:HD12	1:H:697:ILE:N	2.28	0.48
1:K:297:ILE:HG13	11:K:1381:HOH:O	2.14	0.48
1:B:35:ALA:HB1	1:B:324:LYS:HE3	1.95	0.48
1:B:949:ARG:HG3	1:B:1015:THR:OG1	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	2:L:212:ARG:NH1	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:34:THR:HA	2:F:56:THR:OG1	2.14	0.48
2:F:266:PHE:HB2	2:F:370:PHE:CD1	2.49	0.48
2:F:324:ASN:HD22	2:F:324:ASN:N	1.97	0.48
1:K:382:GLU:OE2	1:K:603:GLU:OE2	2.31	0.48
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:713:VAL:CG2	1:H:727:VAL:HG21	2.44	0.48
1:H:1036:LYS:HE2	11:H:1338:HOH:O	2.13	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: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
1:H:1019:ARG:HD2	1:H:1019:ARG:HA	1.51	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:48:TYR:HA	2:C:51:GLN:HE21	1.79	0.48
2:C:376:GLN:O	2:C:379:LYS:HB2	2.14	0.48
1:E:1020[B]:ARG:HG2	1:E:1020[B]:ARG:NH1	2.15	0.48
2:F:212:ARG:HB3	2:F:371:ILE:CD1	2.44	0.48
1:H:8:SER:OG	1:H:83:ASP:N	2.45	0.48
1:H:171:PHE:HB3	1:H:199:PRO:HG2	1.95	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:B:714:ARG:CG	1:B:724:MET:HE2	2.44	0.47
1:E:487:PHE:O	1:E:491:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:295:HIS:HE1	2:I:331:SER:CB	2.27	0.47
2:L:50:ARG:HE	2:L:50:ARG:HB3	1.36	0.47
1:B:699:MET:O	1:B:703:LYS:HB2	2.13	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
1:B:384:MET:HE2	1:B:617:PHE:CE1	2.49	0.47
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
1:B:338:ILE:O	1:B:537:THR:OG1	2.32	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:165:CYS:C	1:H:166:ILE:HD12	2.39	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:I:121:LEU:C	2:I:121:LEU:HD12	2.38	0.47
1:B:695:THR:H	1:B:699:MET:HE2	1.79	0.47
2:C:190:LEU:HD11	2:C:210:VAL:HG13	1.97	0.47
2:C:322:PRO:HB2	2:C:324:ASN:HD22	1.79	0.47
1:E:587:ALA:HB2	1:E:862:LYS:HG2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:952:ASP:CB	1:H:1043:LEU:HD22	2.45	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:225:ALA:HB2	2:C:254:ALA:HA	1.97	0.47
1:E:317:PRO:HG3	1:E:609:TYR:OH	2.15	0.47
1:E:478:VAL:HB	1:E:482:GLY:HA3	1.96	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:O	1:B:712:VAL:HG12	2.14	0.47
1:E:993:VAL:HG22	1:E:999:HIS:CG	2.50	0.47
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:346:SER:O	2:L:296:PRO:HB3	2.15	0.47
1:K:990:VAL:CG2	1:K:1003[A]:ARG:HD2	2.45	0.47
2:L:324:ASN:C	2:L:343:THR:HG23	2.40	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:55:LEU:HA	2:F:55:LEU:HD23	1.76	0.47
2:F:277:LEU:HD23	2:F:281:ALA:O	2.15	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:H:1025:SER:HB3	7:H:1090:GLN:HB3	1.97	0.47
1:K:480:ILE:O	1:K:480:ILE:HG13	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
1:E:819:LEU:O	1:E:820:GLN:HB2	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:58:GLU:HB3	11:E:1312:HOH:O	2.14	0.46
1:E:478:VAL:HG23	1:E:479:GLY:N	2.29	0.46
1:E:713:VAL:HG23	1:E:727:VAL:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	2:I:121:LEU:O	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:45:ASP:HB2	11:L:4256:HOH:O	2.15	0.46
2:L:201:ALA:HB2	2:L:239:SER:HB2	1.98	0.46
2:L:212:ARG:HG3	2:L:212:ARG:HH11	1.79	0.46
2:L:341:HIS:CD2	2:L:348:PHE:HB3	2.51	0.46
1:B:44:ILE:HG23	1:B:62:ALA:HB3	1.97	0.46
2:F:170:TRP:C	2:F:171:THR:HG23	2.39	0.46
1:H:153:GLU:O	1:H:157:VAL:HG23	2.15	0.46
2:I:57:TYR:CE1	2:I:58:PRO:HD2	2.49	0.46
2:I:298:LYS:HB2	2:I:332:LEU:HD21	1.98	0.46
2:L:212:ARG:HB3	2:L:371:ILE:CD1	2.45	0.46
2:C:350:PHE:CG	2:C:366:LEU:CD2	2.98	0.46
1:H:3:ARG:HD3	1:H:6:ILE:HD12	1.97	0.46
1:H:157:VAL:HG11	1:H:205:ILE:HB	1.97	0.46
1:H:749:VAL:O	1:H:749:VAL:HG12	2.14	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:HD23	2:F:158:LEU:HA	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:44:ILE:HA	1:E:62:ALA:O	2.16	0.46
1:E:856:THR:O	1:E:1071:ILE:HD12	2.15	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:5:ASP:N	1:K:5:ASP:OD1	2.49	0.46
1:K:16:PRO:HG3	1:K:916:VAL:CG1	2.46	0.46
1:B:714:ARG:HB2	1:B:750:LEU:CB	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:8:SER:HB3	1:B:42:ARG:HB3	1.97	0.46
1:B:671:ALA:CB	1:B:843:PRO:HG3	2.46	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
1:K:692:ALA:CB	1:K:707:ILE:HD11	2.46	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
2:I:237:PHE:HZ	2:I:268:ILE:HD12	1.81	0.46
2:L:46:PRO:HA	2:L:76:HIS:CG	2.50	0.46
1:E:492:LYS:HD2	1:E:492:LYS:HA	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:39:GLU:OE1	1:B:329:TYR:OH	2.32	0.45
1:B:725:GLU:CG	1:B:726:ILE:N	2.79	0.45
1:B:839:ILE:O	1:B:840:GLU:HB3	2.14	0.45
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:74:ARG:HG2	1:K:74:ARG:NH1	2.20	0.45
1:K:362:ASN:OD1	1:K:380:VAL:HG21	2.16	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:HG3	1:B:949:ARG:H	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:74:GLN:HG3	2:L:76:HIS:NE2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:GLN:C	1:B:681:VAL:HG12	2.40	0.45
2:C:191:PRO:HD2	2:C:213:GLY:O	2.16	0.45
1:E:825:MET:HE2	1:E:827:VAL:CG2	2.47	0.45
2:F:232:ASN:N	2:F:233:PRO:CD	2.80	0.45
1:K:74:ARG:HH11	1:K:74:ARG:CG	2.24	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
2:L:324:ASN:ND2	2:L:324:ASN:N	2.61	0.45
1:B:138:ILE:HG21	1:B:273:GLU:HB2	1.98	0.45
1:B:173:MET:HB2	5:B:1078:PO4:O1	2.15	0.45
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
1:E:1020[B]:ARG:NH2	1:E:1023:GLU:CG	2.77	0.45
2:I:267:GLY:HA3	2:I:271:GLY:O	2.17	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:K:1035:TYR:HA	11:K:1859:HOH:O	2.15	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
1:B:695:THR:H	1:B:699:MET:CE	2.29	0.45
2:C:232:ASN:N	2:C:233:PRO:CD	2.79	0.45
1:H:475:VAL:HG13	1:H:483:LEU:HD21	1.97	0.45
1:H:1027:VAL:O	1:H:1031:SER:HB2	2.16	0.45
2:I:285:LYS:HG3	2:I:314:PHE:CZ	2.50	0.45
2:L:306:MET:HE2	2:L:329:HIS:CD2	2.51	0.45
1:E:157:VAL:HG11	1:E:205:ILE:HB	1.98	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: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:B:805:GLN:HA	1:B:808:MET:HE2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:492:LYS:HD2	1:H:492:LYS:HA	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
1:B:953:LYS:C	1:B:956:VAL:HG12	2.42	0.45
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:HD12	2:F:321:LEU:HA	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
2:C:286:MET:CE	2:C:312:HIS:ND1	2.78	0.44
2:C:364:ALA:C	2:C:366:LEU:H	2.26	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:1000:ILE:HG21	1:E:1028:ILE:HG12	1.99	0.44
1:E:1003:ARG:CB	1:E:1008:GLU:HG3	2.46	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:533:ALA:HB2	2:L:116:ARG:NH1	2.31	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:B:0:MET:N	1:B:223:LYS:HZ2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:795:LEU:C	1:E:795:LEU:HD23	2.42	0.44
1:H:697:ILE:O	1:H:700:ALA:HB3	2.17	0.44
1:K:966:GLN:O	1:K:966:GLN:HG3	2.17	0.44
1:B:221:ARG:NH2	1:B:272:ARG:HG2	2.32	0.44
1:E:342[B]:ARG:HH12	1:E:536:ALA:C	2.25	0.44
2:I:26:ALA:O	2:I:131:CYS:HA	2.16	0.44
2:I:279:SER:CB	2:I:325:LEU:HD11	2.48	0.44
2:I:284:VAL:O	2:I:315:ALA:N	2.43	0.44
1:K:702:GLU:OE1	1:K:702:GLU:HA	2.17	0.44
2:L:273:GLN:HE21	2:L:351:GLN:HE22	1.65	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:59:MET:HE2	11:B:1942:HOH:O	2.16	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
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:378:LYS:HE2	11:K:1329:HOH:O	2.17	0.44
1:K:691:ASN:N	1:K:691:ASN:HD22	2.14	0.44
1:K:947:SER:O	1:K:1014:ASN:HA	2.16	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:HA	1:H:104:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:126:GLU:HB2	1:H:171:PHE:CZ	2.52	0.44
1:H:673:ASP:CG	1:H:676:ARG:HB2	2.43	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:HD12	2:C:332:LEU:HA	1.41	0.44
1:E:39:GLU:OE1	1:E:329:TYR:OH	2.29	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
2:C:113:ILE:HD12	2:C:113:ILE:C	2.43	0.43
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
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:70:TRP:CE2	1:K:71:GLU:HG3	2.53	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
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:810[B]:GLN:HE21	1:K:810[B]:GLN:HB2	1.31	0.43
1:K:1053:LEU:HD23	1:K:1053:LEU:HA	1.71	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:81:ARG:HD3	11:E:2311:HOH:O	2.18	0.43
1:E:636:GLY:HA2	1:E:659:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:334:ASP:CG	2:L:336:THR:HG23	2.44	0.43
1:B:165:CYS:C	1:B:166:ILE:HD12	2.43	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:NE2	1:H:783:GLN:N	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
1:H:825:MET:HE3	1:H:825:MET:HB2	1.87	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:H	1:H:58:GLU:HG2	0.80	0.43
1:K:239:MET:HE3	8:K:1095:ADP:C4	2.54	0.43
2:L:163:THR:HB	2:L:221:ALA:HB2	2.01	0.43
1:B:360:ARG:CZ	1:B:570:ARG:HG2	2.49	0.43
1:B:1016:THR:CG2	1:B:1017:SER:N	2.81	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
1:H:805:GLN:HA	1:H:808:MET:HE3	1.99	0.43
2:I:246:ALA:C	2:I:248:CYS:H	2.26	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: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:227:CYS:O	1:B:268:MET:HE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:862:LYS:O	1:B:866:ARG:HG3	2.19	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:H:966:GLN:HG2	1:H:1053:LEU:HD13	2.01	0.43
1:K:58:GLU:CG	1:K:59:MET:HE2	2.48	0.43
1:K:151:MET:HE2	1:K:151:MET:HB2	1.77	0.43
2:L:208:MET:HE2	2:L:367:PHE:CD2	2.52	0.43
1:B:270:VAL:HG12	1:B:299:MET:HE3	2.00	0.42
1:B:645:THR:HB	1:B:646:PRO:HD3	2.01	0.42
1:B:1020:ARG:HD3	1:B:1020:ARG:HA	1.54	0.42
1:E:989:LEU:HD23	1:H:978:ILE:HG12	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
2:I:363:ALA:C	2:I:365:PRO:HD2	2.44	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:F:334:ASP:CG	2:F:336:THR:HG23	2.43	0.42
2:L:83:ARG:O	2:L:112:ASP:HA	2.19	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
1:B:299:MET:O	1:B:299:MET:HG3	2.18	0.42
1:B:478:VAL:CG2	1:B:482:GLY:HA3	2.49	0.42
1:E:733:LEU:HD22	1:E:737:PHE:HD2	1.85	0.42
1:H:824:LEU:HG	1:H:864:ALA:CB	2.49	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:K:7:LYS:HB2	1:K:83:ASP:OD2	2.18	0.42
1:K:517:ASP:HB2	11:K:1585:HOH:O	2.19	0.42
1:K:736:TYR:C	1:K:738:GLN:N	2.76	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:58:PRO:HA	2:I:83:ARG:HB3	2.00	0.42
2:I:380:THR:HG22	2:I:380:THR:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:LEU:HB3	2:L:15:PHE:HB2	2.01	0.42
2:C:48:TYR:HA	2:C:51:GLN:NE2	2.35	0.42
2:C:295:HIS:CE1	2:C:333:PHE:HD2	2.37	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
1:H:549:GLU:OE1	2:I:117:LYS:HA	2.19	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
10:H:1095:NET:H72	10:H:1095:NET:H62	1.76	0.42
2:I:45:ASP:HB3	2:I:48:TYR:HD2	1.84	0.42
2:I:332:LEU:HA	2:I:332:LEU:HD12	1.68	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:B:562:MET:HE3	1:B:634:PRO:CG	2.36	0.42
1:E:901:GLY:HA2	1:E:1030:ARG:NH1	2.34	0.42
2:F:78:GLN:HA	2:F:78:GLN:NE2	2.34	0.42
2:F:332:LEU:HA	2:F:332:LEU:HD12	1.64	0.42
2:F:351:GLN:O	2:F:351:GLN:HG3	2.20	0.42
1:H:733:LEU:HA	1:H:733:LEU:HD23	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:HD23	2:C:158:LEU:HA	1.90	0.42
2:C:198:ASP:O	2:C:221:ALA:HB2	2.19	0.42
2:C:363:ALA:O	2:C:366:LEU:HB2	2.19	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:265:ASN:ND2	11:E:1539:HOH:O	2.44	0.42
1:E:342[B]:ARG:NH1	1:E:536:ALA:C	2.77	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
1:E:901:GLY:O	1:E:1026:ARG:NH2	2.53	0.42
2:F:7:LEU:HB3	2:F:15:PHE:HB2	2.00	0.42
2:F:269:CYS:HB2	11:F:2274:HOH:O	2.18	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
2:I:237:PHE:C	2:I:238:LEU:HD23	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:270:VAL:HG12	1:B:299:MET:CE	2.50	0.42
1:B:408:PHE:O	1:B:443:ARG:NH2	2.49	0.42
1:B:949:ARG:HD2	1:B:952:ASP:CG	2.45	0.42
1:E:1036:LYS:HE2	11:E:1447:HOH:O	2.19	0.42
2:F:28:GLY:HA3	2:F:50:ARG:O	2.20	0.42
2:F:249:ASP:N	2:F:249:ASP:OD1	2.50	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
1:K:69:HIS:O	1:K:73:VAL:HG23	2.19	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:B:348:GLU:O	2:C:294:ASN:HB2	2.20	0.42
1:B:1050:ALA:HA	1:B:1053:LEU:HD12	2.02	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: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:55:LEU:HD13	2:I:60:ILE:HD12	2.02	0.42
2:I:350:PHE:HB2	2:I:366:LEU:HD23	2.01	0.42
1:K:201:LYS:NZ	1:K:201:LYS:HB3	2.35	0.42
1:K:802:GLN:HE21	1:K:802:GLN:HB2	1.56	0.42
1:K:1019:ARG:HD2	1:K:1019:ARG:HA	1.50	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:HD23	1:E:140:LEU:HA	1.85	0.42
1:E:980:LEU:HD23	1:E:980:LEU:HA	1.86	0.42
1:H:137:LYS:HE3	1:H:273:GLU:OE2	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:K:364:GLU:CD	1:K:364:GLU:H	2.28	0.42
1:B:187:PHE:HZ	1:B:205:ILE:HD13	1.84	0.41
1:B:290:LYS:NZ	11:B:1364:HOH:O	2.50	0.41
1:B:418[B]:GLU:OE1	1:B:421:THR:HB	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:969:GLU:O	1:B:970:LEU:HD23	2.20	0.41
1:E:641:TYR:OH	1:E:864:ALA:HB3	2.19	0.41
1:E:703:LYS:HD2	1:E:703:LYS:HA	1.37	0.41
1:E:997:ARG:HA	1:E:998:PRO:C	2.42	0.41
1:E:1023:GLU:HG2	1:E:1023:GLU:H	1.67	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:65:ILE:CG2	1:K:917:MET:HB3	2.49	0.41
1:K:330:THR:OG1	1:K:333:GLU:HG3	2.20	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:9:LEU:O	2:F:12:GLY:N	2.50	0.41
2:F:350:PHE:CG	2:F:366:LEU:HD21	2.55	0.41
1:H:378:LYS:HB3	1:H:899:PHE:HE1	1.85	0.41
1:H:894:LEU:HA	1:H:895:PRO:HD3	1.92	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
2:C:11:ASP:CG	2:C:128:GLN:HE22	2.28	0.41
2:C:228:VAL:C	2:C:230:LYS:H	2.27	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
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:HD23	1:K:733:LEU:HA	1.73	0.41
1:K:894:LEU:HA	1:K:895:PRO:HD3	1.75	0.41
1:B:6:ILE:HD13	1:B:6:ILE:HG21	1.78	0.41
1:B:234:GLU:HB2	1:B:252:ALA:HA	2.01	0.41
1:B:526:LYS:HB2	1:B:543:TYR:CZ	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:808:MET:HE3	1:K:808:MET:HB2	1.77	0.41
1:H:75:LYS:HD2	1:H:75:LYS:HA	1.73	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
10:H:1095:NET:H63	10:H:1095:NET:H31	1.92	0.41
1:K:23:CYS:HB3	1:K:575:ILE:HD12	2.01	0.41
1:K:213:LYS:O	1:K:286:ALA:HA	2.21	0.41
1:B:677:PHE:C	1:B:679:HIS:N	2.77	0.41
1:B:991:ASN:HD21	1:K:974:HIS:HE2	1.66	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:OD1	2:C:344:ASP:N	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:N	2:I:366:LEU:HD12	2.35	0.41
1:K:105:GLY:HA2	11:K:1247:HOH:O	2.21	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: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:93:ARG:HH11	2:C:93:ARG:HD3	1.72	0.41
2:C:364:ALA:N	2:C:365:PRO:CD	2.83	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
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
1:B:725:GLU:CD	1:B:735:ARG:NH2	2.79	0.41
2:C:43:LEU:HD21	2:C:80:LEU:HD13	2.03	0.41
2:C:246:ALA:HB3	2:C:247:PRO:HD3	2.01	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:HD13	1:H:228:ILE:HG21	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:630:ARG:HD3	11:B:1570:HOH:O	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:771:MET:HG3	1:B:873:LEU:HD12	2.02	0.41
1:B:781:ILE:HD12	1:B:781:ILE:N	2.36	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: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
2:C:373:LEU:HA	2:C:373:LEU:HD23	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:749:VAL:HG12	1:E:751:LEU:HD13	2.03	0.41
1:E:804:ILE:HD13	1:E:804:ILE:HA	1.67	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
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:738:GLN:C	1:H:738:GLN:HE21	2.28	0.41
1:H:810:GLN:HG3	11:H:1702:HOH:O	2.21	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
2:I:223:THR:HG22	2:I:224:SER:N	2.35	0.41
2:I:238:LEU:HB2	2:I:267:GLY:CA	2.51	0.41
1:K:630:ARG:HH11	1:K:630:ARG:HD3	1.57	0.41
1:K:738:GLN:NE2	1:K:739:THR:CG2	2.84	0.41
2:L:38:GLY:HA3	2:L:358:PRO:CB	2.50	0.41
2:L:192:PHE:O	2:L:215:ARG:HG2	2.21	0.41
1:B:117:ALA:HA	11:B:1239:HOH:O	2.20	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:HD12	1:E:420:LEU:HA	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:H:997:ARG:HA	1:H:998:PRO:C	2.44	0.41
1:K:464:GLN:O	1:K:468:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:MET:HB3	1:B:341:GLY:HA2	2.03	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:E:955:ARG:NH2	1:E:1044:ASN:OD1	2.47	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
1:B:658:VAL:HG13	1:B:659:PRO:HD2	2.02	0.40
10:B:1096:NET:H63	10:B:1096:NET:H31	1.82	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:969:GLU:HG2	11:E:2042:HOH:O	2.21	0.40
1:E:1071:ILE:HG22	1:E:1072:LYS:HD2	2.03	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:HE21	2:I:376:GLN:HB3	1.60	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
1:B:709:TYR:CE2	1:B:729:ASP:C	3.00	0.40
2:C:82:ILE:O	2:C:111:ALA:HA	2.20	0.40
1:E:707:ILE:CG2	1:E:711:LEU:CD2	2.99	0.40
1:E:1016:THR:HG21	1:E:1022:ILE:HA	2.04	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
1:H:900:PRO:HD2	6:H:1085:CL:CL	2.59	0.40
2:I:215:ARG:NH1	2:I:215:ARG:CG	2.80	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
1:K:1001:GLN:HG3	11:K:1783:HOH:O	2.21	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
1:B:1001:GLN:C	1:B:1001:GLN:NE2	2.80	0.40
2:C:246:ALA:C	2:C:248:CYS:N	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:10:GLU:C	2:F:12:GLY:H	2.28	0.40
1:H:443:ARG:HH11	1:H:443:ARG:HD2	1.53	0.40
1:H:704:ALA:C	1:H:706:GLU:N	2.79	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:74:ARG:NH1	1:K:74:ARG:CG	2.82	0.40
1:K:699:MET:HE2	1:K:703:LYS:NZ	2.36	0.40
1:K:714:ARG:HB2	1:K:750:LEU:HB2	2.02	0.40
1:B:369:ALA:HA	6:B:1086:CL:CL	2.58	0.40
1:B:734:ARG:O	1:B:738:GLN:N	2.40	0.40
2:C:191:PRO:O	2:C:378:ARG:NH1	2.55	0.40
2:C:228:VAL:CG1	2:C:258:PHE:CE1	3.05	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:HD23	1:H:964:LEU:HA	1.91	0.40
1:H:981:GLY:HA2	1:H:985:ILE:O	2.22	0.40
2:I:32:PHE:CD1	2:I:32:PHE:C	2.99	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1059/1073 (99%)	1008 (95%)	48 (4%)	3 (0%)	36 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	1064/1073 (99%)	1008 (95%)	54 (5%)	2 (0%)	43	44
1	H	1057/1073 (98%)	1016 (96%)	38 (4%)	3 (0%)	36	36
1	K	1059/1073 (99%)	1012 (96%)	43 (4%)	4 (0%)	30	28
2	C	377/382 (99%)	356 (94%)	19 (5%)	2 (0%)	24	22
2	F	379/382 (99%)	359 (95%)	19 (5%)	1 (0%)	36	36
2	I	377/382 (99%)	354 (94%)	21 (6%)	2 (0%)	24	22
2	L	377/382 (99%)	362 (96%)	15 (4%)	0	100	100
All	All	5749/5820 (99%)	5475 (95%)	257 (4%)	17 (0%)	36	36

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%)	797 (91%)	76 (9%)	9	7
1	E	878/878 (100%)	816 (93%)	62 (7%)	13	11
1	H	871/878 (99%)	796 (91%)	75 (9%)	10	7
1	K	872/878 (99%)	803 (92%)	69 (8%)	11	9
2	C	308/310 (99%)	271 (88%)	37 (12%)	5	3
2	F	309/310 (100%)	274 (89%)	35 (11%)	5	3
2	I	308/310 (99%)	271 (88%)	37 (12%)	5	3
2	L	308/310 (99%)	279 (91%)	29 (9%)	8	6
All	All	4727/4752 (100%)	4307 (91%)	420 (9%)	9	6

All (420) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	0	MET
1	B	42	ARG
1	B	44	ILE
1	B	45	LEU
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	235	ASN
1	B	277	GLU
1	B	282	ASN
1	B	296	VAL
1	B	325	LEU
1	B	362	ASN
1	B	383	VAL
1	B	411	LYS
1	B	412	VAL
1	B	425	ARG
1	B	478	VAL
1	B	520[A]	ASP
1	B	520[B]	ASP
1	B	521	LEU
1	B	547	GLU

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Mol	Chain	Res	Type
1	B	556	THR
1	B	559	GLU
1	B	570	ARG
1	B	644	GLN
1	B	651	ARG
1	B	674	ARG
1	B	676	ARG
1	B	679	HIS
1	B	685	LYS
1	B	687	LYS
1	B	688	GLN
1	B	698	GLU
1	B	707	ILE
1	B	714	ARG
1	B	726	ILE
1	B	734	ARG
1	B	750	LEU
1	B	751	LEU
1	B	770	GLU
1	B	783	GLN
1	B	799	THR
1	B	803	GLU
1	B	804	ILE
1	B	808	MET
1	B	811	GLN
1	B	837	TYR
1	B	854	LYS
1	B	880	LYS
1	B	883	ILE
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	962	LYS
1	B	965	LYS
1	B	1005	LYS
1	B	1017	SER
1	B	1019	ARG

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Mol	Chain	Res	Type
1	B	1020	ARG
1	B	1043	LEU
1	B	1051	MET
1	B	1060	LYS
1	B	1062	ILE
1	B	1071	ILE
1	B	1072	LYS
2	C	2	ILE
2	C	6	LEU
2	C	18	ARG
2	C	74	GLN
2	C	87	LEU
2	C	104	ARG
2	C	106	ASN
2	C	146	LYS
2	C	153	LEU
2	C	160	LYS
2	C	166	GLU
2	C	169	SER
2	C	175	TRP
2	C	183	GLN
2	C	186	LYS
2	C	187	GLU
2	C	194	VAL
2	C	204	ASN
2	C	215	ARG
2	C	217	THR
2	C	222	GLN
2	C	227	ASP
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	366	LEU

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Mol	Chain	Res	Type
2	C	371	ILE
2	C	376	GLN
1	E	0	MET
1	E	45	LEU
1	E	137	LYS
1	E	161	VAL
1	E	201	LYS
1	E	274	ILE
1	E	298	GLU
1	E	324	LYS
1	E	332	ASP
1	E	338	ILE
1	E	357	LYS
1	E	413	SER
1	E	415	ASP
1	E	416	ASP
1	E	420	LEU
1	E	421	THR
1	E	427	LEU
1	E	478	VAL
1	E	486	ASP
1	E	503	LYS
1	E	508[A]	ARG
1	E	508[B]	ARG
1	E	557	ASP
1	E	558	ARG
1	E	562	MET
1	E	633	LYS
1	E	644	GLN
1	E	651	ARG
1	E	674	ARG
1	E	682	GLU
1	E	687	LYS
1	E	694	VAL
1	E	698	GLU
1	E	703	LYS
1	E	713	VAL
1	E	732	ASP
1	E	733	LEU
1	E	734	ARG
1	E	762	ASP
1	E	783	GLN

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Mol	Chain	Res	Type
1	E	804	ILE
1	E	813	GLN
1	E	834	ASN
1	E	854	LYS
1	E	882	VAL
1	E	883	ILE
1	E	890	LYS
1	E	911	ARG
1	E	939	LYS
1	E	949	ARG
1	E	953	LYS
1	E	1013	ILE
1	E	1017	SER
1	E	1019	ARG
1	E	1020[A]	ARG
1	E	1020[B]	ARG
1	E	1023	GLU
1	E	1026	ARG
1	E	1049	THR
1	E	1060	LYS
1	E	1071	ILE
1	E	1072	LYS
2	F	18	ARG
2	F	25	SER
2	F	70	GLU
2	F	73	SER
2	F	106	ASN
2	F	113	ILE
2	F	131	CYS
2	F	136	ASP
2	F	137	ASN
2	F	154	ASN
2	F	161	GLU
2	F	174	SER
2	F	175	TRP
2	F	188	ASP
2	F	189	GLU
2	F	217	THR
2	F	218	ILE
2	F	222	GLN
2	F	230	LYS
2	F	236	ILE

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Mol	Chain	Res	Type
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	371	ILE
2	F	378	ARG
2	F	380	THR
1	H	0	MET
1	H	45	LEU
1	H	54	MET
1	H	58	GLU
1	H	89	MET
1	H	100	GLU
1	H	127	ASP
1	H	147	ILE
1	H	173	MET
1	H	185[A]	GLU
1	H	185[B]	GLU
1	H	274	ILE
1	H	277	GLU
1	H	295	ILE
1	H	312	LYS
1	H	332	ASP
1	H	343	THR
1	H	357	LYS
1	H	362	ASN
1	H	411	LYS
1	H	421	THR
1	H	427	LEU
1	H	446	LEU
1	H	470	ARG
1	H	478	VAL
1	H	480	ILE
1	H	514	LYS

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Mol	Chain	Res	Type
1	H	547	GLU
1	H	548	GLU
1	H	561	ILE
1	H	570	ARG
1	H	575	ILE
1	H	590	GLU
1	H	644	GLN
1	H	672	GLU
1	H	674	ARG
1	H	675	GLU
1	H	677	PHE
1	H	683	ARG
1	H	698	GLU
1	H	702	GLU
1	H	707	ILE
1	H	711	LEU
1	H	713	VAL
1	H	727	VAL
1	H	733	LEU
1	H	734	ARG
1	H	738	GLN
1	H	749	VAL
1	H	750	LEU
1	H	751	LEU
1	H	752	ASP
1	H	771	MET
1	H	783	GLN
1	H	804	ILE
1	H	808	MET
1	H	834	ASN
1	H	854	LYS
1	H	871	LYS
1	H	875	GLU
1	H	883	ILE
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	992	LYS
1	H	1013	ILE

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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	74	GLN
2	I	78	GLN
2	I	113	ILE
2	I	136	ASP
2	I	145	GLU
2	I	166	GLU
2	I	183	GLN
2	I	186	LYS
2	I	198	ASP
2	I	202	LYS
2	I	215	ARG
2	I	218	ILE
2	I	222	GLN
2	I	257	LYS
2	I	263	ILE
2	I	282	LYS
2	I	284	VAL
2	I	301	GLU
2	I	306	MET
2	I	318	GLU
2	I	321	LEU
2	I	330	LYS
2	I	331	SER
2	I	332	LEU
2	I	333	PHE
2	I	340	ILE
2	I	371	ILE
2	I	374	ILE
2	I	379	LYS

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Mol	Chain	Res	Type
2	I	380	THR
1	K	2	LYS
1	K	23	CYS
1	K	45	LEU
1	K	54	MET
1	K	74	ARG
1	K	102	GLU
1	K	136	LYS
1	K	147	ILE
1	K	184	ARG
1	K	201	LYS
1	K	235	ASN
1	K	274	ILE
1	K	282	ASN
1	K	362	ASN
1	K	364	GLU
1	K	411	LYS
1	K	413	SER
1	K	421	THR
1	K	427	LEU
1	K	478	VAL
1	K	480	ILE
1	K	481	THR
1	K	521	LEU
1	K	547	GLU
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	687	LYS
1	K	691	ASN
1	K	694	VAL
1	K	698	GLU
1	K	703	LYS
1	K	706	GLU
1	K	724	MET
1	K	733	LEU
1	K	737	PHE
1	K	738	GLN

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Mol	Chain	Res	Type
1	K	750	LEU
1	K	762	ASP
1	K	773	LEU
1	K	781	ILE
1	K	783	GLN
1	K	803	GLU
1	K	804	ILE
1	K	810[A]	GLN
1	K	810[B]	GLN
1	K	813	GLN
1	K	814	LYS
1	K	838	LEU
1	K	854	LYS
1	K	890	LYS
1	K	939	LYS
1	K	949	ARG
1	K	950	GLU
1	K	954	GLU
1	K	992	LYS
1	K	1000	ILE
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	1062	ILE
1	K	1072	LYS
2	L	4	SER
2	L	6	LEU
2	L	23	THR
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	215	ARG
2	L	218	ILE
2	L	222	GLN
2	L	226	GLU

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Mol	Chain	Res	Type
2	L	239	SER
2	L	257	LYS
2	L	268	ILE
2	L	318	GLU
2	L	321	LEU
2	L	324	ASN
2	L	326	ARG
2	L	332	LEU
2	L	340	ILE
2	L	357	SER
2	L	371	ILE
2	L	372	GLU
2	L	375	GLU
2	L	376	GLN
2	L	379	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) 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	897	ASN
1	B	935	ASN
1	B	991	ASN
1	B	994	HIS
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	137	ASN
2	C	154	ASN
2	C	204	ASN

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Mol	Chain	Res	Type
2	C	291	HIS
2	C	324	ASN
1	E	224	ASN
1	E	265	ASN
1	E	490	GLN
1	E	553	ASN
1	E	678	GLN
1	E	783	GLN
1	E	802	GLN
1	E	820	GLN
1	E	842	ASN
1	E	897	ASN
1	E	935	ASN
1	E	986	ASN
1	E	991	ASN
1	E	994	HIS
1	E	999	HIS
1	E	1034	GLN
1	E	1054	ASN
1	E	1070	GLN
2	F	78	GLN
2	F	154	ASN
2	F	324	ASN
1	H	104	GLN
1	H	265	ASN
1	H	691	ASN
1	H	738	GLN
1	H	783	GLN
1	H	802	GLN
1	H	813	GLN
1	H	834	ASN
1	H	897	ASN
1	H	935	ASN
1	H	991	ASN
1	H	999	HIS
1	H	1001	GLN
1	H	1034	GLN
1	H	1070	GLN
2	I	51	GLN
2	I	66	ASN
2	I	105	HIS
2	I	129	ASN

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Mol	Chain	Res	Type
2	I	222	GLN
2	I	295	HIS
2	I	351	GLN
2	I	376	GLN
1	K	104	GLN
1	K	265	ASN
1	K	336	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	897	ASN
1	K	935	ASN
1	K	966	GLN
1	K	986	ASN
1	K	991	ASN
1	K	994	HIS
1	K	999	HIS
1	K	1001	GLN
1	K	1034	GLN
1	K	1070	GLN
2	L	51	GLN
2	L	183	GLN
2	L	324	ASN
2	L	351	GLN
2	L	361	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
10	NET	H	1095	-	8,8,8	0.74	0	10,10,10	0.63	0
7	GLN	E	1093	-	8,9,9	1.34	1 (12%)	8,11,11	0.94	1 (12%)
7	GLN	H	1090	-	8,9,9	1.42	1 (12%)	8,11,11	1.18	1 (12%)
5	PO4	E	1082	-	4,4,4	2.17	2 (50%)	6,6,6	1.17	0
5	PO4	K	1092	-	4,4,4	0.56	0	6,6,6	1.38	1 (16%)
8	ADP	E	1095	3	28,29,29	1.35	4 (14%)	43,45,45	0.83	1 (2%)
9	ORN	E	1097	-	7,8,8	0.91	0	6,9,9	2.56	2 (33%)
10	NET	E	1098	-	8,8,8	0.79	0	10,10,10	0.43	0
8	ADP	H	1093	3	28,29,29	1.37	5 (17%)	43,45,45	1.31	6 (13%)
9	ORN	K	1097	-	7,8,8	1.04	0	6,9,9	1.58	1 (16%)
7	GLN	E	1094	-	8,9,9	1.89	3 (37%)	8,11,11	1.17	0
5	PO4	K	1078	4,3	4,4,4	2.01	2 (50%)	6,6,6	1.35	1 (16%)
7	GLN	K	1093	-	8,9,9	1.31	1 (12%)	8,11,11	1.07	1 (12%)
5	PO4	H	1082	-	4,4,4	2.01	1 (25%)	6,6,6	1.04	0
9	ORN	H	1094	-	7,8,8	0.97	0	6,9,9	1.99	2 (33%)
7	GLN	B	1092	-	8,9,9	1.92	3 (37%)	8,11,11	1.29	1 (12%)
8	ADP	E	1096	3	28,29,29	1.57	5 (17%)	43,45,45	1.15	5 (11%)
5	PO4	B	1078	4,3	4,4,4	2.07	3 (75%)	6,6,6	0.97	0
7	GLN	H	1091	-	8,9,9	1.36	1 (12%)	8,11,11	1.33	1 (12%)
7	GLN	B	1091	-	8,9,9	1.87	3 (37%)	8,11,11	2.31	4 (50%)
10	NET	B	1096	-	8,8,8	0.69	0	10,10,10	0.72	0
7	GLN	K	1094	-	8,9,9	1.28	1 (12%)	8,11,11	1.13	0
8	ADP	B	1094	3	28,29,29	1.38	4 (14%)	43,45,45	0.88	0
8	ADP	H	1092	3	28,29,29	1.21	3 (10%)	43,45,45	0.91	1 (2%)
5	PO4	E	1078	4,3	4,4,4	2.23	2 (50%)	6,6,6	0.85	0
10	NET	K	1098	-	8,8,8	0.62	0	10,10,10	0.93	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	H	1078	4,3	4,4,4	2.26	3 (75%)	6,6,6	0.65	0
8	ADP	K	1095	3	28,29,29	1.00	2 (7%)	43,45,45	1.02	1 (2%)
5	PO4	K	1082	-	4,4,4	2.04	2 (50%)	6,6,6	0.68	0
8	ADP	K	1096	3	28,29,29	1.24	3 (10%)	43,45,45	0.90	1 (2%)
8	ADP	B	1093	3	28,29,29	1.44	5 (17%)	43,45,45	0.95	0
9	ORN	B	1095	-	7,8,8	1.23	1 (14%)	6,9,9	1.38	0
5	PO4	B	1082	-	4,4,4	2.44	2 (50%)	6,6,6	0.87	0

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
10	NET	H	1095	-	-	3/12/12/12	-
7	GLN	E	1093	-	-	5/9/9/9	-
7	GLN	H	1090	-	-	6/9/9/9	-
9	ORN	E	1097	-	-	5/8/8/8	-
8	ADP	E	1095	3	-	2/16/32/32	0/3/3/3
10	NET	E	1098	-	-	1/12/12/12	-
8	ADP	H	1093	3	-	0/16/32/32	0/3/3/3
9	ORN	K	1097	-	-	7/8/8/8	-
7	GLN	E	1094	-	-	0/9/9/9	-
7	GLN	K	1093	-	-	6/9/9/9	-
9	ORN	H	1094	-	-	7/8/8/8	-
7	GLN	B	1092	-	-	0/9/9/9	-
8	ADP	E	1096	3	-	2/16/32/32	0/3/3/3
7	GLN	H	1091	-	-	1/9/9/9	-
7	GLN	B	1091	-	-	6/9/9/9	-
10	NET	B	1096	-	-	0/12/12/12	-
7	GLN	K	1094	-	-	0/9/9/9	-
8	ADP	B	1094	3	-	4/16/32/32	0/3/3/3
8	ADP	H	1092	3	-	2/16/32/32	0/3/3/3
10	NET	K	1098	-	-	0/12/12/12	-
8	ADP	K	1095	3	-	2/16/32/32	0/3/3/3
8	ADP	K	1096	3	-	4/16/32/32	0/3/3/3
8	ADP	B	1093	3	-	1/16/32/32	0/3/3/3
9	ORN	B	1095	-	-	6/8/8/8	-

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	1096	ADP	PA-O3A	-4.92	1.54	1.59
8	B	1093	ADP	PA-O3A	-4.32	1.54	1.59
8	E	1095	ADP	PA-O3A	-4.07	1.55	1.59
8	H	1093	ADP	PA-O3A	-4.03	1.55	1.59
8	B	1094	ADP	PA-O3A	-3.90	1.55	1.59
5	B	1082	PO4	P-O4	-3.67	1.44	1.54
5	E	1078	PO4	P-O4	-3.59	1.44	1.54
8	K	1096	ADP	C2-N1	3.30	1.39	1.33
8	E	1096	ADP	O3'-C3'	3.25	1.51	1.43
7	B	1092	GLN	OE1-CD	3.17	1.33	1.23
7	E	1094	GLN	CA-N	-3.12	1.32	1.48
7	H	1090	GLN	CA-N	-3.11	1.32	1.48
7	E	1094	GLN	OE1-CD	3.08	1.33	1.23
5	H	1082	PO4	P-O4	-3.08	1.45	1.54
5	K	1082	PO4	P-O4	-3.03	1.45	1.54
7	B	1091	GLN	CA-N	-2.98	1.33	1.48
7	K	1093	GLN	CA-N	-2.93	1.33	1.48
8	H	1092	ADP	PA-O3A	-2.93	1.56	1.59
7	E	1093	GLN	CA-N	-2.92	1.33	1.48
7	K	1094	GLN	CA-N	-2.90	1.33	1.48
7	B	1092	GLN	CA-N	-2.78	1.34	1.48
7	H	1091	GLN	CA-N	-2.74	1.34	1.48
5	H	1078	PO4	P-O2	-2.70	1.46	1.54
8	H	1093	ADP	C2-N3	-2.69	1.29	1.33
8	E	1096	ADP	O2'-C2'	2.69	1.49	1.43
5	E	1082	PO4	P-O2	-2.67	1.46	1.54
5	E	1082	PO4	P-O4	-2.61	1.47	1.54
5	H	1078	PO4	P-O4	-2.61	1.47	1.54
7	B	1091	GLN	CB-CA	2.57	1.58	1.53
5	B	1078	PO4	P-O2	-2.56	1.47	1.54
8	K	1096	ADP	O2'-C2'	2.50	1.49	1.43
5	K	1078	PO4	P-O2	-2.47	1.47	1.54
5	B	1078	PO4	P-O4	-2.45	1.47	1.54
5	K	1078	PO4	P-O3	-2.45	1.47	1.54
8	E	1096	ADP	C2-N1	2.44	1.38	1.33
8	B	1093	ADP	O3'-C3'	2.39	1.48	1.43
8	K	1096	ADP	PA-O3A	-2.36	1.56	1.59
5	B	1082	PO4	P-O2	-2.35	1.47	1.54
8	B	1094	ADP	C2-N1	2.32	1.38	1.33
8	H	1093	ADP	O2'-C2'	2.29	1.48	1.43
8	B	1094	ADP	C2-N3	-2.28	1.29	1.33
8	K	1095	ADP	O3'-C3'	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1092	ADP	C2-N3	-2.28	1.29	1.33
8	K	1095	ADP	C2-N1	2.27	1.38	1.33
7	B	1092	GLN	CD-NE2	-2.24	1.25	1.32
5	H	1078	PO4	P-O3	-2.18	1.48	1.54
9	B	1095	ORN	O-C	2.17	1.28	1.22
8	B	1093	ADP	C8-N7	2.16	1.35	1.31
7	E	1094	GLN	CD-NE2	-2.12	1.25	1.32
8	H	1093	ADP	O3'-C3'	2.12	1.48	1.43
8	B	1093	ADP	C2-N1	2.11	1.37	1.33
7	B	1091	GLN	CB-CG	2.11	1.59	1.52
5	E	1078	PO4	P-O2	-2.11	1.48	1.54
8	H	1093	ADP	O4'-C1'	-2.10	1.37	1.42
8	E	1095	ADP	C2-N1	2.09	1.37	1.33
8	E	1095	ADP	C2-N3	-2.09	1.30	1.33
8	E	1095	ADP	O3'-C3'	2.08	1.48	1.43
5	B	1078	PO4	P-O3	-2.06	1.48	1.54
5	K	1082	PO4	P-O2	-2.05	1.48	1.54
8	E	1096	ADP	C2-N3	-2.03	1.30	1.33
8	B	1093	ADP	O2'-C2'	2.02	1.48	1.43
8	B	1094	ADP	C8-N7	2.02	1.35	1.31
8	H	1092	ADP	O2'-C2'	2.01	1.47	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	1097	ORN	CB-CA-C	-4.98	97.25	110.45
9	H	1094	ORN	CB-CA-C	-3.95	99.97	110.45
7	B	1091	GLN	CG-CB-CA	3.88	122.78	113.86
8	K	1096	ADP	O2A-PA-O3A	3.57	116.93	107.27
8	H	1093	ADP	O2A-PA-O3A	3.37	116.38	107.27
7	B	1091	GLN	CB-CA-N	3.21	118.49	110.12
9	K	1097	ORN	CB-CA-C	-3.19	101.98	110.45
8	H	1093	ADP	O4'-C1'-N9	-3.09	102.15	108.09
8	H	1093	ADP	O3'-C3'-C2'	3.00	121.45	111.82
7	H	1091	GLN	OXT-C-O	-2.89	117.52	124.08
9	E	1097	ORN	CG-CB-CA	2.86	122.45	113.22
8	H	1093	ADP	O2'-C2'-C3'	2.73	120.58	111.82
8	H	1093	ADP	O3B-PB-O3A	2.73	113.78	104.64
7	B	1091	GLN	CB-CG-CD	2.71	121.76	112.55
7	B	1092	GLN	CB-CA-N	2.70	117.15	110.12
7	B	1091	GLN	CB-CA-C	2.60	117.33	110.45
7	K	1093	GLN	CB-CA-N	2.52	116.70	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	1092	PO4	O4-P-O3	2.42	115.45	107.91
8	E	1096	ADP	O4'-C1'-N9	2.35	112.61	108.09
7	H	1090	GLN	CB-CA-N	2.35	116.24	110.12
5	K	1078	PO4	O3-P-O1	-2.31	102.78	110.95
8	E	1096	ADP	C2'-C3'-C4'	-2.30	98.16	102.61
8	E	1096	ADP	O2A-PA-O3A	2.22	113.26	107.27
8	E	1096	ADP	C6-C5-C4	2.18	120.15	117.18
8	K	1095	ADP	O3'-C3'-C2'	2.14	118.66	111.82
8	E	1096	ADP	O3B-PB-O3A	2.11	111.71	104.64
10	K	1098	NET	C6-C5-N1	-2.11	105.23	114.64
9	H	1094	ORN	OXT-C-O	-2.10	119.31	124.08
8	H	1092	ADP	C5-C6-N6	2.07	128.42	123.29
8	E	1095	ADP	O2'-C2'-C3'	2.07	118.44	111.82
8	H	1093	ADP	C4-N9-C8	2.06	107.91	105.74
7	E	1093	GLN	OXT-C-O	-2.05	119.44	124.08

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1091	GLN	N-CA-CB-CG
7	E	1093	GLN	N-CA-CB-CG
7	E	1093	GLN	C-CA-CB-CG
7	H	1090	GLN	N-CA-CB-CG
7	H	1090	GLN	C-CA-CB-CG
7	K	1093	GLN	N-CA-CB-CG
7	K	1093	GLN	C-CA-CB-CG
8	B	1094	ADP	PA-O3A-PB-O3B
8	K	1096	ADP	PA-O3A-PB-O3B
9	B	1095	ORN	N-CA-CB-CG
9	B	1095	ORN	C-CA-CB-CG
9	E	1097	ORN	N-CA-CB-CG
9	E	1097	ORN	C-CA-CB-CG
9	H	1094	ORN	N-CA-CB-CG
9	H	1094	ORN	C-CA-CB-CG
9	K	1097	ORN	N-CA-CB-CG
9	K	1097	ORN	C-CA-CB-CG
7	B	1091	GLN	CA-CB-CG-CD
7	E	1093	GLN	CA-CB-CG-CD
9	B	1095	ORN	OXT-C-CA-N
7	H	1091	GLN	CA-CB-CG-CD
9	H	1094	ORN	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
9	K	1097	ORN	OXT-C-CA-N
9	B	1095	ORN	CA-CB-CG-CD
9	B	1095	ORN	O-C-CA-N
9	H	1094	ORN	O-C-CA-N
9	K	1097	ORN	O-C-CA-N
9	H	1094	ORN	CA-CB-CG-CD
10	H	1095	NET	C8-C7-N1-C1
8	B	1094	ADP	PA-O3A-PB-O1B
8	K	1096	ADP	PA-O3A-PB-O1B
7	B	1091	GLN	C-CA-CB-CG
8	B	1093	ADP	PB-O3A-PA-O1A
8	E	1095	ADP	PB-O3A-PA-O1A
8	H	1092	ADP	PB-O3A-PA-O1A
8	K	1095	ADP	PB-O3A-PA-O1A
8	K	1096	ADP	PB-O3A-PA-O2A
9	B	1095	ORN	NE-CD-CG-CB
7	H	1090	GLN	CA-CB-CG-CD
9	E	1097	ORN	NE-CD-CG-CB
8	B	1094	ADP	PB-O3A-PA-O2A
10	H	1095	NET	C8-C7-N1-C5
7	H	1090	GLN	O-C-CA-CB
9	H	1094	ORN	NE-CD-CG-CB
9	E	1097	ORN	O-C-CA-N
9	K	1097	ORN	CA-CB-CG-CD
7	H	1090	GLN	OXT-C-CA-N
7	H	1090	GLN	OXT-C-CA-CB
7	K	1093	GLN	O-C-CA-CB
7	K	1093	GLN	OXT-C-CA-N
7	B	1091	GLN	O-C-CA-CB
9	E	1097	ORN	OXT-C-CA-N
8	B	1094	ADP	PB-O3A-PA-O1A
8	E	1096	ADP	PB-O3A-PA-O2A
8	K	1096	ADP	PB-O3A-PA-O1A
7	E	1093	GLN	O-C-CA-CB
7	B	1091	GLN	OXT-C-CA-N
7	B	1091	GLN	OXT-C-CA-CB
7	K	1093	GLN	OXT-C-CA-CB
9	H	1094	ORN	O-C-CA-CB
9	K	1097	ORN	O-C-CA-CB
9	K	1097	ORN	NE-CD-CG-CB
10	E	1098	NET	C8-C7-N1-C3
7	E	1093	GLN	OXT-C-CA-CB

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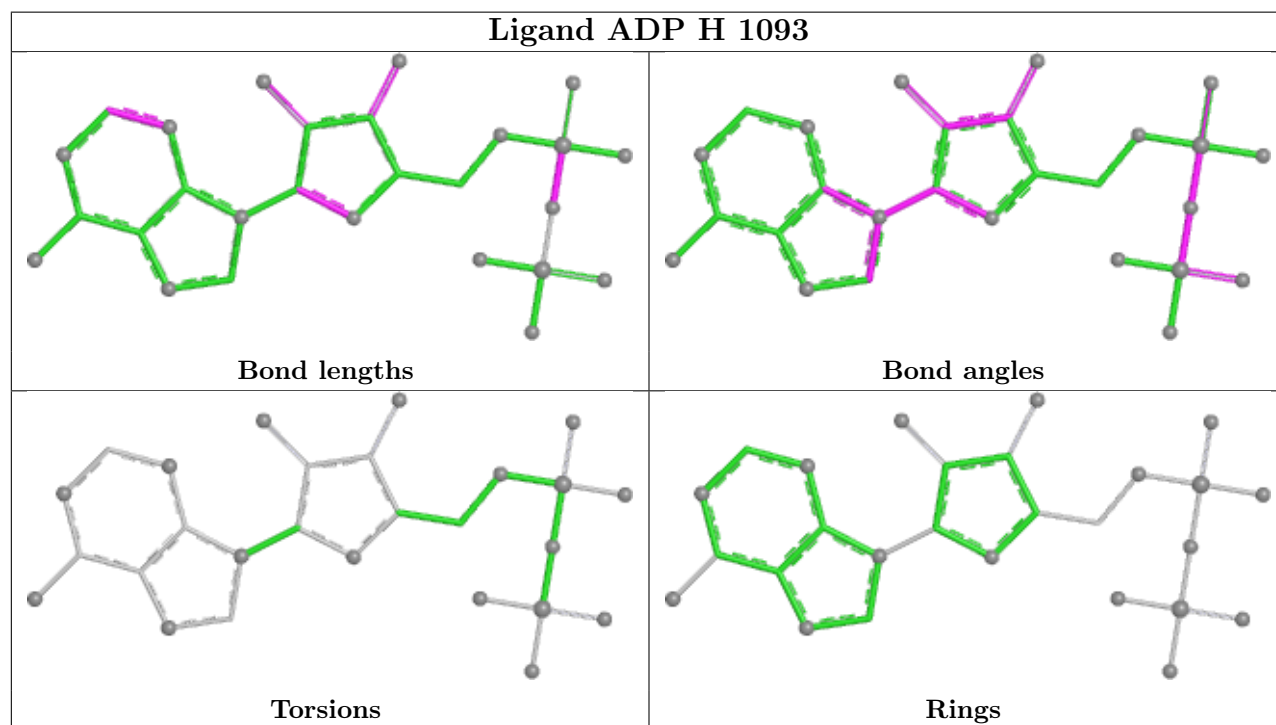
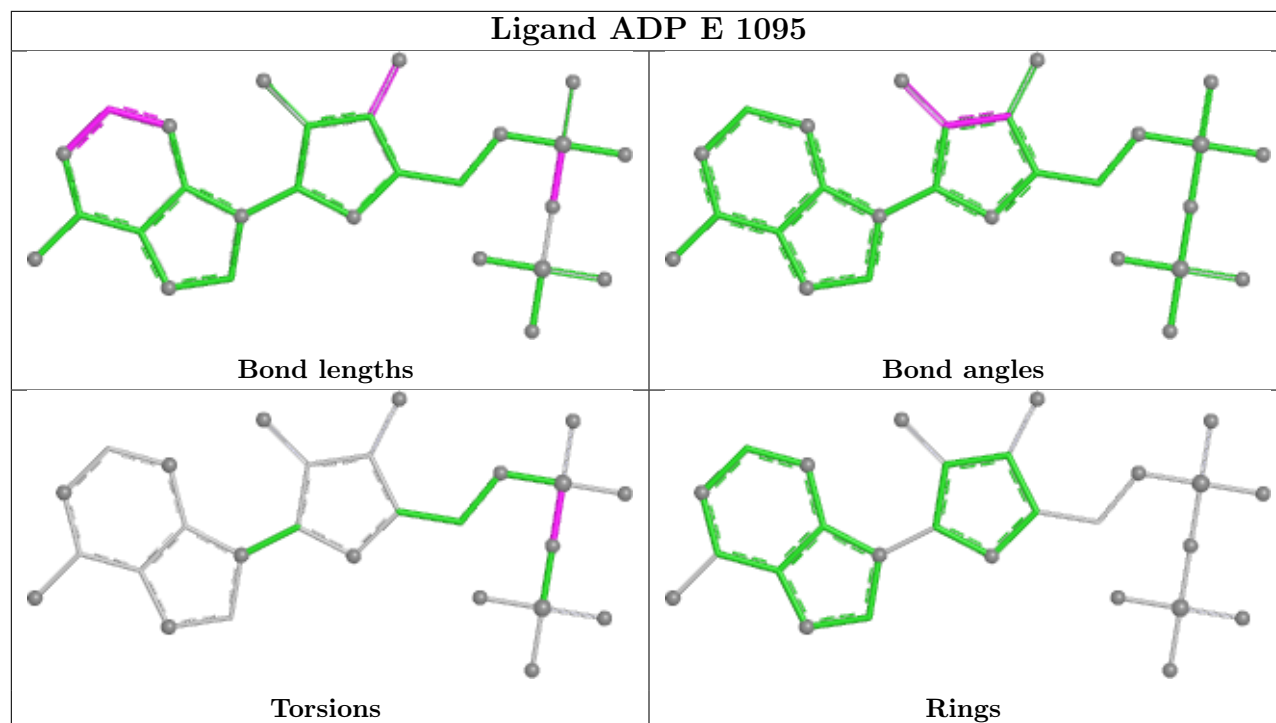
Mol	Chain	Res	Type	Atoms
7	K	1093	GLN	O-C-CA-N
10	H	1095	NET	C8-C7-N1-C3
8	E	1095	ADP	PB-O3A-PA-O2A
8	E	1096	ADP	PB-O3A-PA-O1A
8	H	1092	ADP	PB-O3A-PA-O2A
8	K	1095	ADP	PB-O3A-PA-O2A

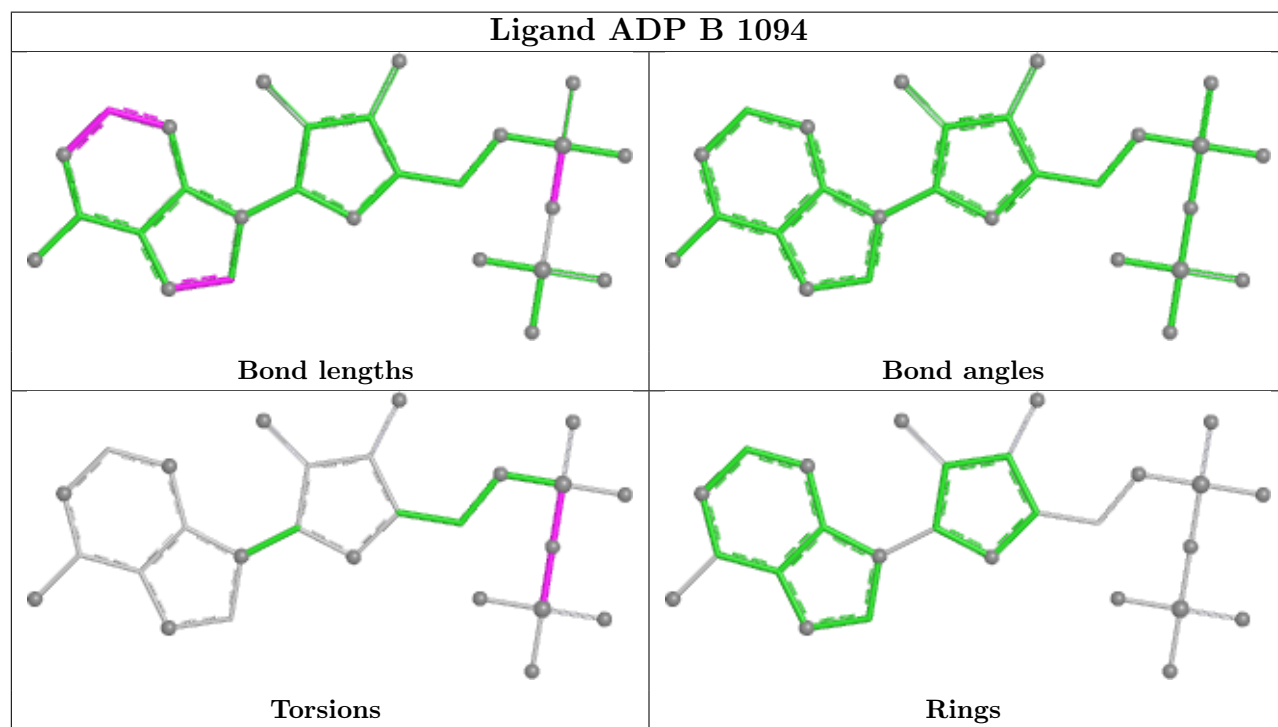
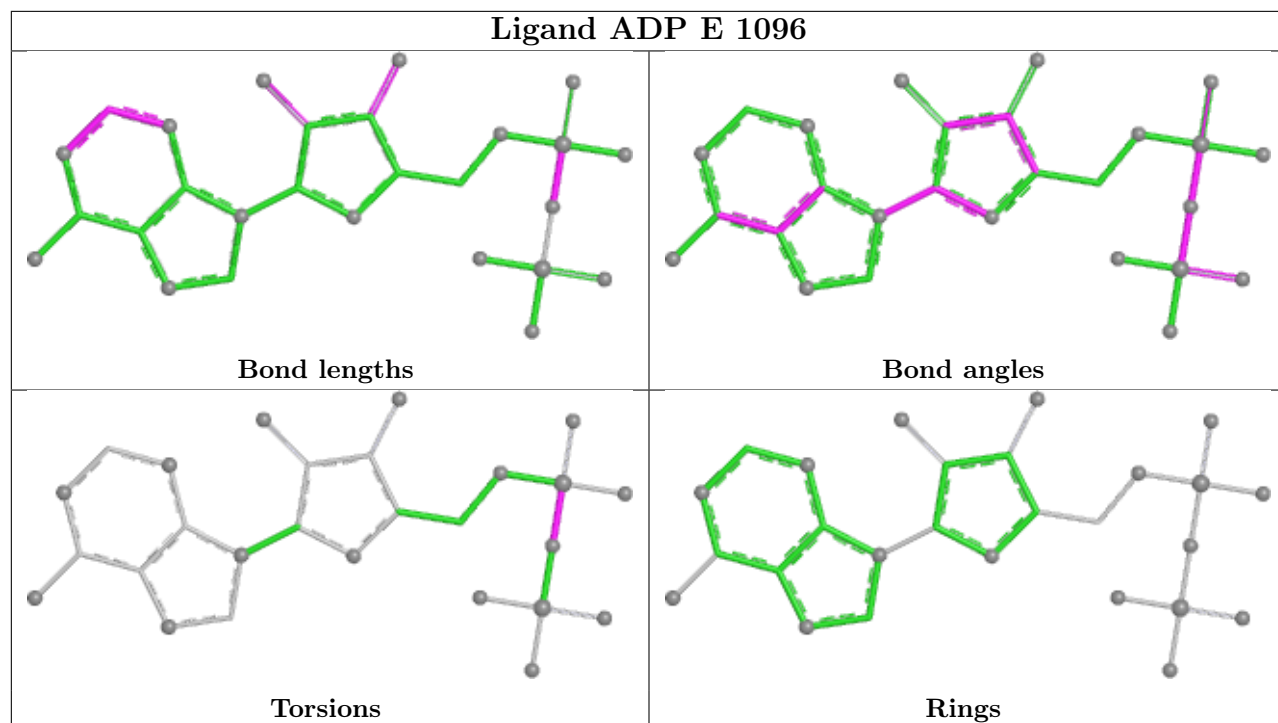
There are no ring outliers.

15 monomers are involved in 24 short contacts:

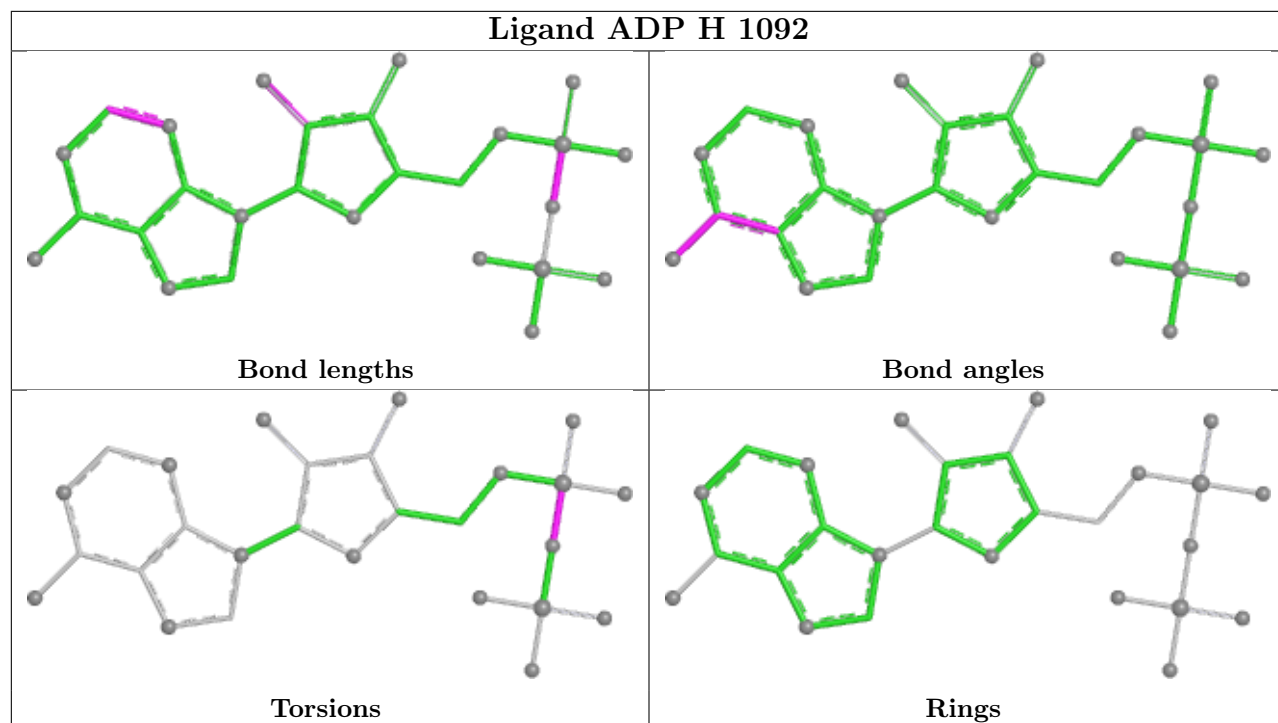
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	1095	NET	2	0
7	E	1093	GLN	1	0
7	H	1090	GLN	2	0
5	E	1082	PO4	2	0
8	E	1095	ADP	1	0
9	E	1097	ORN	3	0
9	K	1097	ORN	1	0
7	K	1093	GLN	1	0
5	H	1082	PO4	2	0
8	E	1096	ADP	1	0
5	B	1078	PO4	1	0
10	B	1096	NET	1	0
8	K	1095	ADP	1	0
5	K	1082	PO4	2	0
9	B	1095	ORN	4	0

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.

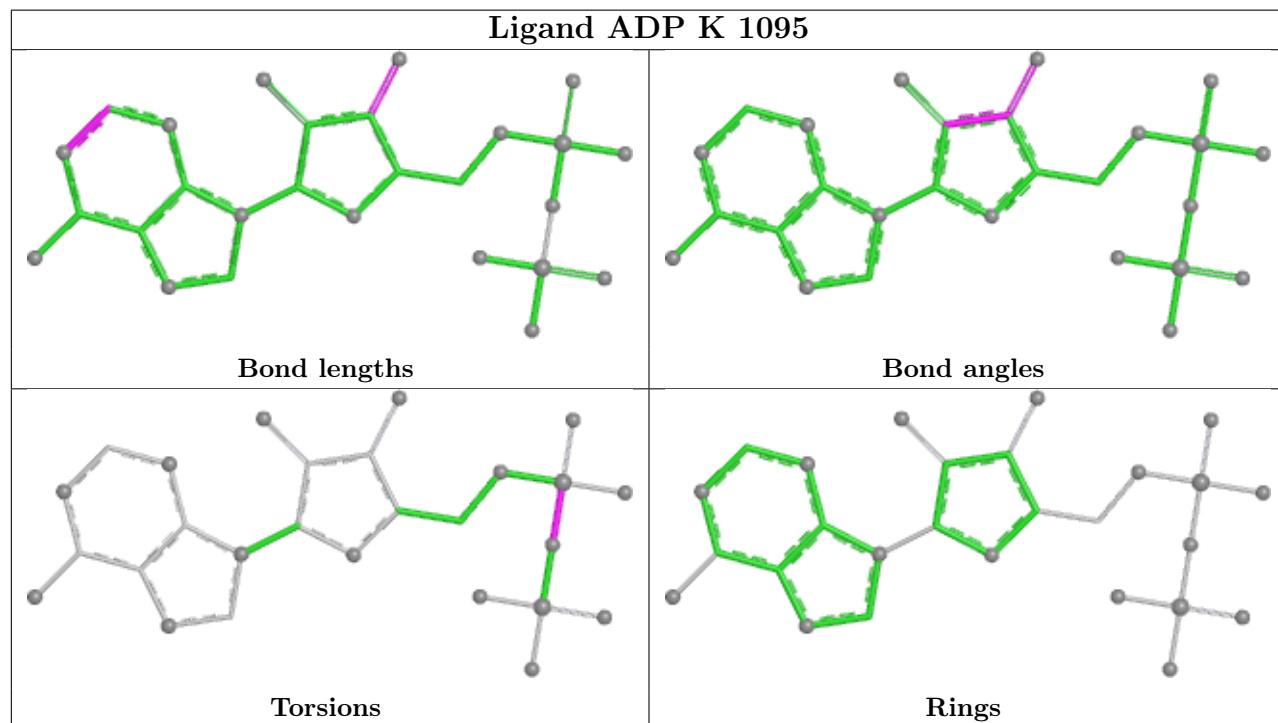


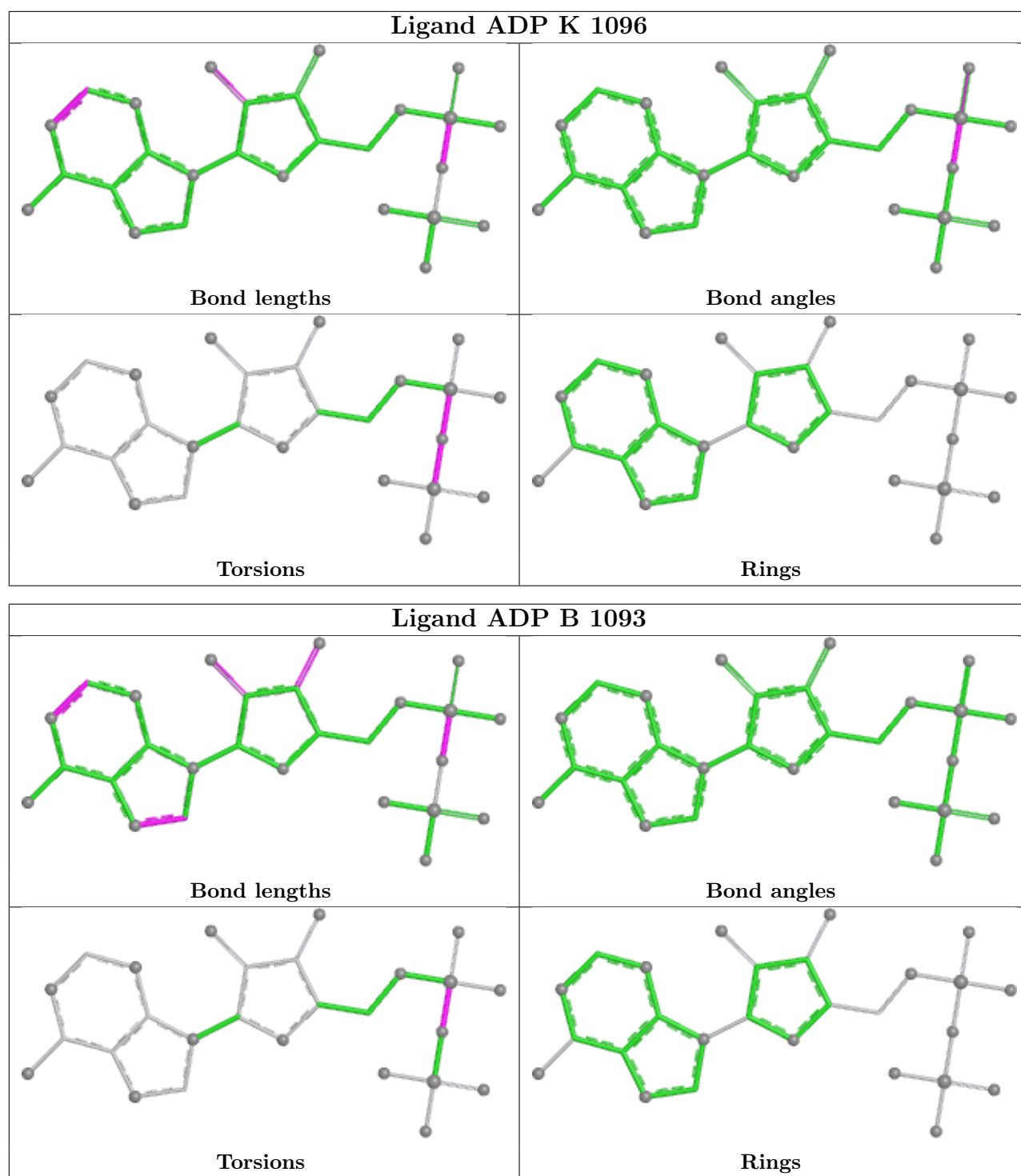


Ligand ADP H 1092



Ligand ADP K 1095





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.