



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:53 PM GMT

PDB ID : 1CS0
Title : Crystal structure of carbamoyl phosphate synthetase complexed at CYS269 in the small subunit with the tetrahedral mimic l-glutamate gamma-semialdehyde
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 1999-08-16
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

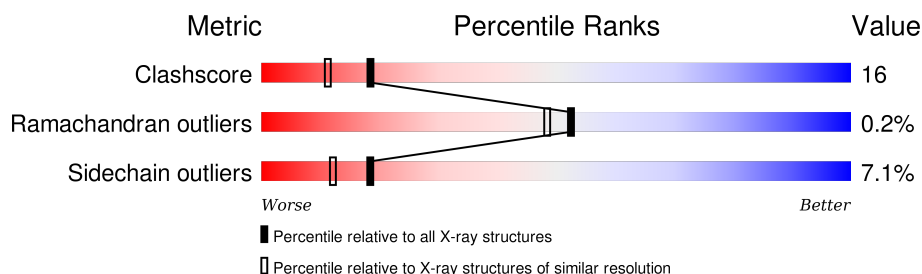
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)


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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	 60% 31% 6% ..
1	C	1073	 60% 31% 6% ..
1	E	1073	 65% 27% 6% ..
1	G	1073	 61% 30% 7% ..
2	B	382	 59% 35% 5% .
2	D	382	 59% 34% 7% .
2	F	382	 60% 35% . .

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Mol	Chain	Length	Quality of chain
2	H	382	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: green (53%), yellow (38%), and orange (8%). The segments are labeled with their respective percentages: 53%, 38%, and 8%. The bar ends with a small black dot.

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 48889 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: LARGE SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	3	0
			8169	5128	1422	1574	45			
1	C	1058	Total	C	N	O	S	0	3	0
			8173	5132	1423	1573	45			
1	E	1058	Total	C	N	O	S	0	6	0
			8186	5140	1424	1576	46			
1	G	1058	Total	C	N	O	S	0	3	0
			8175	5132	1425	1572	46			

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2904	1830	509	555	10			
2	D	379	Total	C	N	O	S	0	1	0
			2909	1833	509	557	10			
2	F	379	Total	C	N	O	S	0	0	0
			2904	1830	509	555	10			
2	H	379	Total	C	N	O	S	0	1	0
			2906	1831	509	556	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total	Mn	0	0
			3	3		
3	A	3	Total	Mn	0	0
			3	3		
3	C	3	Total	Mn	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	3	Total 3	Mn 3	0	0

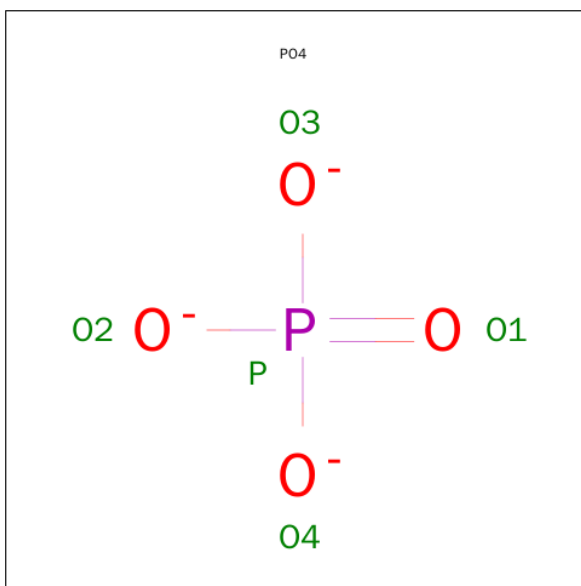
- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	7	Total 7	K 7	0	0
4	D	1	Total 1	K 1	0	0
4	E	8	Total 8	K 8	0	0
4	H	1	Total 1	K 1	0	0
4	B	1	Total 1	K 1	0	0
4	C	7	Total 7	K 7	0	0
4	A	7	Total 7	K 7	0	0
4	F	1	Total 1	K 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

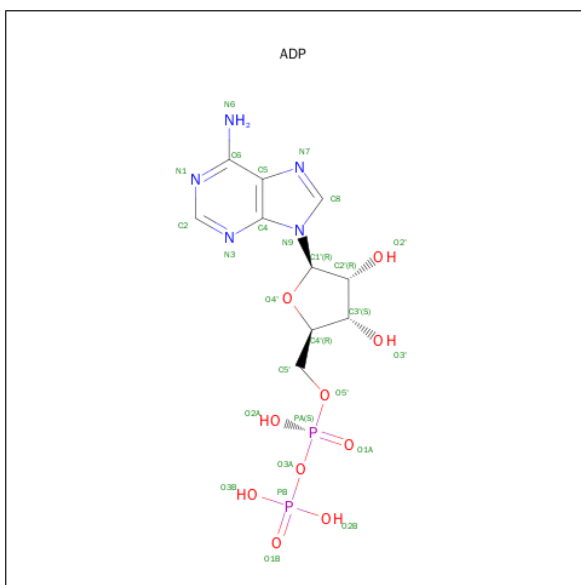
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	5	Total 5	Cl 5	0	0
5	D	2	Total 2	Cl 2	0	0
5	E	5	Total 5	Cl 5	0	0
5	H	2	Total 2	Cl 2	0	0
5	B	2	Total 2	Cl 2	0	0
5	C	5	Total 5	Cl 5	0	0
5	A	6	Total 6	Cl 6	0	0
5	F	2	Total 2	Cl 2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



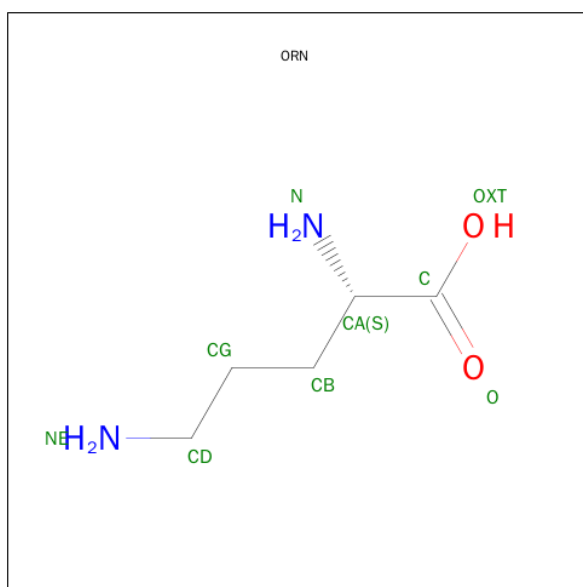
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



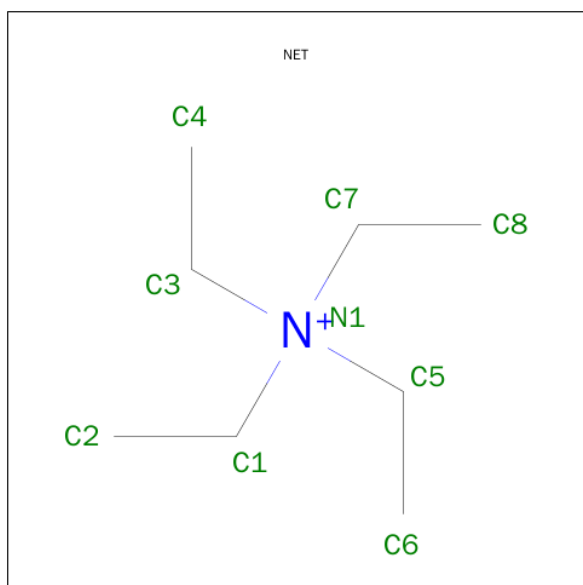
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	G	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 8 is L-ORNITHINE (three-letter code: ORN) (formula: $\text{C}_5\text{H}_{12}\text{N}_2\text{O}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula: $C_8H_{20}N$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N 9 8 1	0	0
9	C	1	Total C N 9 8 1	0	0
9	E	1	Total C N 9 8 1	0	0
9	G	1	Total C N 9 8 1	0	0

- Molecule 10 is water.

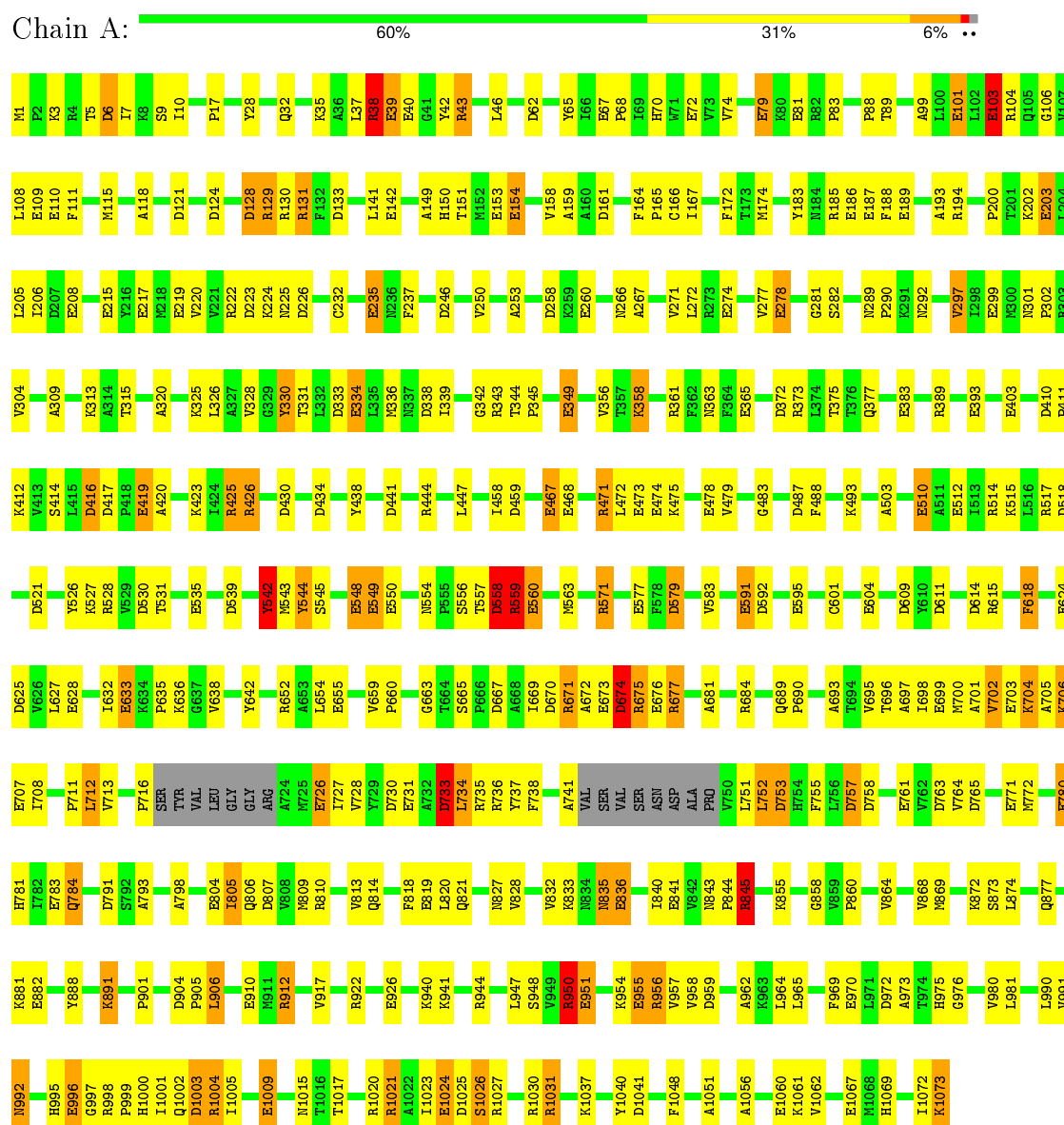
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	869	Total O 869 869	0	0
10	B	213	Total O 213 213	0	0
10	C	784	Total O 784 784	0	0
10	D	275	Total O 275 275	0	0
10	E	864	Total O 864 864	0	0
10	F	235	Total O 235 235	0	0
10	G	743	Total O 743 743	0	0
10	H	193	Total O 193 193	0	0

3 Residue-property plots

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

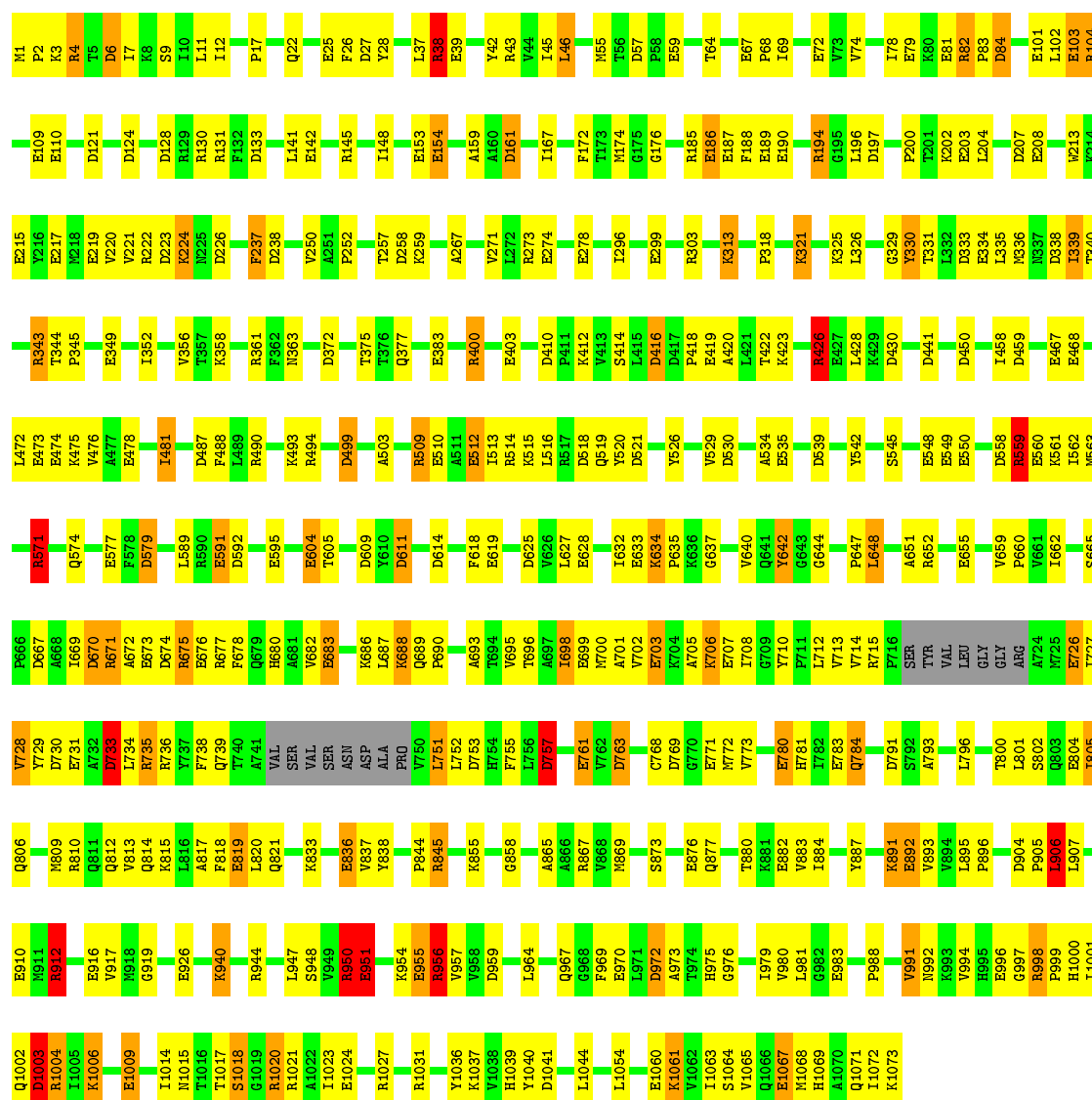
Note EDS was not executed.

• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT



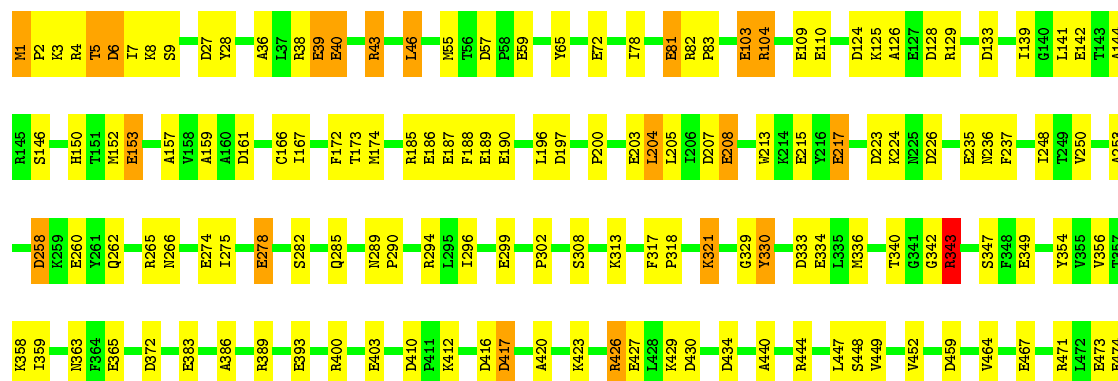
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain C: 



• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

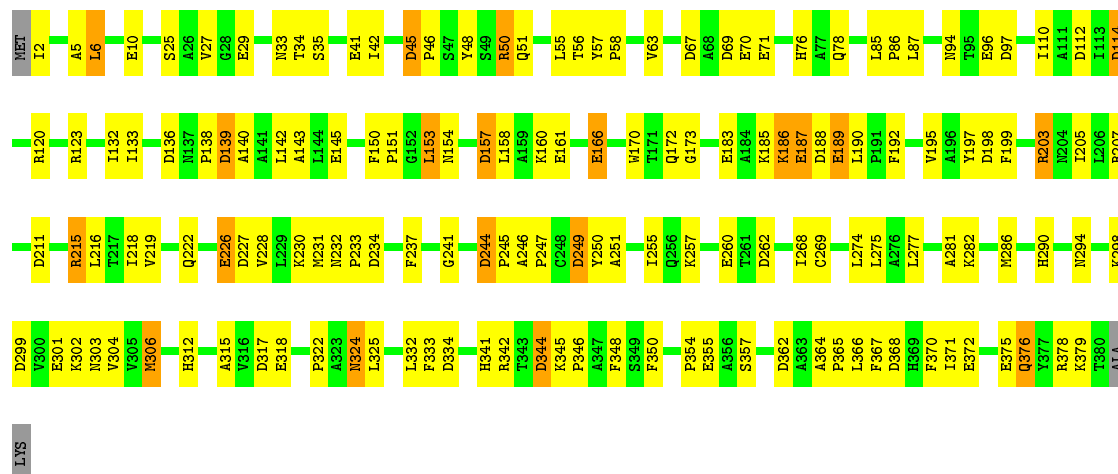
Chain E: 





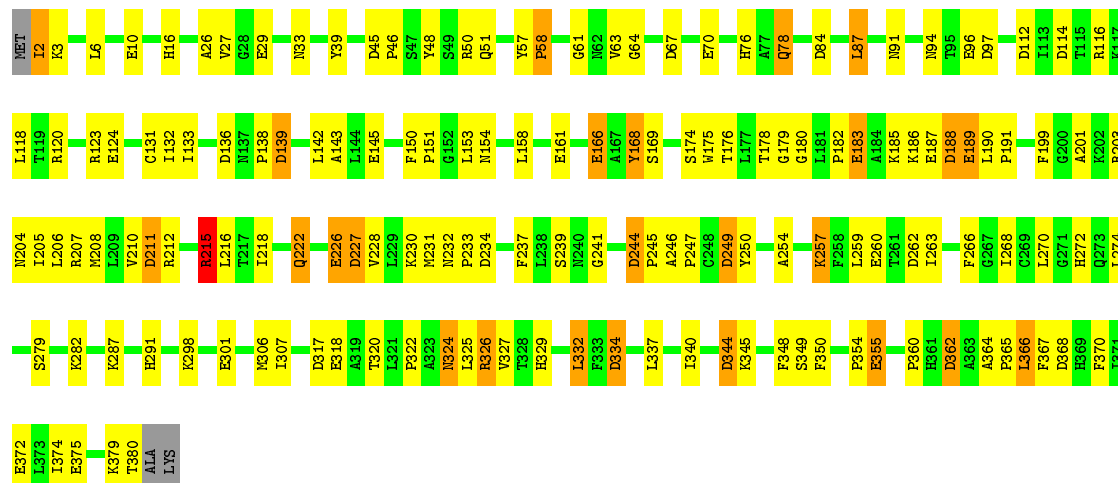
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain B: 59% 35% 5% .



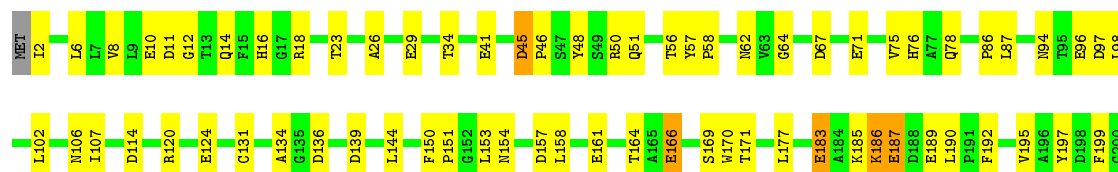
• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

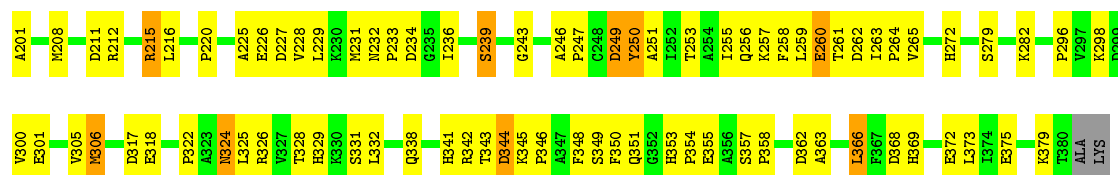
Chain D: 59% 34% 7% .



• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

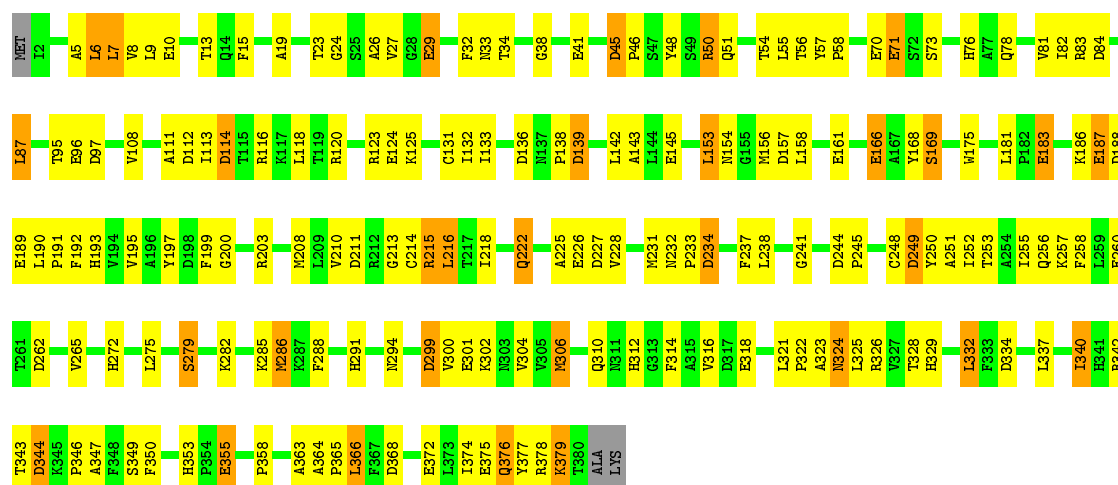
Chain F: 60% 35% . .





• Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain H: 53% 38% 8% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.70Å 163.80Å 332.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.7 (30.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.186 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48889	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.05	72/8307 (0.9%)	1.38	129/11230 (1.1%)
1	C	1.04	70/8311 (0.8%)	1.38	130/11236 (1.2%)
1	E	1.05	64/8336 (0.8%)	1.35	129/11267 (1.1%)
1	G	1.04	71/8313 (0.9%)	1.36	109/11237 (1.0%)
2	B	0.92	18/2950 (0.6%)	1.29	32/4005 (0.8%)
2	D	0.98	15/2959 (0.5%)	1.31	40/4017 (1.0%)
2	F	0.96	16/2950 (0.5%)	1.34	31/4005 (0.8%)
2	H	0.93	19/2956 (0.6%)	1.30	36/4013 (0.9%)
All	All	1.02	345/45082 (0.8%)	1.35	636/61010 (1.0%)

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

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

All (345) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	189	GLU	CD-OE2	13.05	1.40	1.25
1	G	39	GLU	CD-OE1	-9.37	1.15	1.25
1	E	403	GLU	CD-OE2	8.00	1.34	1.25
1	E	819	GLU	CD-OE2	7.90	1.34	1.25
1	E	427	GLU	CD-OE2	7.81	1.34	1.25
2	H	372	GLU	CD-OE2	7.74	1.34	1.25
1	G	676	GLU	CD-OE2	7.65	1.34	1.25
1	A	655	GLU	CD-OE2	7.55	1.33	1.25
1	E	804	GLU	CD-OE2	7.53	1.33	1.25
2	D	355	GLU	CD-OE2	7.49	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	549	GLU	CD-OE2	7.46	1.33	1.25
1	E	676	GLU	CD-OE2	7.35	1.33	1.25
1	G	215	GLU	CD-OE2	7.29	1.33	1.25
1	A	624	GLU	CD-OE2	7.28	1.33	1.25
2	H	226	GLU	CD-OE2	7.27	1.33	1.25
1	E	955	GLU	CD-OE2	7.26	1.33	1.25
1	G	512	GLU	CD-OE2	7.19	1.33	1.25
1	C	1024	GLU	CD-OE2	7.19	1.33	1.25
1	G	707	GLU	CD-OE2	7.18	1.33	1.25
1	G	699	GLU	CD-OE2	7.16	1.33	1.25
1	E	836	GLU	CD-OE2	7.16	1.33	1.25
1	G	1024	GLU	CD-OE2	7.16	1.33	1.25
1	A	633	GLU	CD-OE2	7.13	1.33	1.25
1	E	393	GLU	CD-OE2	7.06	1.33	1.25
2	F	372	GLU	CD-OE2	7.00	1.33	1.25
2	H	41	GLU	CD-OE2	6.99	1.33	1.25
1	C	951	GLU	CD-OE2	6.99	1.33	1.25
1	E	707	GLU	CD-OE2	6.98	1.33	1.25
1	E	970	GLU	CD-OE2	6.96	1.33	1.25
1	C	187	GLU	CD-OE2	6.95	1.33	1.25
1	C	109	GLU	CD-OE2	6.94	1.33	1.25
1	A	217	GLU	CD-OE2	6.91	1.33	1.25
2	H	166	GLU	CD-OE2	6.86	1.33	1.25
1	C	655	GLU	CD-OE2	6.83	1.33	1.25
1	E	478	GLU	CD-OE2	6.82	1.33	1.25
1	A	1009[A]	GLU	CD-OE2	6.81	1.33	1.25
1	A	1009[B]	GLU	CD-OE2	6.81	1.33	1.25
1	E	783	GLU	CD-OE2	6.79	1.33	1.25
1	C	676	GLU	CD-OE2	6.78	1.33	1.25
2	D	183	GLU	CD-OE2	6.77	1.33	1.25
1	G	427	GLU	CD-OE2	6.75	1.33	1.25
1	G	731	GLU	CD-OE2	6.72	1.33	1.25
1	C	804	GLU	CD-OE2	6.71	1.33	1.25
1	E	703	GLU	CD-OE2	6.71	1.33	1.25
1	G	996	GLU	CD-OE2	6.71	1.33	1.25
1	G	926	GLU	CD-OE2	6.69	1.33	1.25
1	C	771	GLU	CD-OE2	6.67	1.32	1.25
1	A	186	GLU	CD-OE2	6.67	1.32	1.25
1	A	1067	GLU	CD-OE2	6.67	1.32	1.25
1	G	819	GLU	CD-OE2	6.67	1.32	1.25
1	E	59	GLU	CD-OE2	6.66	1.32	1.25
2	H	71	GLU	CD-OE2	6.65	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1009	GLU	CD-OE2	6.64	1.32	1.25
2	B	372	GLU	CD-OE2	6.63	1.32	1.25
2	F	183	GLU	CD-OE2	6.62	1.32	1.25
2	B	226	GLU	CD-OE2	6.62	1.32	1.25
1	G	110	GLU	CD-OE2	6.61	1.32	1.25
1	E	683	GLU	CD-OE2	6.61	1.32	1.25
2	D	226	GLU	CD-OE2	6.61	1.32	1.25
1	E	365	GLU	CD-OE2	6.59	1.32	1.25
1	G	153	GLU	CD-OE2	6.59	1.32	1.25
1	G	190	GLU	CD-OE2	6.58	1.32	1.25
2	B	145	GLU	CD-OE2	6.57	1.32	1.25
1	E	190	GLU	CD-OE2	6.57	1.32	1.25
1	C	955	GLU	CD-OE2	6.53	1.32	1.25
1	C	549	GLU	CD-OE2	6.53	1.32	1.25
1	C	699	GLU	CD-OE2	6.52	1.32	1.25
1	A	707	GLU	CD-OE2	6.51	1.32	1.25
1	A	478	GLU	CD-OE2	6.50	1.32	1.25
1	G	186	GLU	CD-OE2	6.50	1.32	1.25
1	G	771	GLU	CD-OE2	6.50	1.32	1.25
1	C	153	GLU	CD-OE2	6.48	1.32	1.25
2	B	166	GLU	CD-OE2	6.46	1.32	1.25
2	D	318	GLU	CD-OE2	6.46	1.32	1.25
1	E	110	GLU	CD-OE2	6.46	1.32	1.25
1	A	560	GLU	CD-OE2	6.46	1.32	1.25
1	E	910	GLU	CD-OE2	6.45	1.32	1.25
1	A	628	GLU	CD-OE2	6.45	1.32	1.25
2	B	29	GLU	CD-OE2	6.45	1.32	1.25
1	G	955	GLU	CD-OE2	6.44	1.32	1.25
1	G	109	GLU	CD-OE2	6.43	1.32	1.25
1	A	365	GLU	CD-OE2	6.42	1.32	1.25
1	A	1024	GLU	CD-OE2	6.42	1.32	1.25
1	E	1009[A]	GLU	CD-OE2	6.42	1.32	1.25
1	E	1009[B]	GLU	CD-OE2	6.42	1.32	1.25
1	G	836	GLU	CD-OE2	6.41	1.32	1.25
1	E	260	GLU	CD-OE2	6.40	1.32	1.25
1	A	110	GLU	CD-OE2	6.39	1.32	1.25
1	C	468	GLU	CD-OE2	6.39	1.32	1.25
1	G	916	GLU	CD-OE2	6.39	1.32	1.25
1	C	110	GLU	CD-OE2	6.37	1.32	1.25
1	E	771	GLU	CD-OE2	6.37	1.32	1.25
1	G	467	GLU	CD-OE2	6.36	1.32	1.25
1	G	683	GLU	CD-OE2	6.36	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	215	GLU	CD-OE2	6.36	1.32	1.25
1	C	473	GLU	CD-OE2	6.36	1.32	1.25
1	A	512	GLU	CD-OE2	6.35	1.32	1.25
2	F	10	GLU	CD-OE2	6.35	1.32	1.25
1	C	67	GLU	CD-OE2	6.35	1.32	1.25
1	C	577	GLU	CD-OE2	6.34	1.32	1.25
1	G	59	GLU	CD-OE2	6.34	1.32	1.25
1	C	892	GLU	CD-OE2	6.34	1.32	1.25
1	A	676	GLU	CD-OE2	6.34	1.32	1.25
1	A	703	GLU	CD-OE2	6.33	1.32	1.25
2	F	71	GLU	CD-OE2	6.32	1.32	1.25
1	A	699	GLU	CD-OE2	6.31	1.32	1.25
1	C	731	GLU	CD-OE2	6.31	1.32	1.25
1	C	535	GLU	CD-OE2	6.31	1.32	1.25
2	F	301	GLU	CD-OE2	6.30	1.32	1.25
2	F	166	GLU	CD-OE2	6.30	1.32	1.25
1	G	549	GLU	CD-OE2	6.29	1.32	1.25
1	C	595	GLU	CD-OE2	6.28	1.32	1.25
1	G	72	GLU	CD-OE2	6.27	1.32	1.25
1	C	349	GLU	CD-OE2	6.26	1.32	1.25
1	G	1060	GLU	CD-OE2	6.26	1.32	1.25
1	G	560	GLU	CD-OE2	6.25	1.32	1.25
1	A	604	GLU	CD-OE2	6.24	1.32	1.25
1	E	72	GLU	CD-OE2	6.24	1.32	1.25
1	G	591	GLU	CD-OE2	6.24	1.32	1.25
1	C	926	GLU	CD-OE2	6.21	1.32	1.25
1	E	103	GLU	CD-OE2	6.21	1.32	1.25
2	D	166	GLU	CD-OE2	6.21	1.32	1.25
2	B	189	GLU	CD-OE2	6.20	1.32	1.25
1	C	203	GLU	CD-OE2	6.20	1.32	1.25
1	E	731	GLU	CD-OE2	6.19	1.32	1.25
2	F	226	GLU	CD-OE2	6.19	1.32	1.25
2	B	301	GLU	CD-OE2	6.17	1.32	1.25
1	A	996	GLU	CD-OE2	6.17	1.32	1.25
1	A	951	GLU	CD-OE2	6.17	1.32	1.25
1	C	983	GLU	CD-OE2	6.16	1.32	1.25
2	D	301	GLU	CD-OE2	6.16	1.32	1.25
1	E	153	GLU	CD-OE2	6.16	1.32	1.25
1	C	142	GLU	CD-OE2	6.15	1.32	1.25
1	C	59	GLU	CD-OE2	6.15	1.32	1.25
1	A	109	GLU	CD-OE2	6.14	1.32	1.25
1	G	79	GLU	CD-OE2	6.13	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	GLU	CD-OE2	6.13	1.32	1.25
1	C	467	GLU	CD-OE2	6.11	1.32	1.25
1	A	219	GLU	CD-OE2	6.10	1.32	1.25
1	G	882	GLU	CD-OE2	6.10	1.32	1.25
1	G	154	GLU	CD-OE2	6.10	1.32	1.25
1	A	955	GLU	CD-OE2	6.09	1.32	1.25
2	H	375	GLU	CD-OE2	6.09	1.32	1.25
1	A	783	GLU	CD-OE2	6.07	1.32	1.25
1	C	726	GLU	CD-OE2	6.05	1.32	1.25
1	A	334	GLU	CD-OE2	6.05	1.32	1.25
1	A	595	GLU	CD-OE2	6.03	1.32	1.25
1	G	189	GLU	CD-OE2	6.03	1.32	1.25
1	C	1067	GLU	CD-OE2	6.03	1.32	1.25
1	C	79	GLU	CD-OE2	6.03	1.32	1.25
1	E	274	GLU	CD-OE2	6.02	1.32	1.25
2	H	10	GLU	CD-OE2	6.00	1.32	1.25
1	E	187	GLU	CD-OE2	6.00	1.32	1.25
1	G	761	GLU	CD-OE2	5.99	1.32	1.25
1	G	67	GLU	CD-OE2	5.98	1.32	1.25
1	E	591	GLU	CD-OE2	5.98	1.32	1.25
1	G	39	GLU	CD-OE2	5.96	1.32	1.25
2	H	301	GLU	CD-OE2	5.96	1.32	1.25
1	A	260	GLU	CD-OE2	5.96	1.32	1.25
1	C	703	GLU	CD-OE2	5.96	1.32	1.25
1	G	673	GLU	CD-OE2	5.95	1.32	1.25
1	A	473	GLU	CD-OE2	5.94	1.32	1.25
2	B	187	GLU	CD-OE2	5.94	1.32	1.25
1	G	703	GLU	CD-OE2	5.94	1.32	1.25
2	H	183	GLU	CD-OE2	5.94	1.32	1.25
1	A	591	GLU	CD-OE2	5.94	1.32	1.25
1	C	103	GLU	CD-OE2	5.93	1.32	1.25
1	E	186	GLU	CD-OE2	5.93	1.32	1.25
1	C	189	GLU	CD-OE2	5.92	1.32	1.25
2	H	70	GLU	CD-OE2	5.92	1.32	1.25
1	C	550	GLU	CD-OE2	5.91	1.32	1.25
1	C	910	GLU	CD-OE2	5.91	1.32	1.25
1	A	274	GLU	CD-OE2	5.90	1.32	1.25
1	G	535	GLU	CD-OE2	5.89	1.32	1.25
1	A	673	GLU	CD-OE2	5.89	1.32	1.25
1	A	731	GLU	CD-OE2	5.88	1.32	1.25
2	D	10	GLU	CD-OE2	5.88	1.32	1.25
1	E	726	GLU	CD-OE2	5.88	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	836	GLU	CD-OE2	5.87	1.32	1.25
1	C	683	GLU	CD-OE2	5.85	1.32	1.25
2	B	161	GLU	CD-OE2	5.83	1.32	1.25
1	C	474	GLU	CD-OE2	5.83	1.32	1.25
2	B	318	GLU	CD-OE2	5.83	1.32	1.25
1	A	403	GLU	CD-OE2	5.83	1.32	1.25
1	A	510	GLU	CD-OE2	5.83	1.32	1.25
1	A	819	GLU	CD-OE2	5.82	1.32	1.25
1	C	478	GLU	CD-OE2	5.82	1.32	1.25
2	B	375	GLU	CD-OE2	5.82	1.32	1.25
1	A	624	GLU	CD-OE1	-5.82	1.19	1.25
2	B	10	GLU	CD-OE2	5.81	1.32	1.25
2	H	355	GLU	CD-OE2	5.81	1.32	1.25
1	G	783	GLU	CD-OE2	5.81	1.32	1.25
2	H	187	GLU	CD-OE2	5.81	1.32	1.25
1	G	473	GLU	CD-OE2	5.80	1.32	1.25
1	C	761	GLU	CD-OE2	5.80	1.32	1.25
1	E	1024	GLU	CD-OE2	5.80	1.32	1.25
2	F	124	GLU	CD-OE2	5.79	1.32	1.25
1	A	780	GLU	CD-OE2	5.78	1.32	1.25
1	A	474	GLU	CD-OE2	5.78	1.32	1.25
1	E	951	GLU	CD-OE2	5.78	1.32	1.25
1	A	804	GLU	CD-OE2	5.77	1.31	1.25
2	H	96	GLU	CD-OE2	5.77	1.31	1.25
1	C	560	GLU	CD-OE2	5.76	1.31	1.25
1	E	673	GLU	CD-OE2	5.75	1.31	1.25
2	D	70	GLU	CD-OE2	5.75	1.31	1.25
1	C	591	GLU	CD-OE2	5.73	1.31	1.25
1	C	707	GLU	CD-OE2	5.73	1.31	1.25
1	G	595	GLU	CD-OE2	5.73	1.31	1.25
1	C	836	GLU	CD-OE2	5.73	1.31	1.25
1	A	771	GLU	CD-OE2	5.72	1.31	1.25
1	E	39	GLU	CD-OE2	5.72	1.31	1.25
1	C	819	GLU	CD-OE2	5.71	1.31	1.25
2	B	70	GLU	CD-OE2	5.71	1.31	1.25
2	D	124	GLU	CD-OE2	5.71	1.31	1.25
2	F	187	GLU	CD-OE2	5.71	1.31	1.25
1	A	349	GLU	CD-OE2	5.70	1.31	1.25
1	E	203	GLU	CD-OE2	5.70	1.31	1.25
1	C	219	GLU	CD-OE2	5.69	1.31	1.25
1	G	970	GLU	CD-OE2	5.68	1.31	1.25
1	A	419	GLU	CD-OE2	5.68	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	882	GLU	CD-OE2	5.67	1.31	1.25
1	G	951	GLU	CD-OE2	5.67	1.31	1.25
1	C	876	GLU	CD-OE2	5.66	1.31	1.25
1	G	365	GLU	CD-OE2	5.66	1.31	1.25
1	G	655	GLU	CD-OE2	5.66	1.31	1.25
1	A	383	GLU	CD-OE2	5.65	1.31	1.25
1	G	726	GLU	CD-OE2	5.64	1.31	1.25
1	E	208	GLU	CD-OE2	5.63	1.31	1.25
1	A	926	GLU	CD-OE2	5.63	1.31	1.25
2	D	375	GLU	CD-OE2	5.63	1.31	1.25
2	F	96	GLU	CD-OE2	5.62	1.31	1.25
1	C	39	GLU	CD-OE2	5.61	1.31	1.25
1	G	474	GLU	CD-OE2	5.61	1.31	1.25
1	C	780	GLU	CD-OE2	5.60	1.31	1.25
1	G	334	GLU	CD-OE2	5.60	1.31	1.25
1	C	403	GLU	CD-OE2	5.60	1.31	1.25
1	E	699	GLU	CD-OE2	5.59	1.31	1.25
2	H	29	GLU	CD-OE2	5.59	1.31	1.25
1	C	673	GLU	CD-OE2	5.59	1.31	1.25
1	G	910	GLU	CD-OE2	5.58	1.31	1.25
1	E	841	GLU	CD-OE2	5.58	1.31	1.25
1	C	334	GLU	CD-OE2	5.58	1.31	1.25
2	H	260	GLU	CD-OE2	5.57	1.31	1.25
1	G	403	GLU	CD-OE2	5.56	1.31	1.25
1	C	628	GLU	CD-OE2	5.55	1.31	1.25
1	G	208	GLU	CD-OE2	5.55	1.31	1.25
1	C	604	GLU	CD-OE2	5.55	1.31	1.25
1	C	215	GLU	CD-OE2	5.54	1.31	1.25
2	H	161	GLU	CD-OE2	5.54	1.31	1.25
1	E	299	GLU	CD-OE1	-5.54	1.19	1.25
1	A	203	GLU	CD-OE2	5.54	1.31	1.25
2	B	41	GLU	CD-OE2	5.53	1.31	1.25
2	H	124	GLU	CD-OE2	5.53	1.31	1.25
1	E	109	GLU	CD-OE2	5.52	1.31	1.25
1	A	726	GLU	CD-OE2	5.52	1.31	1.25
1	C	81	GLU	CD-OE2	5.52	1.31	1.25
2	F	375	GLU	CD-OE2	5.49	1.31	1.25
1	G	876	GLU	CD-OE2	5.49	1.31	1.25
1	A	535	GLU	CD-OE2	5.47	1.31	1.25
1	C	882	GLU	CD-OE2	5.47	1.31	1.25
1	C	190	GLU	CD-OE2	5.47	1.31	1.25
2	B	96	GLU	CD-OE2	5.46	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	334	GLU	CD-OE2	5.46	1.31	1.25
2	F	355	GLU	CD-OE2	5.45	1.31	1.25
1	E	278	GLU	CD-OE2	5.45	1.31	1.25
1	A	549	GLU	CD-OE2	5.45	1.31	1.25
1	A	970	GLU	CD-OE2	5.44	1.31	1.25
2	B	260	GLU	CD-OE2	5.44	1.31	1.25
2	D	96	GLU	CD-OE1	-5.44	1.19	1.25
1	E	467	GLU	CD-OE2	5.44	1.31	1.25
1	C	278	GLU	CD-OE2	5.44	1.31	1.25
1	A	101	GLU	CD-OE2	5.43	1.31	1.25
1	C	783	GLU	CD-OE2	5.41	1.31	1.25
1	A	187	GLU	CD-OE2	5.41	1.31	1.25
1	C	217	GLU	CD-OE2	5.40	1.31	1.25
1	E	217	GLU	CD-OE2	5.40	1.31	1.25
2	H	318	GLU	CD-OE2	5.39	1.31	1.25
2	F	161	GLU	CD-OE2	5.39	1.31	1.25
1	A	1060	GLU	CD-OE2	5.39	1.31	1.25
1	E	761	GLU	CD-OE2	5.38	1.31	1.25
1	G	103	GLU	CD-OE2	5.38	1.31	1.25
1	A	278	GLU	CD-OE2	5.38	1.31	1.25
1	E	619	GLU	CD-OE2	5.37	1.31	1.25
2	D	145	GLU	CD-OE2	5.36	1.31	1.25
1	G	219	GLU	CD-OE2	5.33	1.31	1.25
1	C	1060	GLU	CD-OE2	5.33	1.31	1.25
2	H	145	GLU	CD-OE2	5.33	1.31	1.25
1	G	393	GLU	CD-OE2	5.33	1.31	1.25
2	F	41	GLU	CD-OE2	5.32	1.31	1.25
1	A	467	GLU	CD-OE2	5.32	1.31	1.25
1	E	1060	GLU	CD-OE2	5.31	1.31	1.25
2	B	183	GLU	CD-OE2	5.31	1.31	1.25
1	E	892	GLU	CD-OE2	5.29	1.31	1.25
1	C	512	GLU	CD-OE2	5.29	1.31	1.25
1	G	577	GLU	CD-OE2	5.28	1.31	1.25
2	F	260	GLU	CD-OE2	5.28	1.31	1.25
2	B	355	GLU	CD-OE2	5.27	1.31	1.25
1	A	72	GLU	CD-OE2	5.27	1.31	1.25
1	G	217	GLU	CD-OE2	5.27	1.31	1.25
1	E	142	GLU	CD-OE2	5.26	1.31	1.25
1	C	619	GLU	CD-OE2	5.26	1.31	1.25
1	A	577	GLU	CD-OE2	5.25	1.31	1.25
1	C	274	GLU	CD-OE2	5.25	1.31	1.25
1	E	474	GLU	CD-OE2	5.25	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	552	GLU	CD-OE2	5.25	1.31	1.25
1	C	916	GLU	CD-OE2	5.25	1.31	1.25
1	E	40	GLU	CD-OE2	5.25	1.31	1.25
1	C	186	GLU	CD-OE2	5.24	1.31	1.25
1	G	892	GLU	CD-OE2	5.23	1.31	1.25
1	G	510	GLU	CD-OE2	5.22	1.31	1.25
1	A	550	GLU	CD-OE2	5.22	1.31	1.25
1	A	819	GLU	CD-OE1	-5.22	1.20	1.25
1	G	419	GLU	CD-OE2	5.21	1.31	1.25
1	E	577	GLU	CD-OE2	5.21	1.31	1.25
1	A	103	GLU	CD-OE2	5.21	1.31	1.25
1	A	208	GLU	CD-OE2	5.20	1.31	1.25
1	E	535	GLU	CD-OE2	5.20	1.31	1.25
1	G	40	GLU	CD-OE2	5.20	1.31	1.25
1	G	101	GLU	CD-OE2	5.19	1.31	1.25
1	E	876	GLU	CD-OE2	5.19	1.31	1.25
1	G	278	GLU	CD-OE2	5.19	1.31	1.25
1	A	142	GLU	CD-OE2	5.18	1.31	1.25
1	G	624	GLU	CD-OE2	5.17	1.31	1.25
1	G	478	GLU	CD-OE2	5.17	1.31	1.25
1	G	187	GLU	CD-OE2	5.17	1.31	1.25
1	C	72	GLU	CD-OE2	5.16	1.31	1.25
1	G	628	GLU	CD-OE2	5.16	1.31	1.25
1	C	970	GLU	CD-OE2	5.15	1.31	1.25
1	E	550	GLU	CD-OE2	5.13	1.31	1.25
1	A	154	GLU	CD-OE2	5.11	1.31	1.25
1	A	215	GLU	CD-OE2	5.10	1.31	1.25
1	A	79	GLU	CD-OE2	5.09	1.31	1.25
2	D	29	GLU	CD-OE2	5.08	1.31	1.25
1	E	1067	GLU	CD-OE2	5.08	1.31	1.25
1	E	81	GLU	CD-OE2	5.07	1.31	1.25
1	E	349	GLU	CD-OE2	5.07	1.31	1.25
1	A	235	GLU	CD-OE2	5.07	1.31	1.25
1	A	393	GLU	CD-OE2	5.06	1.31	1.25
1	G	468	GLU	CD-OE2	5.06	1.31	1.25
1	C	25	GLU	CD-OE1	-5.05	1.20	1.25
1	A	882	GLU	CD-OE2	5.04	1.31	1.25
1	G	983	GLU	CD-OE2	5.03	1.31	1.25
1	A	910	GLU	CD-OE2	5.02	1.31	1.25
2	F	318	GLU	CD-OE2	5.01	1.31	1.25
2	D	260	GLU	CD-OE2	5.01	1.31	1.25

All (636) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	956	ARG	NE-CZ-NH2	-12.15	114.22	120.30
1	A	677	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	A	677	ARG	NE-CZ-NH2	-10.47	115.07	120.30
1	G	43	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	G	43	ARG	NE-CZ-NH2	-10.24	115.18	120.30
2	F	368	ASP	CB-CG-OD2	-10.04	109.26	118.30
2	D	334	ASP	CB-CG-OD2	-10.02	109.28	118.30
1	E	104	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	G	265	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	C	956	ARG	NE-CZ-NH2	-9.47	115.57	120.30
1	G	410	ASP	CB-CG-OD2	-9.37	109.86	118.30
1	E	343	ARG	NE-CZ-NH1	9.35	124.97	120.30
2	D	334	ASP	CB-CG-OD1	9.19	126.57	118.30
1	A	468	GLU	CG-CD-OE2	-9.18	99.93	118.30
1	E	43	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	A	128	ASP	CB-CG-OD1	9.08	126.47	118.30
2	D	211	ASP	CB-CG-OD2	-9.04	110.17	118.30
2	B	203	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	G	1021	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	C	514	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	C	131	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	G	1031	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	944	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	670	ASP	CB-CG-OD2	-8.86	110.32	118.30
1	C	670	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	C	223	ASP	CB-CG-OD2	-8.85	110.34	118.30
1	A	128	ASP	CB-CG-OD2	-8.77	110.40	118.30
1	G	75	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	C	972	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	E	82	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	A	223	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	G	6	ASP	CB-CG-OD2	-8.72	110.46	118.30
1	E	625	ASP	CB-CG-OD1	8.55	126.00	118.30
1	C	810	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	A	625	ASP	CB-CG-OD2	-8.44	110.71	118.30
2	H	97	ASP	CB-CG-OD2	-8.44	110.71	118.30
2	F	139	ASP	CB-CG-OD1	8.37	125.83	118.30
1	A	517	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	A	642	TYR	CB-CG-CD1	8.33	126.00	121.00
1	E	333	ASP	CB-CG-OD1	8.29	125.76	118.30
1	G	444	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	642	TYR	CB-CG-CD2	-8.15	116.11	121.00
1	G	579	ASP	CB-CG-OD2	-8.15	110.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	361	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	E	530	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	E	333	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	G	972	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	E	625	ASP	CB-CG-OD2	-8.06	111.04	118.30
1	A	338	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	E	558	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	A	223	ASP	CB-CG-OD1	8.04	125.53	118.30
1	G	956	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	G	674	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	C	494	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	E	38	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	E	265	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	625	ASP	CB-CG-OD1	7.92	125.43	118.30
1	C	128	ASP	CB-CG-OD1	7.88	125.39	118.30
1	C	131	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	G	223	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	C	223	ASP	CB-CG-OD1	7.81	125.33	118.30
1	A	791	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	E	956	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	C	571	ARG	NE-CZ-NH1	7.76	124.18	120.30
2	H	211	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	E	128	ASP	CB-CG-OD2	-7.72	111.36	118.30
1	C	258	ASP	CB-CG-OD2	-7.71	111.36	118.30
2	B	368	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	A	468	GLU	CG-CD-OE1	7.67	133.65	118.30
1	A	670	ASP	CB-CG-OD1	7.63	125.17	118.30
1	G	757	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	G	956	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	C	972	ASP	CB-CG-OD1	7.60	125.14	118.30
2	H	344	ASP	CB-CG-OD1	7.59	125.13	118.30
1	E	133	ASP	CB-CG-OD2	-7.56	111.50	118.30
2	F	368	ASP	CB-CG-OD1	7.56	125.10	118.30
1	G	625	ASP	CB-CG-OD1	7.54	125.08	118.30
1	C	959	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	E	372	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	E	1041	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	G	769	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	C	361	ARG	NE-CZ-NH1	7.49	124.04	120.30
2	B	211	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	E	791	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	A	43	ARG	NE-CZ-NH2	-7.45	116.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	E	400	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	G	670	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	A	1041	ASP	CB-CG-OD1	7.44	124.99	118.30
1	C	154	GLU	OE1-CD-OE2	-7.43	114.38	123.30
2	F	120	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	F	262	ASP	CB-CG-OD1	7.42	124.97	118.30
2	D	212	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	C	333	ASP	CB-CG-OD1	7.37	124.93	118.30
2	D	368	ASP	CB-CG-OD2	-7.37	111.67	118.30
2	H	249	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	G	959	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	G	444	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	C	128	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	A	514	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	G	944	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	1041	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	E	959	ASP	CB-CG-OD1	7.26	124.84	118.30
1	G	848	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	C	558	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	G	133	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	E	611	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	A	956	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	558	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	C	609	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	G	128	ASP	CB-CG-OD2	-7.18	111.83	118.30
1	E	959	ASP	CB-CG-OD2	-7.16	111.86	118.30
2	B	262	ASP	CB-CG-OD2	-7.15	111.86	118.30
2	D	112	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	E	530	ASP	CB-CG-OD1	7.13	124.72	118.30
1	C	197	ASP	CB-CG-OD2	-7.12	111.90	118.30
1	A	611	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	G	1031	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	514	ARG	NE-CZ-NH2	-7.07	116.77	120.30
2	F	317	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	904	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	G	716	PRO	N-CA-CB	7.06	111.78	103.30
1	A	667	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	C	736	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	G	416	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	E	416	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	A	791	ASP	CB-CG-OD1	7.04	124.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	211	ASP	CB-CG-OD1	7.04	124.64	118.30
2	F	234	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	E	609	ASP	CB-CG-OD2	-7.03	111.97	118.30
2	B	317	ASP	CB-CG-OD2	-7.03	111.98	118.30
1	C	161	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	E	129	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	D	112	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	592	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	G	959	ASP	CB-CG-OD1	6.99	124.59	118.30
1	C	592	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	410	ASP	CB-CG-OD2	-6.97	112.02	118.30
1	E	487	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	E	735	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	G	425	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	C	810	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	E	6	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	E	226	ASP	CB-CG-OD1	6.93	124.54	118.30
2	B	227	ASP	CB-CG-OD2	-6.93	112.07	118.30
1	A	674	ASP	CB-CG-OD2	-6.91	112.08	118.30
2	D	368	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	129	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	E	539	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	A	972	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	C	84	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	G	530	ASP	CB-CG-OD1	6.83	124.45	118.30
1	G	625	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	A	471	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	C	539	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	609	ASP	CB-CG-OD1	6.82	124.44	118.30
2	H	139	ASP	CB-CG-OD1	6.82	124.44	118.30
1	C	674	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	C	6	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	E	128	ASP	CB-CG-OD1	6.79	124.42	118.30
1	E	417	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	E	736	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	539	ASP	CB-CG-OD2	-6.76	112.22	118.30
2	B	249	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	G	133	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	614	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	A	614	ASP	CB-CG-OD1	6.74	124.37	118.30
1	G	667	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	C	226	ASP	CB-CG-OD1	6.73	124.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	ASP	CB-CG-OD2	-6.72	112.25	118.30
2	D	188	ASP	CB-CG-OD2	-6.72	112.25	118.30
2	B	97	ASP	CB-CG-OD1	6.72	124.35	118.30
1	E	670	ASP	CB-CG-OD2	-6.72	112.25	118.30
2	H	139	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	C	194	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	C	400	ARG	NE-CZ-NH1	6.69	123.64	120.30
2	F	262	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	A	530	ASP	CB-CG-OD1	6.68	124.31	118.30
1	G	539	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	C	333	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	C	579	ASP	CB-CG-OD1	6.67	124.30	118.30
1	E	730	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	E	611	ASP	CB-CG-OD1	6.67	124.30	118.30
1	C	104	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	C	459	ASP	CB-CG-OD1	6.66	124.30	118.30
1	C	416	ASP	CB-CG-OD2	-6.64	112.32	118.30
2	D	67	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	G	753	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	E	667	ASP	CB-CG-OD2	-6.63	112.33	118.30
2	B	244	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	C	558	ASP	N-CA-CB	-6.62	98.68	110.60
1	C	956	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	736	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	667	ASP	CB-CG-OD1	6.61	124.25	118.30
2	H	112	ASP	CB-CG-OD1	6.61	124.25	118.30
1	E	765	ASP	CB-CG-OD1	6.61	124.25	118.30
1	G	75	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	C	372	ASP	CB-CG-OD2	-6.60	112.36	118.30
2	B	114	ASP	CB-CG-OD2	-6.58	112.37	118.30
1	A	131	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	579	ASP	CB-CG-OD2	-6.57	112.39	118.30
2	D	262	ASP	CB-CG-OD2	-6.57	112.39	118.30
2	H	249	ASP	CB-CG-OD1	6.57	124.21	118.30
1	C	124	ASP	CB-CG-OD1	6.57	124.21	118.30
1	G	121	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	E	904	ASP	CB-CG-OD2	-6.56	112.39	118.30
2	H	188	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	E	410	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	E	471	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	G	6	ASP	CB-CG-OD1	6.53	124.18	118.30
2	D	234	ASP	CB-CG-OD2	-6.52	112.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	757	ASP	CB-CG-OD1	6.52	124.17	118.30
1	E	1003	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	611	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	246	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	C	667	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	194	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	C	441	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	490	ARG	NE-CZ-NH1	6.48	123.54	120.30
2	B	139	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	753	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	530	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	A	333	ASP	CB-CG-OD2	-6.46	112.49	118.30
2	H	262	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	E	124	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	716	PRO	N-CA-CB	6.45	111.04	103.30
1	C	133	ASP	CB-CG-OD1	6.45	124.11	118.30
1	G	183	TYR	CB-CG-CD1	-6.44	117.14	121.00
1	G	674	ASP	CB-CG-OD1	6.43	124.09	118.30
1	C	518	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	G	609	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	E	1021	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	57	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	959	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	E	972	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	E	434	ASP	CB-CG-OD2	-6.39	112.54	118.30
1	E	579	ASP	CB-CG-OD2	-6.39	112.54	118.30
1	C	912	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	A	372	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	124	ASP	CB-CG-OD2	-6.38	112.55	118.30
1	G	530	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	1003	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	765	ASP	CB-CG-OD1	6.38	124.04	118.30
1	C	753	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	609	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	E	558	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	642	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	C	6	ASP	CB-CG-OD1	6.35	124.01	118.30
1	A	389	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	G	246	ASP	CB-CG-OD1	6.33	124.00	118.30
1	E	487	ASP	CB-CG-OD1	6.32	123.99	118.30
1	G	499	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	333	ASP	CB-CG-OD1	6.32	123.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ASP	CB-CG-OD1	6.31	123.98	118.30
1	C	487	ASP	CB-CG-OD2	-6.29	112.64	118.30
2	D	139	ASP	CB-CG-OD1	6.29	123.96	118.30
1	C	330	TYR	CB-CG-CD2	-6.28	117.23	121.00
2	H	286	MET	CG-SD-CE	-6.28	90.16	100.20
2	D	139	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	C	1041	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	592	ASP	CB-CG-OD1	6.26	123.93	118.30
1	G	416	ASP	CB-CG-OD1	6.25	123.93	118.30
1	G	1004	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	E	733	ASP	CB-CG-OD2	-6.24	112.68	118.30
2	F	326	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	B	317	ASP	CB-CG-OD1	6.24	123.91	118.30
2	H	368	ASP	CB-CG-OD2	-6.24	112.69	118.30
2	F	139	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	A	226	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	124	ASP	CB-CG-OD1	6.22	123.89	118.30
2	B	244	ASP	CB-CG-OD1	6.21	123.89	118.30
2	F	249	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	H	112	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	F	97	ASP	CB-CG-OD1	6.20	123.88	118.30
2	F	344	ASP	CB-CG-OD1	6.19	123.87	118.30
1	G	558	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	C	791	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	6	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	E	509	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	B	45	ASP	CB-CG-OD1	6.17	123.85	118.30
1	G	609	ASP	CB-CG-OD1	6.16	123.85	118.30
1	G	124	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	C	459	ASP	CB-CG-OD2	-6.15	112.76	118.30
2	F	234	ASP	CB-CG-OD1	6.15	123.84	118.30
1	C	753	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	E	124	ASP	CB-CG-OD2	-6.15	112.76	118.30
2	H	136	ASP	CB-CG-OD1	6.14	123.83	118.30
2	H	188	ASP	CB-CG-OD1	6.14	123.83	118.30
2	F	97	ASP	CB-CG-OD2	-6.14	112.78	118.30
2	B	344	ASP	CB-CG-OD1	6.14	123.82	118.30
1	E	1004	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	G	128	ASP	CB-CG-OD1	6.14	123.82	118.30
1	G	730	ASP	CB-CG-OD1	6.13	123.82	118.30
1	E	791	ASP	CB-CG-OD1	6.13	123.82	118.30
1	C	518	ASP	CB-CG-OD1	6.13	123.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	84	ASP	CB-CG-OD1	6.13	123.81	118.30
1	G	487	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	416	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	430	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	E	753	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	C	121	ASP	CB-CG-OD1	6.11	123.80	118.30
2	H	136	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	E	1057	ASP	CB-CG-OD2	-6.11	112.80	118.30
2	F	227	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	C	124	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	E	133	ASP	CB-CG-OD1	6.09	123.78	118.30
2	H	114	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	226	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	39	GLU	CB-CA-C	-6.07	98.25	110.40
1	G	258	ASP	CB-CG-OD1	6.06	123.75	118.30
2	D	67	ASP	CB-CG-OD1	6.05	123.74	118.30
1	E	810	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	C	611	ASP	CB-CG-OD1	6.04	123.74	118.30
1	E	539	ASP	CB-CG-OD1	6.04	123.74	118.30
1	C	27	ASP	CB-CG-OD1	6.04	123.73	118.30
2	H	227	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	G	246	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	C	197	ASP	CB-CG-OD1	6.01	123.71	118.30
1	C	400	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	487	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	C	736	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	E	223	ASP	CB-CG-OD1	5.99	123.69	118.30
2	F	227	ASP	CB-CG-OD1	5.99	123.69	118.30
1	G	161	ASP	CB-CG-OD2	-5.99	112.91	118.30
2	D	168	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	E	670	ASP	CB-CG-OD1	5.99	123.69	118.30
1	E	1041	ASP	CB-CG-OD1	5.98	123.69	118.30
2	B	368	ASP	CB-CG-OD1	5.98	123.68	118.30
1	C	222	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	G	333	ASP	CB-CG-OD1	5.98	123.68	118.30
1	G	333	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	C	499	ASP	CB-CG-OD1	5.98	123.68	118.30
1	E	226	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	A	459	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	810	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	517	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	E	57	ASP	CB-CG-OD1	5.96	123.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	326	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	G	667	ASP	CB-CG-OD1	5.95	123.66	118.30
2	F	67	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	E	416	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	149	ALA	N-CA-CB	5.93	118.40	110.10
2	D	326	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	D	344	ASP	CB-CG-OD1	5.92	123.63	118.30
1	E	386	ALA	N-CA-CB	5.92	118.39	110.10
1	C	43	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	544	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	A	416	ASP	CB-CG-OD2	-5.91	112.98	118.30
2	H	215	ARG	NE-CZ-NH1	5.91	123.25	120.30
2	B	344	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	E	434	ASP	CB-CG-OD1	5.90	123.61	118.30
1	C	499	ASP	CB-CG-OD2	-5.90	112.99	118.30
2	D	227	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	530	ASP	CB-CG-OD2	-5.89	112.99	118.30
1	E	1027	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	G	410	ASP	CB-CG-OD1	5.89	123.61	118.30
2	H	234	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	609	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	757	ASP	CB-CG-OD2	-5.88	113.00	118.30
2	B	136	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	G	730	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	C	614	ASP	CB-CG-OD1	5.87	123.59	118.30
1	E	677	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	62	ASP	CB-CG-OD1	5.87	123.58	118.30
1	C	733	ASP	CB-CG-OD2	-5.87	113.02	118.30
2	B	249	ASP	CB-CG-OD1	5.87	123.58	118.30
1	E	517	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	C	912	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	765	ASP	CB-CG-OD2	-5.86	113.03	118.30
2	B	112	ASP	CB-CG-OD1	5.85	123.57	118.30
2	D	249	ASP	CB-CG-OD1	5.85	123.56	118.30
1	E	609	ASP	CB-CG-OD1	5.85	123.56	118.30
1	E	730	ASP	CB-CG-OD1	5.85	123.56	118.30
1	E	758	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	579	ASP	CB-CG-OD1	5.84	123.56	118.30
2	F	136	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	G	590	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	674	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	521	ASP	CB-CG-OD1	5.82	123.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	670	ASP	CB-CG-OD1	5.82	123.53	118.30
1	C	410	ASP	CB-CG-OD2	-5.80	113.08	118.30
2	F	11	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	258	ASP	CB-CG-OD1	5.79	123.52	118.30
1	A	956	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	38	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	C	867	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	G	944	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	G	758	ASP	CB-CG-OD2	-5.77	113.11	118.30
2	H	368	ASP	CB-CG-OD1	5.77	123.49	118.30
1	E	27	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	C	1041	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	43	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	1004	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	G	579	ASP	CB-CG-OD1	5.76	123.48	118.30
2	H	45	ASP	CB-CG-OD1	5.75	123.48	118.30
1	G	490	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	194	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	133	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	E	82	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	E	579	ASP	CB-CG-OD1	5.73	123.46	118.30
2	H	116	ARG	NE-CZ-NH1	5.73	123.17	120.30
2	H	262	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	950	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	133	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	C	207	ASP	CB-CG-OD2	-5.72	113.15	118.30
2	F	250	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	C	38	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	G	758	ASP	CB-CG-OD1	5.70	123.43	118.30
1	E	343	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	G	769	ASP	CB-CG-OD1	5.70	123.42	118.30
1	A	615	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	C	43	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	G	1021	ARG	NE-CZ-NH2	-5.68	117.46	120.30
2	D	362	ASP	CB-CG-OD2	-5.68	113.19	118.30
2	B	97	ASP	CB-CG-OD2	-5.67	113.20	118.30
2	D	262	ASP	CB-CG-OD1	5.67	123.40	118.30
1	E	38	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	129	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	C	950	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	E	372	ASP	CB-CG-OD1	5.66	123.40	118.30
1	E	674	ASP	CB-CG-OD1	5.66	123.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	D	234	ASP	CB-CG-OD1	5.65	123.39	118.30
1	G	912	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	E	197	ASP	CB-CG-OD1	5.65	123.39	118.30
2	F	136	ASP	CB-CG-OD1	5.65	123.39	118.30
2	F	157	ASP	CB-CG-OD1	5.65	123.38	118.30
2	H	84	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	C	674	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	518	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	518	ASP	CB-CG-OD1	5.64	123.38	118.30
2	H	157	ASP	CB-CG-OD1	5.64	123.38	118.30
1	G	57	ASP	CB-CG-OD1	5.64	123.37	118.30
2	H	299	ASP	CB-CG-OD2	-5.64	113.23	118.30
2	F	18	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	C	530	ASP	CB-CG-OD1	5.62	123.36	118.30
1	E	27	ASP	CB-CG-OD1	5.62	123.36	118.30
1	E	258	ASP	CB-CG-OD1	5.62	123.36	118.30
1	E	758	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	733	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	E	972	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	558	ASP	N-CA-CB	-5.61	100.51	110.60
2	H	334	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	E	43	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	G	611	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	E	674	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	E	677	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	246	ASP	CB-CG-OD1	5.58	123.32	118.30
1	G	1041	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	C	426	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	D	203	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	330	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	A	807	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	303	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	E	807	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	E	631	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	D	207	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	E	757	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	E	499	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	E	592	ASP	CB-CG-OD1	5.53	123.27	118.30
1	C	1039	HIS	CA-CB-CG	-5.53	104.21	113.60
1	G	753	ASP	CB-CG-OD1	5.52	123.27	118.30
2	F	344	ASP	CB-CG-OD2	-5.50	113.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	592	ASP	CB-CG-OD2	-5.50	113.35	118.30
2	D	188	ASP	CB-CG-OD1	5.50	123.25	118.30
2	D	227	ASP	CB-CG-OD1	5.50	123.25	118.30
1	G	57	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	C	558	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	763	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	G	373	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	C	625	ASP	CB-CG-OD1	5.48	123.23	118.30
1	G	807	ASP	CB-CG-OD1	5.48	123.23	118.30
2	F	211	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	G	592	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	C	991[A]	VAL	N-CA-CB	5.47	123.54	111.50
1	C	991[B]	VAL	N-CA-CB	5.47	123.54	111.50
1	E	223	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	521	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	C	887	TYR	CB-CG-CD1	-5.45	117.73	121.00
1	A	1004	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	B	45	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	E	614	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	C	430	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	670	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	757	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	410	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	559	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	G	642	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	C	959	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	38	ARG	CD-NE-CZ	5.42	131.20	123.60
1	A	514	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	E	265	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	425	ARG	NE-CZ-NH1	5.41	123.01	120.30
2	F	45	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	6	ASP	CB-CG-OD1	5.41	123.16	118.30
2	D	215	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	E	459	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	G	733	ASP	CB-CG-OD2	-5.39	113.45	118.30
2	B	157	ASP	CB-CG-OD1	5.39	123.15	118.30
1	C	430	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	338	ASP	CB-CG-OD1	5.38	123.14	118.30
2	H	211	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	226	ASP	CB-CG-OD2	-5.38	113.46	118.30
2	H	299	ASP	N-CA-C	-5.38	96.48	111.00
1	E	735	ARG	NE-CZ-NH1	5.38	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	614	ASP	CB-CG-OD1	5.37	123.14	118.30
2	H	378	ARG	NE-CZ-NH1	5.37	122.98	120.30
2	D	249	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	559	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	G	4	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	G	885	PRO	N-CA-CB	5.36	109.73	103.30
1	A	542	TYR	CB-CG-CD2	-5.36	117.78	121.00
1	C	539	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	906	LEU	CB-CA-C	5.36	120.38	110.20
1	E	207	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	G	614	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	459	ASP	CB-CG-OD1	5.36	123.12	118.30
1	G	111	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	A	972	ASP	CB-CG-OD1	5.36	123.12	118.30
1	E	953	ASP	CB-CG-OD1	5.36	123.12	118.30
1	G	223	ASP	CB-CG-OD1	5.35	123.11	118.30
2	D	84	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	E	867	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	C	614	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	E	204	LEU	CB-CA-C	-5.33	100.08	110.20
1	E	904	ASP	CB-CG-OD1	5.33	123.09	118.30
2	B	262	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	667	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	434	ASP	CB-CG-OD1	5.32	123.08	118.30
1	G	39	GLU	CB-CA-C	-5.31	99.78	110.40
1	C	273	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	618	PHE	CB-CG-CD2	-5.31	117.09	120.80
1	E	1057	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	65	TYR	CB-CG-CD2	-5.30	117.82	121.00
2	B	188	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	E	514	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	F	45	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	G	258	ASP	CB-CG-OD2	-5.30	113.53	118.30
2	D	212	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	557	THR	CA-C-N	-5.29	105.56	117.20
1	E	161	ASP	CB-CG-OD2	-5.29	113.54	118.30
2	D	97	ASP	CB-CG-OD1	5.27	123.05	118.30
2	B	69	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	C	338	ASP	CB-CG-OD2	-5.27	113.56	118.30
2	D	45	ASP	CB-CG-OD1	5.26	123.04	118.30
1	E	557	THR	CA-CB-CG2	-5.26	105.04	112.40
1	C	559	ARG	NE-CZ-NH1	5.26	122.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	145	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	615	ARG	NE-CZ-NH1	5.25	122.93	120.30
2	B	188	ASP	CB-CG-OD1	5.25	123.03	118.30
1	E	944	ARG	NE-CZ-NH2	-5.25	117.68	120.30
2	H	116	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	E	584	HIS	CA-CB-CG	-5.25	104.68	113.60
1	G	38	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	121	ASP	CB-CG-OD1	5.25	123.02	118.30
2	D	136	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	E	6	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	373	ARG	NE-CZ-NH2	-5.23	117.68	120.30
2	D	136	ASP	CB-CG-OD1	5.23	123.01	118.30
1	G	904	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	1003	ASP	CB-CG-OD1	5.22	123.00	118.30
1	G	27	ASP	CB-CG-OD2	-5.22	113.61	118.30
1	A	618	PHE	CB-CG-CD1	5.21	124.45	120.80
2	H	97	ASP	CB-CG-OD1	5.20	122.98	118.30
2	H	234	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	642	TYR	CB-CG-CD1	5.20	124.12	121.00
1	A	726	GLU	N-CA-CB	5.20	119.95	110.60
1	G	145	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	C	998	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	E	765	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	C	1003	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	E	517	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	G	518[A]	ASP	CB-CG-OD1	5.18	122.96	118.30
1	G	518[B]	ASP	CB-CG-OD1	5.18	122.96	118.30
2	F	50	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	434	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	888	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	H	227	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	121	ASP	CB-CG-OD2	-5.16	113.66	118.30
2	B	136	ASP	CB-CG-OD1	5.16	122.94	118.30
1	G	459	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	757	ASP	CB-CG-OD1	5.15	122.93	118.30
1	A	758	ASP	CB-CG-OD1	5.15	122.93	118.30
1	G	27	ASP	CB-CG-OD1	5.15	122.93	118.30
1	G	1016	THR	CA-CB-CG2	-5.15	105.20	112.40
1	A	671	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	B	50	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	338	ASP	CB-CG-OD1	5.13	122.92	118.30
2	F	114	ASP	CB-CG-OD1	5.13	122.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	343	ARG	CD-NE-CZ	5.13	130.78	123.60
1	C	487	ASP	CB-CG-OD1	5.13	122.92	118.30
1	G	539	ASP	CB-CG-OD1	5.13	122.91	118.30
1	G	520	TYR	CB-CG-CD2	-5.12	117.92	121.00
1	E	173	THR	N-CA-CB	5.12	120.03	110.30
1	A	730	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	82	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	330	TYR	CB-CG-CD2	-5.11	117.93	121.00
2	D	344	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	E	733	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	237	PHE	CB-CG-CD1	-5.10	117.23	120.80
1	C	769	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	E	185	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	G	558	ASP	N-CA-CB	-5.09	101.44	110.60
1	C	238	ASP	CB-CG-OD1	5.08	122.87	118.30
1	E	389	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	769	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	1031	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	G	161	ASP	CB-CG-OD1	5.07	122.86	118.30
1	G	1025	ASP	CB-CG-OD1	5.07	122.87	118.30
2	D	203	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	E	410	ASP	CB-CG-OD1	5.07	122.86	118.30
2	B	139	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	1025	ASP	CB-CG-OD1	5.06	122.85	118.30
1	E	944	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	57	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	C	611	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	G	972	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	416	ASP	CB-CG-OD1	5.04	122.84	118.30
1	E	161	ASP	CB-CG-OD1	5.04	122.84	118.30
1	E	185	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	845	ARG	NE-CZ-NH1	5.03	122.82	120.30
2	B	67	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	C	450	ASP	CB-CG-OD2	-5.03	113.77	118.30
2	D	244	ASP	CB-CG-OD1	5.03	122.83	118.30
1	E	354	TYR	CB-CG-CD2	5.03	124.02	121.00
1	C	1003	ASP	N-CA-CB	5.02	119.64	110.60
1	E	197	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	753	ASP	CB-CG-OD2	-5.02	113.78	118.30
2	D	114	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	E	430	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	G	791	ASP	CB-CG-OD2	-5.02	113.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	400	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	758	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	G	736	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	E	953	ASP	CB-CG-OD2	-5.01	113.79	118.30
2	B	227	ASP	CB-CG-OD1	5.00	122.80	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	339	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	A	8169	0	8201	245	0
1	C	8173	0	8207	259	0
1	E	8186	0	8220	206	0
1	G	8175	0	8210	282	0
2	B	2904	0	2867	95	0
2	D	2909	0	2869	95	0
2	F	2904	0	2867	86	0
2	H	2906	0	2868	129	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0
4	E	8	0	0	0	0
4	F	1	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	0	2	0
5	B	2	0	0	0	0
5	C	5	0	0	2	0
5	D	2	0	0	0	0
5	E	5	0	0	2	0
5	F	2	0	0	0	0
5	G	5	0	0	3	0
5	H	2	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	10	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	0	0
7	C	54	0	24	0	0
7	E	54	0	24	1	0
7	G	54	0	24	3	0
8	A	9	0	11	0	0
8	C	9	0	11	2	0
8	E	9	0	11	3	0
8	G	9	0	11	0	0
9	A	9	0	20	2	0
9	C	9	0	20	0	0
9	E	9	0	20	1	0
9	G	9	0	20	0	0
10	A	869	0	0	26	0
10	B	213	0	0	3	0
10	C	784	0	0	16	0
10	D	275	0	0	6	0
10	E	864	0	0	22	0
10	F	235	0	0	2	0
10	G	743	0	0	25	0
10	H	193	0	0	6	0
All	All	48889	0	44529	1385	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (1385) 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)
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.21	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.30	1.14
2:F:228:VAL:HA	2:F:231:MET:HE2	1.35	1.06
2:F:187:GLU:HG2	2:F:215:ARG:HD2	1.35	1.05
1:G:1027[B]:ARG:HE	1:G:1031:ARG:HD3	1.17	1.05
1:E:559:ARG:HG3	1:E:559:ARG:HH11	1.19	1.02
1:A:472:LEU:HG	10:A:5510:HOH:O	1.59	1.01
1:A:38:ARG:HH11	1:A:38:ARG:HG3	1.26	1.00
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.44	0.99
1:C:814:GLN:HG3	1:C:818:PHE:HE2	1.30	0.96
1:A:563:MET:HE3	1:A:635:PRO:HG3	1.48	0.95
2:D:78:GLN:HE21	2:D:78:GLN:HA	1.32	0.94
1:E:784:GLN:H	1:E:784:GLN:HE21	1.07	0.94
1:G:784:GLN:HE21	1:G:784:GLN:H	0.96	0.94
1:A:784:GLN:HE21	1:A:784:GLN:H	1.15	0.93
1:C:38:ARG:HH11	1:C:38:ARG:HG3	1.34	0.92
1:C:784:GLN:H	1:C:784:GLN:HE21	1.16	0.92
2:H:54:THR:HG21	2:H:118:LEU:HD23	1.51	0.92
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.50	0.92
1:C:728:VAL:HG12	1:C:733:ASP:HB3	1.49	0.92
1:A:713:VAL:HG23	1:A:755:PHE:HB2	1.53	0.91
1:G:784:GLN:NE2	1:G:784:GLN:H	1.68	0.90
1:G:693:ALA:HB2	1:G:708:ILE:HD11	1.53	0.90
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.52	0.90
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.88	0.88
1:A:728:VAL:HG13	1:A:733:ASP:HB3	1.55	0.88
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.03	0.88
1:G:1001:ILE:HD12	1:G:1002:GLN:N	1.89	0.88
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.56	0.87
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.10	0.87
1:C:814:GLN:HG3	1:C:818:PHE:CE2	2.10	0.87
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.09	0.87
1:A:784:GLN:NE2	1:A:784:GLN:H	1.72	0.86
1:G:728:VAL:CG1	1:G:733:ASP:HB3	2.04	0.86
1:A:1:MET:HB2	1:A:224:LYS:NZ	1.90	0.86
1:E:714:VAL:HG13	1:E:752:LEU:CD1	2.05	0.85
1:G:950:ARG:HD3	5:G:5087:CL:CL	2.14	0.85
1:G:663:GLY:CA	1:G:869:MET:HG2	2.07	0.85
1:G:728:VAL:HG13	1:G:733:ASP:HB3	1.56	0.85
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.40	0.85
2:B:322:PRO:HB2	2:B:324:ASN:ND2	1.93	0.84
1:G:1:MET:HB2	1:G:224:LYS:NZ	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:324:ASN:N	2:B:324:ASN:HD22	1.74	0.83
2:B:286:MET:CE	2:B:315:ALA:HB2	2.08	0.83
1:G:76:LYS:HE3	10:G:5232:HOH:O	1.78	0.83
1:E:784:GLN:H	1:E:784:GLN:NE2	1.77	0.83
1:A:695:VAL:HG13	1:A:700:MET:HB3	1.59	0.83
1:G:1027[B]:ARG:NE	1:G:1031:ARG:HD3	1.93	0.82
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.61	0.82
1:G:682:VAL:HG13	1:G:687:LEU:HB2	1.61	0.82
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.60	0.82
1:G:695:VAL:HG21	1:G:701:ALA:HA	1.61	0.81
1:C:4:ARG:HD3	1:C:7:ILE:HD12	1.63	0.81
2:H:50:ARG:HG3	2:H:158:LEU:HD11	1.61	0.81
1:G:901:PRO:HD2	5:G:5085:CL:CL	2.17	0.81
2:B:324:ASN:H	2:B:324:ASN:ND2	1.78	0.80
1:C:981:LEU:HD12	1:C:988:PRO:HG3	1.62	0.80
1:E:1:MET:H3	1:E:224:LYS:HE3	1.48	0.79
1:G:563:MET:CE	1:G:635:PRO:HG3	2.12	0.79
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.65	0.79
1:G:70:HIS:HE1	1:G:72:GLU:HG3	1.48	0.79
1:A:728:VAL:CG1	1:A:733:ASP:HB3	2.12	0.79
2:D:226:GLU:O	2:D:230:LYS:HG3	1.83	0.79
1:C:1001:ILE:HD12	1:C:1002:GLN:N	1.98	0.79
2:B:324:ASN:H	2:B:324:ASN:HD22	1.31	0.78
2:H:324:ASN:O	2:H:342:ARG:HD2	1.84	0.78
1:G:873:SER:O	1:G:877:GLN:HG3	1.83	0.78
1:C:784:GLN:H	1:C:784:GLN:NE2	1.82	0.78
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.66	0.78
1:E:684:ARG:HG3	1:E:684:ARG:HH11	1.49	0.78
1:G:726:GLU:HG3	1:G:727:ILE:N	1.99	0.77
1:C:967:GLN:HG2	1:C:1054:LEU:HD13	1.65	0.77
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.66	0.77
2:B:269:CYG:N1	10:B:5022:HOH:O	2.17	0.77
1:C:1001:ILE:HD12	1:C:1002:GLN:H	1.46	0.77
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.65	0.77
1:G:967:GLN:HG3	1:G:1054:LEU:HD13	1.67	0.77
2:H:248:CYS:O	2:H:252:ILE:HG13	1.84	0.76
1:E:1:MET:N	1:E:224:LYS:HE3	2.00	0.76
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.12	0.76
1:G:472:LEU:O	1:G:476:VAL:HG23	1.85	0.76
1:C:734:LEU:HD11	1:C:738:PHE:CE2	2.21	0.75
2:B:226:GLU:O	2:B:230:LYS:HG3	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:322:PRO:HG2	2:H:324:ASN:HD21	1.49	0.75
2:H:346:PRO:HG3	10:H:3959:HOH:O	1.87	0.75
1:G:784:GLN:N	1:G:784:GLN:HE21	1.80	0.75
1:A:726:GLU:HG3	1:A:727:ILE:N	2.02	0.75
1:G:714:VAL:HG13	1:G:752:LEU:CD1	2.16	0.75
1:E:714:VAL:HG13	1:E:752:LEU:HD11	1.67	0.75
1:A:873:SER:O	1:A:877:GLN:HG3	1.86	0.75
2:D:133:ILE:HG22	2:D:138:PRO:HB3	1.69	0.74
1:A:726:GLU:HG3	1:A:727:ILE:H	1.51	0.74
2:B:150:PHE:CD2	2:B:151:PRO:HD2	2.21	0.74
2:H:285:LYS:HG3	2:H:314:PHE:CE1	2.23	0.74
1:A:1001:ILE:HD12	1:A:1002:GLN:N	2.03	0.74
1:A:38:ARG:HG3	1:A:38:ARG:NH1	1.98	0.74
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.22	0.74
1:C:1004:ARG:HB3	1:C:1009[A]:GLU:HG3	1.68	0.74
2:B:286:MET:HE2	2:B:315:ALA:HB2	1.68	0.74
2:F:322:PRO:HB2	2:F:324:ASN:ND2	2.03	0.74
1:A:563:MET:CE	1:A:635:PRO:HG3	2.18	0.73
1:G:482:THR:HB	10:G:5525:HOH:O	1.87	0.73
2:F:225:ALA:O	2:F:229:LEU:HG	1.88	0.73
1:C:726:GLU:HG3	1:C:727:ILE:N	2.03	0.73
2:F:236:ILE:HB	2:F:265:VAL:HG22	1.70	0.73
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.69	0.73
1:C:773:VAL:HG23	1:C:818:PHE:CZ	2.24	0.73
1:A:734:LEU:O	1:A:734:LEU:HD12	1.87	0.73
1:C:780:GLU:HG3	1:C:801:LEU:HD11	1.71	0.73
1:G:70:HIS:CE1	1:G:72:GLU:HG3	2.23	0.73
1:E:912:ARG:HD2	10:E:5689:HOH:O	1.88	0.73
1:G:693:ALA:CB	1:G:708:ILE:HD11	2.17	0.73
2:D:206:LEU:O	2:D:210:VAL:HG23	1.88	0.72
1:C:728:VAL:HG11	1:C:734:LEU:HA	1.71	0.72
2:B:324:ASN:N	2:B:324:ASN:ND2	2.37	0.72
1:A:992:ASN:ND2	1:A:996:GLU:HB3	2.03	0.72
1:G:225:ASN:ND2	1:G:331:THR:HG21	2.05	0.72
1:G:663:GLY:HA3	1:G:869:MET:HG2	1.72	0.72
2:H:34:THR:HA	2:H:56:THR:OG1	1.89	0.72
1:A:954:LYS:O	1:A:957:VAL:HG12	1.89	0.72
1:G:475:LYS:O	1:G:479:VAL:HG13	1.89	0.72
2:D:78:GLN:NE2	2:D:78:GLN:HA	2.05	0.72
1:C:154:GLU:OE1	10:C:2077:HOH:O	2.06	0.72
2:D:233:PRO:HG2	2:D:263:ILE:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:714:VAL:HG13	1:G:752:LEU:HD11	1.70	0.71
1:C:559:ARG:HH11	1:C:559:ARG:HG3	1.54	0.71
1:C:998:ARG:HG2	1:C:999:PRO:HA	1.71	0.71
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.21	0.71
1:G:64:THR:O	1:G:1065:VAL:HG23	1.91	0.71
1:G:698:ILE:HD12	1:G:698:ILE:H	1.56	0.71
2:B:228:VAL:HA	2:B:231:MET:CE	2.21	0.71
1:G:809:MET:O	1:G:813:VAL:HG23	1.90	0.71
1:G:563:MET:HE1	1:G:635:PRO:HG3	1.73	0.70
1:A:1001:ILE:HD12	1:A:1002:GLN:H	1.57	0.70
2:H:187:GLU:CG	2:H:215:ARG:HD2	2.19	0.70
1:G:954:LYS:O	1:G:957:VAL:HG12	1.92	0.70
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.27	0.70
1:E:224:LYS:HE2	1:E:329:GLY:O	1.91	0.70
1:E:726:GLU:HG3	1:E:727:ILE:N	2.07	0.70
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.72	0.70
1:C:648:LEU:HD13	1:C:845:ARG:HD2	1.73	0.70
1:G:490:ARG:HD3	10:G:5702:HOH:O	1.90	0.70
1:G:733:ASP:HA	1:G:736:ARG:HH11	1.56	0.70
1:E:714:VAL:HG13	1:E:752:LEU:HD12	1.73	0.70
1:A:700:MET:O	1:A:704:LYS:HB2	1.92	0.70
2:H:228:VAL:HA	2:H:231:MET:HE3	1.73	0.70
2:H:186:LYS:O	2:H:189:GLU:HB2	1.92	0.70
1:G:878:GLY:O	10:G:5645:HOH:O	2.09	0.70
1:A:1:MET:HB2	1:A:224:LYS:HZ2	1.57	0.69
1:G:2:PRO:HB2	10:G:5791:HOH:O	1.92	0.69
2:F:6:LEU:HD13	2:F:16:HIS:CE1	2.27	0.69
1:E:956:ARG:HB3	1:E:1044:LEU:CD2	2.22	0.69
1:A:1:MET:HB2	1:A:224:LYS:HZ1	1.55	0.69
1:C:726:GLU:HG3	1:C:727:ILE:H	1.57	0.69
1:C:145:ARG:HH12	1:C:161:ASP:CG	1.95	0.69
1:C:172:PHE:HB3	1:C:200:PRO:HG2	1.75	0.69
1:A:151:THR:OG1	1:A:154:GLU:HG3	1.93	0.69
1:C:1004:ARG:CB	1:C:1009[A]:GLU:HG3	2.23	0.69
1:C:991[A]:VAL:HG11	1:C:1004:ARG:HE	1.56	0.69
1:G:427:GLU:HG3	1:G:438:TYR:CE1	2.28	0.69
1:A:675:ARG:CD	1:A:675:ARG:H	2.02	0.69
1:C:648:LEU:CD1	1:C:845:ARG:HD2	2.24	0.68
1:G:344:THR:HB	1:G:345:PRO:HD2	1.75	0.68
1:E:684:ARG:NH1	1:E:684:ARG:HG3	2.07	0.68
1:G:998:ARG:HA	1:G:999:PRO:C	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:955:GLU:HB2	10:E:5928:HOH:O	1.93	0.68
2:D:222:GLN:H	2:D:222:GLN:HE21	1.42	0.68
1:E:1001:ILE:HD12	1:E:1002:GLN:N	2.09	0.68
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.76	0.68
1:C:1009[B]:GLU:HG3	10:C:1999:HOH:O	1.93	0.68
1:G:828:VAL:HG22	1:G:842:VAL:HG13	1.76	0.67
2:B:186:LYS:O	2:B:189:GLU:HB2	1.94	0.67
1:G:734:LEU:HD11	1:G:738:PHE:CE2	2.28	0.67
1:E:728:VAL:HG13	1:E:733:ASP:HB3	1.76	0.67
2:H:95:THR:HG21	10:H:3945:HOH:O	1.94	0.67
1:C:509:ARG:HD3	10:C:1979:HOH:O	1.94	0.67
1:G:43:ARG:NH2	1:G:81:GLU:OE2	2.27	0.67
2:B:71:GLU:O	2:B:203:ARG:HG3	1.93	0.67
1:C:416:ASP:O	1:C:418:PRO:HD3	1.94	0.67
1:G:671:ARG:HG2	1:G:677:ARG:NH1	2.08	0.67
1:A:698:ILE:H	1:A:698:ILE:HD12	1.60	0.67
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.29	0.67
1:E:950:ARG:HD3	5:E:5062:CL:CL	2.32	0.67
1:C:695:VAL:HG13	1:C:700:MET:HB3	1.76	0.67
1:A:695:VAL:HG21	1:A:701:ALA:HA	1.76	0.67
1:E:417:ASP:OD1	1:E:423:LYS:NZ	2.27	0.67
2:H:322:PRO:HB2	2:H:324:ASN:ND2	2.10	0.67
1:C:973:ALA:O	1:C:991[B]:VAL:HG12	1.95	0.67
2:H:300:VAL:HG22	2:H:328:THR:O	1.95	0.67
1:A:38:ARG:HH11	1:A:38:ARG:CG	2.06	0.67
1:G:1:MET:HB2	1:G:224:LYS:HZ2	1.57	0.67
2:F:322:PRO:HG2	2:F:324:ASN:HD21	1.58	0.67
1:A:315:THR:O	1:A:531:THR:HG22	1.95	0.66
1:A:40:GLU:CG	1:A:325:LYS:HE2	2.25	0.66
1:E:1020:ARG:O	1:E:1024:GLU:HG3	1.95	0.66
1:A:997:GLY:O	1:A:998:ARG:HG3	1.95	0.66
1:E:698:ILE:HG13	1:E:738:PHE:CD1	2.30	0.66
2:B:228:VAL:HA	2:B:231:MET:HE2	1.76	0.66
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.57	0.66
1:E:1:MET:HB2	1:E:224:LYS:NZ	2.11	0.66
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.77	0.66
1:C:1004:ARG:CA	1:C:1009[A]:GLU:HG3	2.26	0.66
2:D:174:SER:O	2:D:182:PRO:HD3	1.96	0.66
1:C:559:ARG:NH2	10:C:1994:HOH:O	2.28	0.66
1:E:726:GLU:HG3	1:E:727:ILE:H	1.60	0.66
1:G:423:LYS:HB3	10:G:5480:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:VAL:O	2:D:231:MET:HG3	1.96	0.66
1:A:471:ARG:HD2	10:A:5515:HOH:O	1.95	0.66
2:H:50:ARG:HG3	2:H:158:LEU:CD1	2.25	0.66
1:A:40:GLU:HG2	1:A:325:LYS:HE2	1.76	0.66
2:B:133:ILE:HD12	2:B:143:ALA:HB2	1.78	0.66
1:G:1:MET:HB2	1:G:224:LYS:HZ1	1.61	0.65
1:G:682:VAL:CG1	1:G:687:LEU:HB2	2.26	0.65
1:E:734:LEU:O	1:E:734:LEU:HD12	1.96	0.65
1:C:975:HIS:O	1:C:979:ILE:HG12	1.96	0.65
1:C:1061:LYS:HG2	10:C:1883:HOH:O	1.96	0.65
2:H:232:ASN:N	2:H:233:PRO:HD3	2.10	0.65
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.77	0.65
1:G:663:GLY:HA2	1:G:869:MET:HG2	1.79	0.65
1:C:865:ALA:O	1:C:869:MET:HG3	1.96	0.65
1:E:976:GLY:O	1:E:980:VAL:HG23	1.97	0.65
2:H:275:LEU:HD23	2:H:349:SER:OG	1.96	0.65
1:A:1001:ILE:O	1:A:1005:ILE:HG13	1.97	0.65
1:C:954:LYS:HG2	1:C:980:VAL:HG21	1.79	0.65
2:F:34:THR:HA	2:F:56:THR:OG1	1.97	0.65
1:A:814:GLN:NE2	10:A:5628:HOH:O	2.29	0.65
1:G:701:ALA:O	1:G:705:ALA:N	2.29	0.65
2:H:228:VAL:HA	2:H:231:MET:CE	2.27	0.65
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.78	0.65
1:C:780:GLU:HG3	1:C:801:LEU:CD1	2.27	0.65
1:A:38:ARG:NH2	10:A:5735:HOH:O	2.29	0.65
1:E:956:ARG:HB3	1:E:1044:LEU:HD21	1.77	0.65
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.26	0.64
1:C:802:SER:OG	1:C:805:ILE:HB	1.96	0.64
1:C:734:LEU:O	1:C:734:LEU:HD12	1.96	0.64
2:B:286:MET:HE1	2:B:315:ALA:HB2	1.77	0.64
2:H:322:PRO:CG	2:H:324:ASN:HD21	2.10	0.64
2:F:259:LEU:HD13	2:F:342:ARG:NH1	2.12	0.64
1:E:728:VAL:CG1	1:E:733:ASP:HB3	2.27	0.64
1:G:146:SER:HB2	1:G:205:LEU:HD11	1.79	0.64
1:G:698:ILE:N	1:G:698:ILE:HD12	2.12	0.64
2:D:233:PRO:HG2	2:D:263:ILE:HD13	1.79	0.64
1:C:321:LYS:NZ	1:C:611:ASP:OD1	2.30	0.64
1:C:509:ARG:NH1	1:C:512:GLU:OE1	2.30	0.64
1:C:954:LYS:O	1:C:957:VAL:HG12	1.98	0.64
1:E:559:ARG:NH1	10:E:5798:HOH:O	2.29	0.64
1:G:905:PRO:HB2	1:G:1040:TYR:OH	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:897:PHE:HB3	10:E:5859:HOH:O	1.98	0.64
2:B:46:PRO:HA	2:B:76:HIS:CG	2.33	0.64
1:E:6:ASP:N	1:E:6:ASP:OD2	2.30	0.64
1:A:528:ARG:HG2	1:A:543:MET:HG2	1.78	0.64
2:F:324:ASN:O	2:F:342:ARG:HD2	1.98	0.63
1:C:812:GLN:NE2	10:C:1654:HOH:O	2.31	0.63
1:A:189:GLU:HB3	10:A:5919:HOH:O	1.98	0.63
1:G:548:GLU:HG2	2:H:114:ASP:CG	2.18	0.63
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.32	0.63
1:A:734:LEU:HD11	1:A:738:PHE:CE2	2.33	0.63
2:H:249:ASP:OD2	2:H:249:ASP:N	2.31	0.63
1:C:761:GLU:HG2	1:C:781:HIS:CE1	2.33	0.63
1:C:1:MET:HB2	1:C:224:LYS:NZ	2.14	0.63
1:E:998:ARG:HA	1:E:999:PRO:C	2.18	0.63
1:G:6:ASP:OD2	1:G:6:ASP:N	2.29	0.63
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.80	0.63
1:G:734:LEU:HD12	1:G:734:LEU:O	1.97	0.63
1:A:698:ILE:O	1:A:702:VAL:HG23	1.99	0.63
1:E:998:ARG:CB	1:E:999:PRO:HA	2.27	0.63
1:G:318:PRO:HG3	1:G:610:TYR:OH	1.99	0.63
1:G:340:THR:O	1:G:343:ARG:NE	2.31	0.62
1:E:1027:ARG:HE	1:E:1031:ARG:HE	1.45	0.62
1:G:947:LEU:N	1:G:947:LEU:HD12	2.12	0.62
1:G:702:VAL:HG11	1:G:735:ARG:NH2	2.14	0.62
2:H:142:LEU:HD12	2:H:142:LEU:O	1.97	0.62
1:C:698:ILE:H	1:C:698:ILE:HD12	1.64	0.62
1:G:833:LYS:O	1:G:836:GLU:HB2	1.98	0.62
2:D:78:GLN:NE2	10:D:1778:HOH:O	2.31	0.62
1:A:632:ILE:HG13	1:A:633:GLU:N	2.14	0.62
1:G:994:VAL:HG22	1:G:1000:HIS:CG	2.34	0.62
1:E:1001:ILE:HD13	1:E:1029:ILE:HG13	1.81	0.62
1:E:698:ILE:O	1:E:702:VAL:HG23	2.00	0.62
1:G:963:LYS:HE2	10:G:5691:HOH:O	1.99	0.62
1:G:680:HIS:O	1:G:683:GLU:HB2	1.99	0.62
1:G:667:ASP:CG	1:G:677:ARG:HH22	2.03	0.62
1:A:905:PRO:HB2	1:A:1040:TYR:OH	1.98	0.62
2:B:173:GLY:O	2:B:207:ARG:HG2	2.00	0.62
1:G:224:LYS:HE2	1:G:329:GLY:O	1.98	0.62
1:C:519[A]:GLN:NE2	10:C:1959:HOH:O	2.33	0.62
1:G:1017:THR:HG22	1:G:1018:SER:N	2.14	0.62
1:C:675:ARG:CD	1:C:675:ARG:H	2.09	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1021:ARG:CG	1:E:1021:ARG:HH11	2.13	0.62
1:G:728:VAL:HG11	1:G:734:LEU:HA	1.81	0.61
1:G:343:ARG:HG3	1:G:344:THR:HG23	1.82	0.61
1:A:266:ASN:ND2	10:A:5382:HOH:O	2.30	0.61
1:C:677:ARG:O	1:C:680:HIS:HB2	2.00	0.61
1:C:713:VAL:HG23	1:C:755:PHE:HB2	1.82	0.61
1:G:1021:ARG:CG	1:G:1021:ARG:HH11	2.14	0.61
1:A:43:ARG:NH2	1:A:81:GLU:OE2	2.30	0.61
1:C:991[A]:VAL:HG11	1:C:1004:ARG:NE	2.15	0.61
1:E:43:ARG:NH1	10:E:5867:HOH:O	2.24	0.61
2:F:300:VAL:HG22	2:F:328:THR:O	2.01	0.61
2:H:78:GLN:NE2	10:H:3934:HOH:O	2.29	0.61
2:H:58:PRO:HA	2:H:83:ARG:HB3	1.81	0.61
2:H:71:GLU:O	2:H:203:ARG:HG3	2.00	0.61
1:E:559:ARG:NH1	1:E:559:ARG:HG3	1.99	0.61
2:H:168:TYR:CE1	2:H:218:ILE:HB	2.36	0.61
1:E:967:GLN:HG3	1:E:1054:LEU:HD13	1.82	0.61
1:G:1026:SER:HB2	1:G:1030:ARG:HH12	1.65	0.61
2:D:46:PRO:HA	2:D:76:HIS:CG	2.35	0.61
2:H:322:PRO:HG2	2:H:324:ASN:ND2	2.15	0.61
1:A:780:GLU:OE2	1:A:798:ALA:HB1	2.00	0.61
1:E:669:ILE:O	1:E:673:GLU:HG2	2.01	0.61
1:E:873:SER:O	1:E:877:GLN:HG3	2.01	0.61
1:C:998:ARG:CG	1:C:999:PRO:HA	2.30	0.61
1:C:698:ILE:N	1:C:698:ILE:HD12	2.16	0.61
1:A:344:THR:HB	1:A:345:PRO:HD2	1.82	0.61
1:A:891:LYS:NZ	10:A:5624:HOH:O	2.34	0.60
2:B:185:LYS:HD2	2:B:190:LEU:HD21	1.82	0.60
2:B:298:LYS:HE2	2:B:303:ASN:OD1	2.02	0.60
1:E:1061[A]:LYS:NZ	10:E:5637:HOH:O	2.29	0.60
1:C:6:ASP:N	1:C:6:ASP:OD2	2.30	0.60
1:G:1001:ILE:HD12	1:G:1002:GLN:HB2	1.82	0.60
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.46	0.60
1:G:671:ARG:NH2	1:G:819:GLU:O	2.34	0.60
1:G:637:GLY:HA2	1:G:660:PRO:HB2	1.83	0.60
1:A:698:ILE:CD1	1:A:698:ILE:H	2.14	0.60
1:C:991[A]:VAL:CG1	1:C:1004:ARG:HE	2.14	0.60
1:G:667:ASP:OD2	1:G:677:ARG:NH2	2.34	0.60
1:G:1021:ARG:HH11	1:G:1021:ARG:HG2	1.67	0.60
1:G:321:LYS:NZ	1:G:611:ASP:OD1	2.31	0.60
1:G:528:ARG:HG2	1:G:543:MET:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:PHE:HB2	2:B:366:LEU:CD2	2.31	0.60
2:D:334:ASP:HB3	10:D:1431:HOH:O	2.00	0.60
1:G:964:LEU:O	1:G:969:PHE:HB2	2.02	0.60
1:C:145:ARG:NH1	1:C:161:ASP:OD1	2.33	0.60
1:E:1061[B]:LYS:NZ	10:E:5860:HOH:O	2.30	0.60
1:A:1004:ARG:O	1:A:1009[B]:GLU:HG2	2.01	0.60
2:F:187:GLU:HG2	2:F:215:ARG:CD	2.23	0.60
1:A:425:ARG:HD3	10:A:5482:HOH:O	2.01	0.60
1:A:950:ARG:HD3	5:A:5015:CL:CL	2.39	0.60
2:F:228:VAL:HA	2:F:231:MET:CE	2.21	0.60
1:E:1021:ARG:HG2	1:E:1021:ARG:HH11	1.65	0.60
1:E:4:ARG:HA	10:E:5150:HOH:O	2.02	0.60
1:C:892:GLU:OE1	8:C:5033:ORN:NE	2.34	0.60
2:F:212:ARG:HH11	2:F:212:ARG:HG3	1.67	0.60
2:H:322:PRO:HD2	2:H:325:LEU:HD12	1.84	0.60
1:C:1061:LYS:HE2	10:C:1737:HOH:O	2.02	0.60
2:F:150:PHE:CD2	2:F:151:PRO:HD2	2.37	0.60
1:A:1021:ARG:HG3	1:A:1021:ARG:HH11	1.67	0.60
1:G:956:ARG:HB3	1:G:1044:LEU:HD21	1.84	0.60
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.84	0.60
1:E:930:LYS:HE3	10:E:5202:HOH:O	2.02	0.60
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.67	0.59
1:G:704:LYS:O	1:G:708:ILE:HD12	2.01	0.59
1:C:695:VAL:HG21	1:C:701:ALA:HA	1.83	0.59
1:C:997:GLY:O	1:C:998:ARG:HG3	2.02	0.59
2:B:139:ASP:OD2	2:B:142:LEU:HB2	2.01	0.59
2:D:189:GLU:OE2	10:D:2123:HOH:O	2.17	0.59
2:F:187:GLU:OE2	2:F:215:ARG:NH1	2.36	0.59
2:B:299:ASP:OD1	2:B:302:LYS:HD2	2.02	0.59
1:A:278:GLU:HG2	10:A:5759:HOH:O	2.02	0.59
1:E:703:GLU:O	1:E:706:LYS:HB2	2.02	0.59
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.37	0.59
2:B:251:ALA:O	2:B:255:ILE:HD12	2.01	0.59
1:G:65:TYR:OH	1:G:80:LYS:HE2	2.03	0.59
2:F:232:ASN:N	2:F:233:PRO:HD3	2.17	0.59
1:A:698:ILE:N	1:A:698:ILE:HD12	2.17	0.59
1:A:224:LYS:NZ	10:A:5169:HOH:O	2.29	0.58
1:C:687:LEU:CD1	1:C:812:GLN:HG2	2.32	0.58
1:C:671:ARG:NH2	1:C:819:GLU:O	2.36	0.58
1:E:905:PRO:HB2	1:E:1040:TYR:OH	2.03	0.58
1:C:561:LYS:NZ	1:C:633:GLU:O	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:926:GLU:HB2	10:E:5838:HOH:O	2.02	0.58
2:F:259:LEU:HD13	2:F:342:ARG:HH12	1.68	0.58
1:C:689:GLN:HG2	1:C:690:PRO:HD2	1.85	0.58
10:G:5445:HOH:O	2:H:87:LEU:HD13	2.04	0.58
1:A:28:TYR:O	1:A:32:GLN:HG3	2.04	0.58
1:C:883:VAL:O	1:C:884:ILE:HD13	2.04	0.58
1:E:473:GLU:HG2	1:E:505:LEU:HD11	1.85	0.58
1:C:906:LEU:O	1:C:912:ARG:NH2	2.29	0.58
2:B:371:ILE:HG13	10:B:5233:HOH:O	2.04	0.58
1:A:906:LEU:O	1:A:912:ARG:NH2	2.32	0.58
1:A:560:GLU:HB3	1:A:636:LYS:HD2	1.85	0.58
1:C:947:LEU:HG	1:C:1014:ILE:HG21	1.84	0.57
2:H:364:ALA:N	2:H:365:PRO:HD2	2.18	0.57
1:E:645[B]:GLN:HG3	1:E:649:LYS:HE3	1.86	0.57
1:G:713:VAL:HG23	1:G:755:PHE:HB2	1.86	0.57
2:F:306:MET:HB3	2:F:362:ASP:HB3	1.85	0.57
1:G:267:ALA:O	1:G:271:VAL:HG23	2.04	0.57
1:C:325:LYS:O	1:C:330:TYR:HB2	2.04	0.57
1:E:670:ASP:HB3	1:E:677:ARG:NH2	2.19	0.57
1:E:282:SER:OG	1:E:302:PRO:HA	2.04	0.57
1:A:106:GLY:HA2	10:A:5910:HOH:O	2.04	0.57
1:C:375:THR:HG23	1:C:377:GLN:H	1.68	0.57
1:C:11:LEU:HA	1:C:45:ILE:O	2.04	0.57
1:A:67:GLU:HB3	1:A:68:PRO:HD2	1.85	0.57
1:E:998:ARG:HB3	1:E:999:PRO:HA	1.87	0.57
1:A:325:LYS:O	1:A:330:TYR:HB2	2.05	0.57
2:D:64:GLY:HA3	2:D:94:ASN:OD1	2.05	0.57
1:A:784:GLN:HE21	1:A:784:GLN:N	1.95	0.57
1:G:224:LYS:NZ	10:G:5173:HOH:O	2.28	0.57
2:H:363:ALA:C	2:H:365:PRO:HD2	2.24	0.57
2:F:8:VAL:HG22	2:F:14:GLN:HG2	1.86	0.57
1:A:150:HIS:N	1:A:154:GLU:OE2	2.37	0.57
1:C:726:GLU:OE1	1:C:1020:ARG:HD3	2.04	0.56
1:A:336:MET:HB3	1:A:342:GLY:HA2	1.86	0.56
2:H:302:LYS:HD2	10:H:3986:HOH:O	2.03	0.56
1:A:813:VAL:HG22	1:A:828:VAL:HG21	1.86	0.56
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.39	0.56
2:D:322:PRO:HD2	2:D:325:LEU:HD12	1.88	0.56
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.51	0.56
1:G:427:GLU:HG3	1:G:438:TYR:CD1	2.40	0.56
1:C:698:ILE:H	1:C:698:ILE:CD1	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:LEU:HD23	1:G:979:ILE:HG12	1.87	0.56
1:A:193:ALA:HA	10:A:5203:HOH:O	2.05	0.56
1:E:691:ALA:HB3	1:E:708:ILE:HG23	1.88	0.56
1:E:336:MET:HB3	1:E:342:GLY:HA2	1.87	0.56
2:F:324:ASN:HD22	2:F:324:ASN:N	2.03	0.56
2:F:263:ILE:CG2	2:F:264:PRO:HD2	2.36	0.56
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.70	0.56
1:G:675:ARG:H	1:G:675:ARG:CD	2.19	0.56
1:E:809:MET:O	1:E:813:VAL:HG23	2.05	0.56
1:E:669:ILE:HA	1:E:844:PRO:HG2	1.87	0.56
1:E:646:THR:HB	1:E:647:PRO:HD3	1.87	0.56
1:G:526:TYR:O	1:G:552:GLU:HB2	2.04	0.56
1:C:710:TYR:HB3	1:C:729:TYR:O	2.05	0.56
1:A:672:ALA:CB	1:A:844:PRO:HG3	2.36	0.56
1:C:1:MET:HB2	1:C:224:LYS:HZ2	1.69	0.56
2:H:46:PRO:HA	2:H:76:HIS:CG	2.41	0.56
1:C:559:ARG:NH1	1:C:559:ARG:HG3	2.18	0.56
1:A:559:ARG:HH11	1:A:559:ARG:HG3	1.71	0.56
1:G:340:THR:O	1:G:343:ARG:HG2	2.06	0.56
1:G:671:ARG:HG2	1:G:677:ARG:CZ	2.36	0.56
1:G:294:ARG:HD2	5:G:5084:CL:CL	2.43	0.56
1:C:905:PRO:HB2	1:C:1040:TYR:OH	2.05	0.56
1:C:1004:ARG:HA	1:C:1009[A]:GLU:HG3	1.88	0.56
1:A:973:ALA:O	1:A:991:VAL:HG12	2.06	0.55
2:D:26:ALA:O	2:D:131:CYS:HA	2.06	0.55
2:H:197:TYR:HB3	2:H:199:PHE:CZ	2.41	0.55
2:F:171:THR:HG22	2:F:215:ARG:HB2	1.87	0.55
1:C:715:ARG:HB2	1:C:751:LEU:HB2	1.87	0.55
1:E:549:GLU:HG2	10:E:5908:HOH:O	2.06	0.55
2:B:234:ASP:OD1	2:B:378:ARG:NH1	2.30	0.55
1:G:259:LYS:HD3	2:H:175:TRP:CE3	2.41	0.55
1:E:784:GLN:HE21	1:E:784:GLN:N	1.91	0.55
1:E:1:MET:HB2	1:E:224:LYS:HZ2	1.70	0.55
1:C:420:ALA:HA	1:C:423:LYS:HD2	1.87	0.55
2:D:244:ASP:OD2	2:D:245:PRO:HD2	2.07	0.55
2:D:139:ASP:OD2	2:D:142:LEU:HB2	2.05	0.55
1:E:831:ALA:HB2	1:E:840:ILE:HD11	1.87	0.55
2:F:298:LYS:O	2:F:329:HIS:HA	2.07	0.55
1:G:726:GLU:HG3	1:G:727:ILE:H	1.71	0.55
1:G:548:GLU:HG2	2:H:114:ASP:OD1	2.07	0.55
2:B:367:PHE:O	2:B:370:PHE:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:HB2	1:A:42:TYR:OH	2.07	0.55
1:C:976:GLY:O	1:C:979:ILE:HB	2.07	0.55
1:G:1000:HIS:HD2	1:G:1003:ASP:H	1.53	0.55
2:D:178:THR:HB	10:D:1823:HOH:O	2.07	0.55
2:D:307:ILE:HG22	2:D:360:PRO:HG2	1.88	0.55
1:A:150:HIS:CD2	1:A:203:GLU:HG3	2.42	0.54
1:C:634:LYS:HG3	10:C:2090:HOH:O	2.07	0.54
1:C:672:ALA:HB3	1:C:844:PRO:HG3	1.88	0.54
2:B:277:LEU:HD23	2:B:281:ALA:O	2.07	0.54
2:D:367:PHE:O	2:D:370:PHE:HB3	2.06	0.54
1:E:440:ALA:O	1:E:444:ARG:HG3	2.07	0.54
1:G:308:SER:HB3	10:G:5356:HOH:O	2.06	0.54
2:H:32:PHE:O	2:H:291:HIS:HB2	2.06	0.54
1:G:840:ILE:O	1:G:841:GLU:HB3	2.07	0.54
1:C:873:SER:O	1:C:877:GLN:HG3	2.07	0.54
1:G:906:LEU:O	1:G:912:ARG:NH2	2.29	0.54
1:A:101:GLU:HA	1:A:101:GLU:OE2	2.08	0.54
2:D:33:ASN:HA	2:D:291:HIS:O	2.07	0.54
1:E:674:ASP:HB3	1:E:677:ARG:HG3	1.89	0.54
1:C:1017:THR:HG21	1:C:1023:ILE:HA	1.89	0.54
1:A:225:ASN:ND2	1:A:331:THR:HG21	2.22	0.54
1:A:976:GLY:O	1:A:980:VAL:HG23	2.08	0.54
1:C:687:LEU:HD13	1:C:812:GLN:HG2	1.89	0.54
1:G:946:LEU:C	1:G:947:LEU:HD12	2.28	0.54
1:G:734:LEU:O	1:G:737:TYR:HB3	2.08	0.54
1:A:675:ARG:H	1:A:675:ARG:HD3	1.69	0.54
1:G:674:ASP:HB3	1:G:677:ARG:HG3	1.89	0.54
2:H:46:PRO:HG2	2:H:200:GLY:O	2.08	0.54
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.72	0.54
1:A:411:PRO:HG3	10:A:5493:HOH:O	2.07	0.54
1:A:515:LYS:HG3	10:A:5845:HOH:O	2.07	0.54
1:G:698:ILE:CD1	1:G:698:ILE:H	2.19	0.54
2:D:204:ASN:ND2	2:D:355:GLU:O	2.35	0.54
1:G:940:LYS:HG3	1:G:1011:THR:HB	1.90	0.54
1:C:994:VAL:HG22	1:C:1000:HIS:CG	2.43	0.54
1:G:868:VAL:HG23	1:G:877:GLN:HE22	1.73	0.54
1:G:679:GLN:HG2	1:G:683:GLU:OE2	2.08	0.54
1:A:956:ARG:HA	10:A:5872:HOH:O	2.08	0.54
1:G:845:ARG:NH1	10:G:5598:HOH:O	2.41	0.54
1:C:257:THR:HG23	2:D:91:ASN:ND2	2.23	0.53
1:C:954:LYS:CG	1:C:980:VAL:HG21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:648:LEU:CD2	1:E:845:ARG:HD3	2.38	0.53
1:G:172:PHE:HB3	1:G:200:PRO:HG2	1.89	0.53
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.38	0.53
1:A:6:ASP:N	1:A:6:ASP:OD2	2.37	0.53
1:G:1000:HIS:CD2	1:G:1002:GLN:HB3	2.44	0.53
1:A:998:ARG:HA	1:A:999:PRO:C	2.25	0.53
1:C:708:ILE:CG2	1:C:712:LEU:HD11	2.38	0.53
1:G:420:ALA:HA	1:G:423:LYS:HD2	1.91	0.53
2:B:34:THR:HA	2:B:56:THR:OG1	2.08	0.53
2:H:324:ASN:HD22	2:H:324:ASN:N	2.05	0.53
1:C:702:VAL:HG11	1:C:735:ARG:NH2	2.22	0.53
1:A:973:ALA:C	1:A:991:VAL:HG12	2.29	0.53
1:E:1017:THR:HG22	1:E:1018:SER:N	2.24	0.53
1:G:695:VAL:HG13	1:G:700:MET:HB3	1.91	0.53
2:B:228:VAL:HA	2:B:231:MET:HE3	1.90	0.53
1:C:805:ILE:HD13	1:C:837:VAL:CG2	2.39	0.53
1:E:289:ASN:OD1	1:E:290:PRO:HD2	2.08	0.53
1:G:734:LEU:HD12	1:G:734:LEU:C	2.29	0.53
1:G:954:LYS:HB3	1:G:980:VAL:HG21	1.91	0.53
2:H:374:ILE:O	2:H:377:TYR:HB3	2.09	0.53
1:C:809:MET:O	1:C:813:VAL:HG23	2.09	0.53
1:A:10:ILE:HD13	1:A:37:LEU:HD13	1.89	0.53
1:E:953:ASP:O	1:E:955:GLU:N	2.42	0.53
1:A:695:VAL:CG2	1:A:752:LEU:HD22	2.39	0.53
1:G:864:VAL:O	1:G:868:VAL:HG23	2.09	0.52
1:E:730:ASP:O	1:E:733:ASP:HB2	2.08	0.52
1:C:512:GLU:OE1	1:C:515:LYS:NZ	2.40	0.52
1:C:82:ARG:HD3	10:C:1225:HOH:O	2.08	0.52
1:A:654:LEU:O	1:A:659:VAL:HG23	2.08	0.52
1:E:675:ARG:H	1:E:675:ARG:CD	2.21	0.52
2:B:286:MET:HE3	2:B:312:HIS:ND1	2.24	0.52
2:D:185:LYS:HD2	2:D:190:LEU:HD21	1.91	0.52
2:F:64:GLY:HA3	2:F:94:ASN:OD1	2.09	0.52
2:H:350:PHE:HB2	2:H:366:LEU:CD2	2.39	0.52
2:H:132:ILE:HG22	2:H:133:ILE:N	2.25	0.52
2:B:306:MET:HB3	2:B:362:ASP:HB3	1.91	0.52
2:F:78:GLN:NE2	10:F:2837:HOH:O	2.43	0.52
1:G:712:LEU:HD23	1:G:752:LEU:HG	1.92	0.52
1:C:130:ARG:HB2	1:C:148:ILE:HD12	1.90	0.52
1:C:1068:MET:O	1:C:1071:GLN:HB2	2.09	0.52
1:G:485:ASN:HB2	10:G:5526:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1001:ILE:HD12	1:G:1002:GLN:CA	2.40	0.52
1:G:714:VAL:HG13	1:G:752:LEU:HD12	1.92	0.52
1:G:954:LYS:O	1:G:980:VAL:HG11	2.10	0.52
2:B:120:ARG:HD2	10:B:5060:HOH:O	2.09	0.52
1:E:757:ASP:O	1:E:833:LYS:NZ	2.30	0.52
2:H:82:ILE:O	2:H:111:ALA:HA	2.10	0.52
1:A:948:SER:O	1:A:1015:ASN:HA	2.09	0.52
1:E:153:GLU:HB2	10:E:5278:HOH:O	2.09	0.52
1:G:167:ILE:HD12	1:G:167:ILE:N	2.25	0.52
2:D:279:SER:O	2:D:322:PRO:HG3	2.09	0.52
1:A:998:ARG:HG2	1:A:999:PRO:HA	1.92	0.52
1:E:1004:ARG:HD3	1:E:1009[B]:GLU:OE2	2.08	0.52
1:G:733:ASP:O	1:G:736:ARG:NH1	2.43	0.52
2:B:350:PHE:HB2	2:B:366:LEU:HD23	1.92	0.52
1:G:29:SER:HB3	1:G:304:VAL:HG21	1.92	0.52
2:D:199:PHE:O	2:D:241:GLY:HA3	2.10	0.52
2:H:355:GLU:N	2:H:355:GLU:OE2	2.34	0.52
2:H:54:THR:HG21	2:H:118:LEU:CD2	2.31	0.52
1:G:344:THR:HB	1:G:345:PRO:CD	2.40	0.52
2:H:218:ILE:N	2:H:218:ILE:HD13	2.25	0.52
1:A:912:ARG:NH1	10:A:5099:HOH:O	2.42	0.52
1:C:956:ARG:HB3	1:C:1044:LEU:CD2	2.40	0.52
1:G:185:ARG:O	1:G:188:PHE:HB3	2.10	0.52
1:C:426:ARG:C	1:C:426:ARG:HD3	2.30	0.52
2:B:57:TYR:CE1	2:B:58:PRO:HD2	2.45	0.51
1:E:698:ILE:O	1:E:701:ALA:HB3	2.09	0.51
1:C:686:LYS:O	1:C:687:LEU:HD23	2.10	0.51
1:G:525:VAL:HG22	1:G:548:GLU:H	1.74	0.51
1:E:448:SER:O	1:E:452:VAL:HG23	2.10	0.51
2:D:176:THR:O	2:D:180:GLY:N	2.34	0.51
2:F:185:LYS:HD2	2:F:190:LEU:HD21	1.92	0.51
2:H:251:ALA:O	2:H:255:ILE:HG13	2.10	0.51
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.28	0.51
2:B:218:ILE:N	2:B:218:ILE:HD13	2.25	0.51
1:A:166:CYS:C	1:A:167:ILE:HD12	2.31	0.51
1:C:964:LEU:O	1:C:969:PHE:HB2	2.10	0.51
2:H:153:LEU:HA	2:H:156:MET:HE3	1.91	0.51
1:G:28:TYR:CZ	1:G:313:LYS:HE3	2.45	0.51
1:E:146:SER:HB2	1:E:205:LEU:HD11	1.92	0.51
1:A:272:LEU:HD11	1:A:282:SER:HB2	1.92	0.51
1:A:141:LEU:HB3	1:A:297:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:195:VAL:HG21	2:F:231:MET:CE	2.40	0.51
1:G:1000:HIS:NE2	1:G:1002:GLN:HB3	2.25	0.51
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.29	0.51
1:A:339:ILE:HD11	1:A:531:THR:HG23	1.92	0.51
1:G:36:ALA:HB1	1:G:325:LYS:HE3	1.91	0.51
1:G:17:PRO:HG3	1:G:917:VAL:CG1	2.40	0.51
1:C:336:MET:HG3	10:C:1423:HOH:O	2.10	0.51
2:B:48:TYR:HA	2:B:51:GLN:HE21	1.74	0.51
2:D:6:LEU:HD13	2:D:16:HIS:CE1	2.45	0.51
1:E:997:GLY:O	1:E:998:ARG:HG3	2.10	0.51
1:E:734:LEU:C	1:E:734:LEU:HD12	2.30	0.51
2:D:2:ILE:HD12	2:D:3:LYS:N	2.25	0.51
1:G:769:ASP:N	1:G:769:ASP:OD2	2.39	0.51
1:A:88:PRO:HB3	1:A:99:ALA:HB2	1.91	0.51
1:E:698:ILE:HG23	1:E:738:PHE:CD2	2.45	0.51
1:A:417:ASP:HB3	1:A:420:ALA:HB2	1.92	0.51
1:A:548:GLU:OE1	2:B:114:ASP:HA	2.11	0.51
1:A:35:LYS:O	1:A:39:GLU:HG3	2.10	0.51
1:E:527:LYS:HB2	1:E:544:TYR:CZ	2.46	0.51
2:F:212:ARG:CG	2:F:212:ARG:HH11	2.23	0.51
2:D:2:ILE:HD12	2:D:3:LYS:H	1.75	0.51
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.26	0.51
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.57	0.51
1:E:509:ARG:NH2	1:E:515:LYS:NZ	2.59	0.51
2:B:187:GLU:HG2	2:B:215:ARG:CD	2.15	0.51
1:A:563:MET:HB3	1:A:638:VAL:HG13	1.93	0.51
2:H:279:SER:O	2:H:322:PRO:HG3	2.11	0.51
2:F:57:TYR:CE1	2:F:58:PRO:HD2	2.46	0.51
2:B:198:ASP:HB2	2:B:218:ILE:CG2	2.41	0.51
1:C:948:SER:O	1:C:1015:ASN:HA	2.10	0.51
2:F:272:HIS:HA	2:F:349:SER:CB	2.41	0.51
1:A:695:VAL:CG1	1:A:700:MET:HB3	2.37	0.51
2:H:324:ASN:HA	2:H:343:THR:OG1	2.10	0.51
1:C:992:ASN:ND2	1:C:996:GLU:HB3	2.25	0.51
2:F:324:ASN:H	2:F:324:ASN:HD22	1.57	0.51
1:C:998:ARG:CB	1:C:999:PRO:HA	2.41	0.51
1:G:29:SER:CB	1:G:304:VAL:HG21	2.41	0.51
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.93	0.51
2:H:81:VAL:CG1	2:H:113:ILE:HD11	2.41	0.51
1:C:344:THR:HB	1:C:345:PRO:HD2	1.92	0.51
1:A:103:GLU:HB3	10:A:5725:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:ARG:C	1:A:426:ARG:HD3	2.31	0.51
1:E:1027:ARG:HE	1:E:1031:ARG:NE	2.09	0.51
1:C:4:ARG:HD3	1:C:7:ILE:CD1	2.38	0.50
1:A:992:ASN:HB2	1:A:999:PRO:O	2.12	0.50
1:C:78:ILE:O	1:C:82:ARG:N	2.35	0.50
2:F:272:HIS:HA	2:F:349:SER:HB2	1.93	0.50
2:H:222:GLN:H	2:H:222:GLN:HE21	1.58	0.50
2:H:195:VAL:O	2:H:237:PHE:N	2.30	0.50
1:A:1023:ILE:HG22	1:A:1024:GLU:N	2.25	0.50
1:E:426:ARG:C	1:E:426:ARG:HD3	2.31	0.50
2:B:42:ILE:HG23	2:B:48:TYR:CE2	2.45	0.50
2:F:45:ASP:HB3	2:F:48:TYR:HD2	1.75	0.50
1:G:730:ASP:H	1:G:733:ASP:HB2	1.76	0.50
1:C:714:VAL:HG21	1:C:728:VAL:HG21	1.93	0.50
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.26	0.50
1:A:141:LEU:HB3	1:A:297:VAL:HG21	1.92	0.50
1:C:659:VAL:HG13	1:C:660:PRO:HD2	1.92	0.50
1:G:1019:GLY:O	1:G:1023:ILE:HG13	2.11	0.50
1:A:964:LEU:O	1:A:969:PHE:HB2	2.11	0.50
1:A:860:PRO:O	1:A:864:VAL:HG23	2.11	0.50
1:E:805:ILE:CD1	1:E:837:VAL:HG23	2.42	0.50
1:G:735:ARG:O	1:G:738:PHE:HB2	2.12	0.50
1:C:224:LYS:HE2	1:C:329:GLY:O	2.09	0.50
1:A:336:MET:HE3	10:A:5795:HOH:O	2.11	0.50
1:C:637:GLY:HA2	1:C:660:PRO:O	2.10	0.50
2:D:118:LEU:O	2:D:118:LEU:HD12	2.12	0.50
1:A:412:LYS:NZ	10:A:5488:HOH:O	2.37	0.50
2:F:354:PRO:HB3	2:F:363:ALA:O	2.11	0.50
2:B:345:LYS:HB3	2:B:346:PRO:HD2	1.93	0.50
1:E:907:LEU:HD11	8:E:5056:ORN:HD3	1.93	0.50
1:E:46:LEU:HD22	1:E:46:LEU:C	2.32	0.50
2:F:322:PRO:CG	2:F:324:ASN:HD21	2.24	0.50
1:A:941:LYS:NZ	1:A:1056:ALA:O	2.30	0.50
1:E:383:GLU:OE2	1:E:604:GLU:OE1	2.30	0.50
1:A:412:LYS:HD2	10:A:5822:HOH:O	2.10	0.50
1:G:802:SER:OG	1:G:805:ILE:HB	2.12	0.50
1:G:423:LYS:NZ	10:G:5476:HOH:O	2.44	0.50
2:H:199:PHE:O	2:H:241:GLY:HA3	2.11	0.50
2:F:369:HIS:O	2:F:373:LEU:HG	2.12	0.50
1:E:785:ALA:HB1	7:E:5052:ADP:N3	2.27	0.50
1:C:186:GLU:HA	10:C:1915:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:702:VAL:HG11	1:E:735:ARG:NH2	2.27	0.49
2:H:323:ALA:C	2:H:325:LEU:H	2.16	0.49
2:B:45:ASP:O	2:B:76:HIS:HB2	2.11	0.49
1:C:751:LEU:C	1:C:752:LEU:HD12	2.32	0.49
2:H:208:MET:SD	2:H:355:GLU:HA	2.52	0.49
2:B:290:HIS:NE2	2:B:334:ASP:OD1	2.40	0.49
1:E:103:GLU:HG3	1:E:104:ARG:N	2.24	0.49
1:E:166:CYS:C	1:E:167:ILE:HD12	2.32	0.49
1:A:1:MET:N	1:A:224:LYS:HE3	2.27	0.49
2:D:63:VAL:O	2:D:94:ASN:HB2	2.12	0.49
2:H:123:ARG:HA	2:H:288:PHE:CD2	2.48	0.49
2:F:257:LYS:O	2:F:260:GLU:HB2	2.11	0.49
1:A:79:GLU:HA	1:A:111:PHE:CE2	2.47	0.49
1:C:383:GLU:OE2	1:C:604:GLU:OE1	2.30	0.49
2:D:237:PHE:CE1	2:D:268:ILE:HD12	2.47	0.49
2:B:33:ASN:HB3	2:B:55:LEU:HD23	1.94	0.49
1:C:690:PRO:HD2	10:C:1875:HOH:O	2.12	0.49
1:A:414:SER:OG	1:A:416:ASP:OD2	2.29	0.49
2:F:201:ALA:HB2	2:F:239:SER:CB	2.43	0.49
1:E:28:TYR:CZ	1:E:313:LYS:HE3	2.48	0.49
2:B:185:LYS:CD	2:B:190:LEU:HD21	2.42	0.49
2:B:27:VAL:O	2:B:78:GLN:HG2	2.12	0.49
1:E:941:LYS:HE2	10:E:5839:HOH:O	2.12	0.49
1:G:82:ARG:N	1:G:83:PRO:HD3	2.28	0.49
1:G:349:GLU:O	2:H:294:ASN:HB2	2.13	0.49
1:C:78:ILE:HG23	1:C:83:PRO:HD2	1.93	0.49
1:G:891:LYS:NZ	10:G:5618:HOH:O	2.46	0.49
1:C:17:PRO:HG3	1:C:917:VAL:CG1	2.42	0.49
1:A:734:LEU:C	1:A:734:LEU:HD12	2.30	0.49
2:F:75:VAL:HG11	2:F:107:ILE:HG13	1.94	0.49
1:G:103:GLU:HG3	1:G:104:ARG:N	2.26	0.49
1:G:1001:ILE:O	1:G:1005:ILE:HG13	2.12	0.49
1:G:1026:SER:CB	1:G:1030:ARG:HH12	2.24	0.49
1:E:509:ARG:HH22	1:E:515:LYS:NZ	2.11	0.49
2:H:6:LEU:HD12	2:H:7:LEU:N	2.28	0.49
1:G:1030:ARG:HH11	1:G:1030:ARG:HG3	1.78	0.49
1:C:1064:SER:O	1:C:1068:MET:HG3	2.12	0.49
1:A:220:VAL:O	1:A:281:GLY:HA2	2.12	0.49
1:A:713:VAL:HG22	1:A:727:ILE:HG12	1.95	0.49
2:H:272:HIS:HB2	2:H:349:SER:HB2	1.94	0.49
2:H:139:ASP:OD2	2:H:142:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:956:ARG:HB3	1:G:1044:LEU:CD2	2.43	0.49
2:B:344:ASP:OD2	2:B:344:ASP:N	2.38	0.49
2:D:201:ALA:HB2	2:D:239:SER:CB	2.43	0.49
2:B:286:MET:HE1	2:B:312:HIS:CE1	2.48	0.49
8:E:5056:ORN:HB3	10:E:5079:HOH:O	2.11	0.49
2:H:244:ASP:OD2	2:H:245:PRO:HD2	2.13	0.49
1:E:682:VAL:HG13	1:E:687:LEU:HB2	1.95	0.49
1:G:475:LYS:NZ	10:G:5513:HOH:O	2.43	0.48
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.76	0.48
1:E:78:ILE:HG23	1:E:83:PRO:HD2	1.95	0.48
1:A:479:VAL:HB	1:A:483:GLY:HA3	1.95	0.48
1:A:689:GLN:HG2	1:A:690:PRO:HD2	1.95	0.48
1:E:659:VAL:CG1	1:E:660:PRO:HD2	2.43	0.48
1:C:640:VAL:HG21	1:C:651:ALA:HB2	1.94	0.48
1:C:563:MET:CE	1:C:635:PRO:HG3	2.34	0.48
1:G:1:MET:CB	1:G:224:LYS:HZ1	2.26	0.48
1:G:755:PHE:CD1	7:G:5077:ADP:C2	3.01	0.48
2:H:38:GLY:HA3	2:H:358:PRO:HB3	1.96	0.48
1:E:125:LYS:NZ	10:E:5739:HOH:O	2.46	0.48
2:H:9:LEU:HD12	2:H:13:THR:HB	1.95	0.48
1:C:46:LEU:C	1:C:46:LEU:HD22	2.34	0.48
2:F:263:ILE:HG23	2:F:264:PRO:HD2	1.95	0.48
2:F:341:HIS:CD2	2:F:348:PHE:HB3	2.47	0.48
1:E:1:MET:CB	1:E:224:LYS:HZ1	2.27	0.48
2:H:325:LEU:HD23	2:H:325:LEU:HA	1.66	0.48
1:G:17:PRO:HG3	1:G:917:VAL:HG13	1.96	0.48
1:G:550:GLU:CD	2:H:120:ARG:HH21	2.16	0.48
1:A:681:ALA:O	1:A:684:ARG:HB3	2.13	0.48
1:G:481:ILE:HD13	1:G:508:VAL:HG11	1.96	0.48
1:E:947:LEU:N	1:E:947:LEU:HD12	2.28	0.48
1:C:956:ARG:HB3	1:C:1044:LEU:HD23	1.96	0.48
1:G:36:ALA:O	1:G:40:GLU:HG2	2.13	0.48
1:A:267:ALA:O	1:A:271:VAL:HG23	2.13	0.48
1:G:569:PRO:O	1:G:571:ARG:HD2	2.14	0.48
1:C:237:PHE:CE2	1:C:458:ILE:HD13	2.49	0.48
1:G:780:GLU:OE2	1:G:798:ALA:HB1	2.14	0.48
1:G:708:ILE:CG2	1:G:754:HIS:HB2	2.44	0.48
1:C:1004:ARG:O	1:C:1009[A]:GLU:HG2	2.13	0.48
1:A:665:SER:O	1:A:669:ILE:HG13	2.14	0.48
2:B:232:ASN:N	2:B:233:PRO:HD3	2.28	0.48
2:F:350:PHE:HB2	2:F:366:LEU:CD2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:ALA:HB3	2:B:247:PRO:HD3	1.96	0.48
1:C:159:ALA:HB2	1:C:188:PHE:CZ	2.49	0.48
1:G:645:GLN:HE21	1:G:649:LYS:HE3	1.79	0.48
1:A:868:VAL:HA	1:A:872:LYS:O	2.14	0.48
1:C:526:TYR:CE1	1:C:545:SER:HB3	2.48	0.48
2:B:228:VAL:O	2:B:231:MET:HB2	2.14	0.48
1:A:167:ILE:N	1:A:167:ILE:HD12	2.28	0.48
1:C:757:ASP:O	1:C:833:LYS:NZ	2.38	0.48
1:C:944:ARG:HD3	1:C:972:ASP:OD1	2.13	0.48
2:F:26:ALA:O	2:F:131:CYS:HA	2.13	0.48
1:G:728:VAL:HG12	1:G:733:ASP:HB3	1.89	0.48
1:C:994:VAL:HG23	1:C:1001:ILE:HD11	1.95	0.48
1:C:3:LYS:HB3	1:C:330:TYR:CE1	2.49	0.48
1:C:74:VAL:HG11	1:C:102:LEU:HD11	1.95	0.48
1:C:22:GLN:HG3	1:C:26:PHE:CE2	2.48	0.48
2:H:5:ALA:HB2	2:H:19:ALA:HB2	1.95	0.48
1:C:1027:ARG:NH1	1:C:1027:ARG:HG3	2.29	0.48
1:C:680:HIS:HA	1:C:683:GLU:OE2	2.14	0.48
1:A:344:THR:HB	1:A:345:PRO:CD	2.43	0.48
2:H:299:ASP:OD1	2:H:302:LYS:HD2	2.14	0.48
2:H:169:SER:HA	2:H:216:LEU:O	2.14	0.48
1:G:640:VAL:HG21	1:G:651:ALA:HB2	1.96	0.48
1:C:267:ALA:O	1:C:271:VAL:HG23	2.14	0.48
1:A:695:VAL:HG11	1:A:701:ALA:CB	2.43	0.47
1:C:637:GLY:HA2	1:C:660:PRO:HB2	1.96	0.47
1:A:772:MET:HG3	1:A:874:LEU:HD12	1.96	0.47
1:G:237:PHE:HB3	1:G:248:ILE:HB	1.96	0.47
1:A:89:THR:O	1:A:304:VAL:HG22	2.14	0.47
1:G:1000:HIS:CD2	1:G:1002:GLN:H	2.32	0.47
2:B:244:ASP:OD2	2:B:245:PRO:HD2	2.15	0.47
1:C:213:TRP:CZ3	1:C:296:ILE:HD12	2.49	0.47
2:B:376:GLN:HG3	2:B:376:GLN:O	2.14	0.47
1:E:1027:ARG:NE	1:E:1031:ARG:HE	2.11	0.47
1:C:419:GLU:O	1:C:423:LYS:HG3	2.14	0.47
1:C:101:GLU:OE2	1:C:104:ARG:NH2	2.42	0.47
1:C:579:ASP:OD1	1:C:605:THR:HB	2.14	0.47
1:A:1048:PHE:O	1:A:1051:ALA:HB3	2.13	0.47
1:E:196:LEU:HG	1:E:204:LEU:HD11	1.97	0.47
1:A:1027:ARG:O	1:A:1031:ARG:HG3	2.14	0.47
2:B:286:MET:HE2	2:B:315:ALA:CB	2.40	0.47
1:E:126:ALA:HB3	1:E:302:PRO:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:ARG:NH2	2:B:344:ASP:OD1	2.39	0.47
1:E:9:SER:OG	1:E:83:PRO:HA	2.15	0.47
1:A:158:VAL:HG11	1:A:206:ILE:HB	1.95	0.47
1:A:764:VAL:O	1:A:827:ASN:HA	2.13	0.47
1:E:308:SER:HB3	10:E:5336:HOH:O	2.14	0.47
1:C:820:LEU:O	1:C:821:GLN:HB2	2.14	0.47
1:A:674:ASP:HB3	1:A:677:ARG:HG3	1.96	0.47
1:E:710:TYR:HB3	1:E:729:TYR:O	2.14	0.47
1:E:152:MET:SD	1:E:189:GLU:HG2	2.55	0.47
1:C:772:MET:SD	1:C:880:THR:HG22	2.55	0.47
2:B:6:LEU:HD21	2:B:140:ALA:HA	1.96	0.47
2:B:199:PHE:O	2:B:241:GLY:HA3	2.13	0.47
1:G:874:LEU:HD22	1:G:879:VAL:O	2.15	0.47
1:A:128:ASP:CG	1:A:131:ARG:HG3	2.35	0.47
2:H:6:LEU:CD1	2:H:8:VAL:HG23	2.32	0.47
1:G:755:PHE:CE1	7:G:5077:ADP:C2	3.02	0.47
1:A:1001:ILE:CD1	1:A:1002:GLN:N	2.77	0.47
1:A:32:GLN:OE1	1:A:320:ALA:HB3	2.15	0.47
2:D:142:LEU:O	2:D:142:LEU:HD12	2.15	0.47
2:F:246:ALA:N	2:F:247:PRO:HD2	2.30	0.47
2:H:316:VAL:CG1	2:H:337:LEU:HD23	2.45	0.47
2:B:205:ILE:HG21	2:B:237:PHE:CZ	2.49	0.47
2:B:354:PRO:HB2	2:B:367:PHE:CE2	2.50	0.47
1:E:213:TRP:CZ3	1:E:296:ILE:HD12	2.50	0.47
1:G:436:ILE:HG23	1:G:437:TRP:CE3	2.50	0.47
1:E:678:PHE:O	1:E:681:ALA:N	2.48	0.47
1:E:340:THR:O	1:E:343:ARG:HB2	2.15	0.47
2:D:350:PHE:HB2	2:D:366:LEU:HD22	1.97	0.47
1:G:1001:ILE:HD12	1:G:1002:GLN:CB	2.44	0.47
2:B:286:MET:CE	2:B:312:HIS:ND1	2.78	0.47
1:G:76:LYS:HA	1:G:76:LYS:HD2	1.69	0.47
1:E:698:ILE:CD1	1:E:698:ILE:N	2.78	0.47
1:C:669:ILE:HA	1:C:844:PRO:HG2	1.97	0.47
1:C:400:ARG:HD3	10:C:1475:HOH:O	2.15	0.47
1:G:803:GLN:HG3	1:G:807:ASP:OD1	2.15	0.47
1:C:196:LEU:HG	1:C:204:LEU:HD11	1.97	0.47
1:E:258:ASP:O	1:E:262:GLN:HG2	2.14	0.47
1:G:951:GLU:OE1	1:G:954:LYS:HD2	2.14	0.46
1:G:1030:ARG:NH1	1:G:1030:ARG:HG3	2.30	0.46
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.95	0.46
1:A:669:ILE:HA	1:A:844:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:ILE:HD13	2:B:354:PRO:HD2	1.96	0.46
1:G:503:ALA:HB1	1:G:508:VAL:O	2.15	0.46
1:E:608:THR:HB	1:E:618:PHE:CE2	2.50	0.46
1:E:695:VAL:HG21	1:E:701:ALA:CA	2.40	0.46
2:F:279:SER:O	2:F:322:PRO:HG3	2.15	0.46
1:E:358:LYS:HG2	1:E:359:ILE:N	2.30	0.46
1:A:232:CYS:HA	10:A:5363:HOH:O	2.16	0.46
1:E:318:PRO:HB2	1:E:321:LYS:HB2	1.97	0.46
2:D:158:LEU:O	2:D:161:GLU:HB2	2.14	0.46
1:E:4:ARG:HD3	1:E:7:ILE:HD12	1.96	0.46
1:C:1036:TYR:C	1:C:1037:LYS:HG2	2.35	0.46
1:C:12:ILE:HD11	1:C:37:LEU:HD12	1.97	0.46
1:A:151:THR:HB	10:A:5297:HOH:O	2.15	0.46
1:C:858:GLY:HA2	1:C:1069:HIS:NE2	2.30	0.46
1:C:1017:THR:HG22	1:C:1018:SER:N	2.31	0.46
1:C:644:GLY:O	1:C:647:PRO:HD2	2.16	0.46
2:H:225:ALA:HA	2:H:258:PHE:CZ	2.50	0.46
2:D:150:PHE:CD2	2:D:151:PRO:HD2	2.51	0.46
1:A:663:GLY:CA	1:A:869:MET:HG2	2.45	0.46
2:B:133:ILE:HG22	2:B:138:PRO:HB3	1.98	0.46
2:D:266:PHE:HB2	2:D:370:PHE:CD1	2.51	0.46
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.34	0.46
1:A:358:LYS:HE3	10:A:5372:HOH:O	2.15	0.46
2:F:195:VAL:HG11	2:F:231:MET:HE1	1.98	0.46
1:G:1017:THR:HG22	1:G:1018:SER:H	1.78	0.46
2:B:195:VAL:HG23	2:B:233:PRO:HB3	1.97	0.46
1:A:663:GLY:HA2	1:A:869:MET:HG2	1.97	0.46
1:G:1039:HIS:HA	10:G:5663:HOH:O	2.15	0.46
1:A:250:VAL:HA	1:A:356:VAL:O	2.16	0.46
1:A:901:PRO:HD2	5:A:5013:CL:CL	2.52	0.46
1:C:38:ARG:NH1	1:C:38:ARG:HG3	2.12	0.46
2:D:133:ILE:CG2	2:D:138:PRO:HB3	2.42	0.46
1:A:998:ARG:CB	1:A:999:PRO:HA	2.43	0.46
1:A:814:GLN:HG3	1:A:818:PHE:CE2	2.51	0.46
1:G:676:GLU:O	1:G:680:HIS:ND1	2.48	0.46
2:D:205:ILE:HG13	2:D:355:GLU:HG3	1.98	0.46
2:F:246:ALA:HB3	2:F:247:PRO:HD3	1.96	0.46
1:A:503:ALA:HB2	1:A:510:GLU:HA	1.97	0.46
2:D:39:TYR:CZ	2:D:61:GLY:HA2	2.51	0.46
1:G:713:VAL:HG22	1:G:727:ILE:HG12	1.98	0.46
2:F:324:ASN:HA	2:F:343:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:ALA:HB3	10:E:5280:HOH:O	2.15	0.46
2:D:249:ASP:OD2	2:D:250:TYR:N	2.49	0.46
1:E:579:ASP:OD1	1:E:605:THR:HB	2.16	0.46
1:C:991[B]:VAL:CG2	1:C:992:ASN:N	2.79	0.46
1:C:559:ARG:CG	1:C:559:ARG:HH11	2.26	0.46
2:F:12:GLY:HA2	2:F:144:LEU:HD13	1.98	0.46
1:E:217:GLU:HG2	1:E:285:GLN:HG2	1.98	0.46
1:G:213:TRP:CZ3	1:G:296:ILE:HD12	2.51	0.46
2:H:286:MET:CE	2:H:312:HIS:CE1	2.99	0.46
1:G:702:VAL:O	1:G:705:ALA:HB3	2.17	0.46
1:A:701:ALA:O	1:A:705:ALA:N	2.47	0.46
1:E:1001:ILE:CD1	1:E:1002:GLN:N	2.79	0.46
1:G:128:ASP:OD1	1:G:130:ARG:HB3	2.16	0.46
1:C:730:ASP:H	1:C:733:ASP:HB2	1.80	0.45
1:C:708:ILE:HG22	1:C:712:LEU:HD11	1.97	0.45
2:H:353:HIS:HB3	2:H:355:GLU:CD	2.37	0.45
1:A:235:GLU:HB2	1:A:253:ALA:HA	1.98	0.45
1:A:542:TYR:HE1	1:A:618:PHE:HB2	1.82	0.45
2:H:376:GLN:O	2:H:376:GLN:HG3	2.16	0.45
1:G:728:VAL:HG11	1:G:734:LEU:CA	2.46	0.45
2:D:27:VAL:O	2:D:78:GLN:HG2	2.16	0.45
1:C:695:VAL:HG11	1:C:701:ALA:CA	2.46	0.45
1:E:751:LEU:O	1:E:752:LEU:HD12	2.16	0.45
1:G:868:VAL:HG23	1:G:877:GLN:NE2	2.31	0.45
2:H:312:HIS:HD2	10:H:3239:HOH:O	1.98	0.45
2:F:169:SER:HA	2:F:216:LEU:O	2.15	0.45
1:E:479:VAL:CG2	1:E:483:GLY:HA3	2.46	0.45
1:E:1068:MET:O	1:E:1071:GLN:HB2	2.16	0.45
2:F:353:HIS:CD2	2:F:353:HIS:N	2.84	0.45
2:H:54:THR:CG2	2:H:118:LEU:HD23	2.36	0.45
1:E:695:VAL:HG13	1:E:700:MET:HB3	1.98	0.45
1:C:693:ALA:CB	1:C:708:ILE:HD11	2.47	0.45
1:A:659:VAL:HG13	1:A:660:PRO:HD2	1.97	0.45
1:C:475:LYS:HD3	1:C:488:PHE:CZ	2.51	0.45
1:C:950:ARG:HD3	5:C:5039:CL:CL	2.53	0.45
1:G:456:THR:O	1:G:457:ASN:HB2	2.17	0.45
1:A:695:VAL:HG21	1:A:752:LEU:HD22	1.99	0.45
2:D:186:LYS:H	2:D:189:GLU:CD	2.20	0.45
1:E:509:ARG:NH2	1:E:515:LYS:HZ1	2.15	0.45
1:A:412:LYS:HG2	1:A:438:TYR:CE1	2.51	0.45
2:F:253:THR:O	2:F:256:GLN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:LEU:HD12	2:B:86:PRO:HD2	1.98	0.45
1:C:194:ARG:NH2	10:C:1870:HOH:O	2.49	0.45
2:H:265:VAL:O	2:H:347:ALA:HA	2.17	0.45
2:B:325:LEU:HA	2:B:325:LEU:HD23	1.80	0.45
1:G:329:GLY:HA2	10:G:5173:HOH:O	2.17	0.45
1:E:726:GLU:OE1	1:E:1020:ARG:HD3	2.16	0.45
1:A:467:GLU:O	1:A:471:ARG:HG2	2.15	0.45
1:C:975:HIS:HD1	1:E:975:HIS:HD1	0.79	0.45
2:H:275:LEU:HD23	2:H:349:SER:CB	2.47	0.45
1:G:947:LEU:N	1:G:947:LEU:CD1	2.79	0.45
2:F:208:MET:O	2:F:212:ARG:HG3	2.17	0.45
1:A:1017:THR:HG21	1:A:1023:ILE:HA	1.98	0.45
2:B:364:ALA:N	2:B:365:PRO:HD2	2.31	0.45
2:D:344:ASP:N	2:D:344:ASP:OD2	2.43	0.45
1:E:150:HIS:HE1	10:E:5882:HOH:O	2.00	0.45
1:C:796:LEU:C	1:C:796:LEU:HD23	2.37	0.45
9:E:5057:NET:H22	9:E:5057:NET:H42	1.97	0.45
2:D:259:LEU:HD23	2:D:259:LEU:HA	1.84	0.45
1:C:768:CYS:HB2	1:C:773:VAL:HG22	1.98	0.45
1:E:648:LEU:HD21	1:E:845:ARG:HD3	1.97	0.45
2:H:353:HIS:N	2:H:353:HIS:CD2	2.85	0.45
1:A:1031:ARG:HE	1:A:1031:ARG:HB3	1.61	0.45
2:F:170:TRP:HB3	2:F:216:LEU:HB2	1.97	0.45
1:A:70:HIS:O	1:A:74:VAL:HG23	2.17	0.45
1:E:854:SER:HA	1:E:859:VAL:O	2.17	0.45
1:G:936:ASN:HB2	10:G:5133:HOH:O	2.15	0.45
1:G:223:ASP:OD2	1:G:227:ASN:HB2	2.17	0.45
1:C:814:GLN:CG	1:C:818:PHE:HE2	2.16	0.45
2:B:350:PHE:CG	2:B:366:LEU:CD2	3.00	0.45
1:G:237:PHE:CE2	1:G:458:ILE:HD13	2.52	0.45
1:G:615:ARG:NE	1:G:633:GLU:OE1	2.46	0.45
1:A:835:ASN:ND2	10:A:5879:HOH:O	2.44	0.45
1:E:781:HIS:HE1	1:E:789:SER:CB	2.30	0.45
1:G:400:ARG:HB3	10:G:5451:HOH:O	2.16	0.45
1:C:773:VAL:HG23	1:C:818:PHE:CE2	2.51	0.45
1:E:728:VAL:HG11	1:E:734:LEU:HA	1.98	0.45
1:G:361:ARG:CZ	1:G:571:ARG:HG2	2.47	0.45
2:F:186:LYS:O	2:F:189:GLU:HB2	2.16	0.45
2:D:87:LEU:HD12	2:D:87:LEU:HA	1.56	0.45
1:G:850:VAL:HB	1:G:851:PRO:HD3	1.98	0.45
1:A:349:GLU:O	2:B:294:ASN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:ILE:HG13	1:C:481:ILE:O	2.16	0.45
1:A:447:LEU:HA	1:A:447:LEU:HD23	1.76	0.45
1:A:947:LEU:N	1:A:947:LEU:HD12	2.31	0.45
1:C:1006:LYS:HB2	1:C:1036:TYR:CZ	2.52	0.45
1:C:950:ARG:HG3	1:C:950:ARG:H	1.45	0.45
2:B:364:ALA:N	2:B:365:PRO:CD	2.79	0.45
2:F:338:GLN:HA	2:F:351:GLN:HB3	1.99	0.45
2:H:210:VAL:HA	2:H:214:CYS:O	2.17	0.45
1:E:144:ALA:HB1	1:E:208:GLU:HG2	1.98	0.45
1:C:167:ILE:HD12	1:C:167:ILE:N	2.32	0.45
2:B:275:LEU:O	2:B:275:LEU:HD12	2.17	0.45
2:D:215:ARG:HH11	2:D:215:ARG:HG3	1.82	0.45
1:C:509:ARG:HB2	1:C:509:ARG:HH11	1.81	0.45
1:C:698:ILE:N	1:C:698:ILE:CD1	2.79	0.45
1:E:1017:THR:CG2	1:E:1018:SER:N	2.80	0.45
1:E:278:GLU:HG2	10:E:5895:HOH:O	2.16	0.45
1:G:517:ARG:HG2	1:G:522:LEU:HD23	1.98	0.45
1:A:289:ASN:HB3	1:A:292:ASN:OD1	2.17	0.45
1:C:69:ILE:O	1:C:69:ILE:HG22	2.16	0.45
1:C:734:LEU:C	1:C:734:LEU:HD12	2.35	0.44
1:A:734:LEU:CD1	1:A:738:PHE:CE2	2.99	0.44
2:D:222:GLN:H	2:D:222:GLN:NE2	2.12	0.44
1:G:947:LEU:HG	1:G:1014:ILE:CG2	2.47	0.44
1:C:675:ARG:HD3	1:C:675:ARG:H	1.82	0.44
1:A:805:ILE:HD12	1:A:832:VAL:CG1	2.47	0.44
1:G:1004:ARG:O	1:G:1009:GLU:HB2	2.17	0.44
1:C:145:ARG:HB2	1:C:208:GLU:OE1	2.17	0.44
1:G:637:GLY:HA2	1:G:660:PRO:O	2.17	0.44
1:G:972:ASP:OD1	1:G:989:ARG:HB3	2.17	0.44
1:A:1037:LYS:HA	10:A:5721:HOH:O	2.18	0.44
1:E:250:VAL:HA	1:E:356:VAL:O	2.17	0.44
1:C:472:LEU:O	1:C:476:VAL:HG23	2.17	0.44
1:G:704:LYS:O	1:G:707:GLU:HB2	2.17	0.44
1:E:726:GLU:CG	1:E:727:ILE:N	2.79	0.44
1:C:883:VAL:CG1	1:C:884:ILE:N	2.80	0.44
1:C:499:ASP:HA	1:C:513:ILE:HG21	1.98	0.44
1:A:1073:LYS:N	1:A:1073:LYS:HD2	2.31	0.44
1:A:712:LEU:O	1:A:727:ILE:HA	2.17	0.44
2:D:190:LEU:HB2	2:D:215:ARG:HB3	1.99	0.44
2:B:232:ASN:N	2:B:233:PRO:CD	2.80	0.44
1:A:579:ASP:O	1:A:583:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:795:SER:HB2	1:E:890:VAL:HG22	1.99	0.44
2:D:168:TYR:O	2:D:218:ILE:N	2.42	0.44
2:D:270:LEU:O	2:D:274:LEU:HG	2.17	0.44
2:B:172:GLN:O	2:B:207:ARG:HA	2.17	0.44
1:C:907:LEU:HD11	8:C:5033:ORN:HD3	1.98	0.44
1:E:213:TRP:HH2	1:E:294:ARG:HD3	1.81	0.44
2:F:350:PHE:HB2	2:F:366:LEU:HD22	1.99	0.44
1:C:9:SER:OG	1:C:84:ASP:N	2.45	0.44
1:E:814:GLN:NE2	10:E:5604:HOH:O	2.49	0.44
1:C:64:THR:O	1:C:1065:VAL:HG23	2.17	0.44
2:F:344:ASP:OD2	2:F:344:ASP:N	2.45	0.44
2:F:305:VAL:HG12	2:F:306:MET:N	2.32	0.44
1:E:659:VAL:HG13	1:E:660:PRO:HD2	2.00	0.44
1:G:240:MET:HE3	7:G:5071:ADP:C4	2.52	0.44
1:A:526:TYR:CE1	1:A:545:SER:HB3	2.53	0.44
1:G:222:ARG:HD3	1:G:277:VAL:O	2.18	0.44
2:D:120:ARG:HD2	10:D:1583:HOH:O	2.18	0.44
1:G:402:LEU:O	1:G:403:GLU:HB2	2.18	0.44
2:B:322:PRO:CB	2:B:324:ASN:HD21	2.20	0.44
2:H:306:MET:CE	2:H:329:HIS:CD2	3.01	0.44
2:F:272:HIS:HB2	2:F:349:SER:HB2	2.00	0.44
1:G:773:VAL:HG23	1:G:818:PHE:CZ	2.53	0.44
1:A:361:ARG:CZ	1:A:571:ARG:HG2	2.48	0.44
2:D:332:LEU:HA	2:D:332:LEU:HD12	1.70	0.44
1:G:735:ARG:O	1:G:738:PHE:N	2.51	0.44
1:C:714:VAL:HG23	1:C:728:VAL:HG23	2.00	0.44
1:C:633:GLU:O	1:C:634:LYS:HB2	2.18	0.44
1:A:693:ALA:CB	1:A:708:ILE:HD11	2.47	0.44
1:A:806:GLN:HA	1:A:809:MET:HE2	2.00	0.44
1:E:652:ARG:NH2	1:E:667:ASP:OD2	2.44	0.44
1:G:273:ARG:HD2	10:G:5275:HOH:O	2.18	0.44
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.52	0.44
1:C:331:THR:O	1:C:335:LEU:HG	2.17	0.44
1:A:737:TYR:CE1	1:A:741:ALA:HB2	2.53	0.44
1:A:843:ASN:HB3	1:A:845:ARG:HD2	1.99	0.44
1:G:671:ARG:CG	1:G:677:ARG:NH1	2.79	0.44
2:H:364:ALA:N	2:H:365:PRO:CD	2.79	0.44
1:C:3:LYS:HB2	1:C:42:TYR:OH	2.18	0.44
1:A:556[A]:SER:HB2	1:A:558:ASP:HB2	1.99	0.44
1:C:833:LYS:O	1:C:836:GLU:HB2	2.18	0.44
1:E:196:LEU:HG	1:E:204:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:425:ARG:NH1	10:G:5479:HOH:O	2.47	0.44
2:F:23:THR:HG23	2:F:134:ALA:O	2.17	0.44
1:A:309:ALA:O	1:A:313:LYS:HG2	2.18	0.44
1:C:703:GLU:O	1:C:706:LYS:HB2	2.18	0.44
1:C:340:THR:O	1:C:343:ARG:HB2	2.17	0.44
1:E:65:TYR:OH	1:E:81:GLU:OE1	2.29	0.44
2:H:332:LEU:HD12	2:H:332:LEU:HA	1.53	0.44
1:C:773:VAL:HG21	1:C:817:ALA:HB3	2.00	0.43
1:G:752:LEU:HA	1:G:752:LEU:HD12	1.72	0.43
2:F:342:ARG:HA	2:F:342:ARG:HD2	1.77	0.43
1:E:793:ALA:HA	1:E:891:LYS:O	2.17	0.43
1:E:892:GLU:OE1	8:E:5056:ORN:NE	2.50	0.43
1:G:550:GLU:OE2	2:H:120:ARG:NH2	2.45	0.43
1:G:436:ILE:HG22	10:G:5368:HOH:O	2.16	0.43
2:D:364:ALA:N	2:D:365:PRO:HD2	2.33	0.43
1:A:697:ALA:HB3	1:A:700:MET:HB2	1.99	0.43
1:E:1:MET:HB2	1:E:224:LYS:HZ1	1.83	0.43
1:A:998:ARG:CG	1:A:999:PRO:HA	2.47	0.43
1:E:648:LEU:HD22	1:E:845:ARG:HD3	2.00	0.43
1:C:534:ALA:HB1	2:D:120:ARG:HG2	2.00	0.43
2:D:298:LYS:O	2:D:329:HIS:HA	2.18	0.43
1:A:698:ILE:O	1:A:701:ALA:HB3	2.18	0.43
2:H:133:ILE:HG22	2:H:138:PRO:HB3	1.99	0.43
1:A:693:ALA:HB2	1:A:708:ILE:HD11	2.00	0.43
1:C:688:LYS:HD2	1:C:838:TYR:CE1	2.54	0.43
2:F:62:ASN:OD1	2:F:86:PRO:HG3	2.18	0.43
2:D:272:HIS:HA	2:D:349:SER:CB	2.49	0.43
2:H:33:ASN:HB3	2:H:55:LEU:HD23	1.99	0.43
1:A:1026:SER:HB2	1:A:1030:ARG:HH12	1.83	0.43
2:H:26:ALA:HB2	2:H:108:VAL:HB	2.00	0.43
1:C:991[B]:VAL:HG22	1:C:992:ASN:N	2.32	0.43
1:E:1001:ILE:HG13	1:E:1002:GLN:H	1.82	0.43
2:H:222:GLN:HA	2:H:250:TYR:CD1	2.54	0.43
1:A:419:GLU:O	1:A:423:LYS:HG3	2.19	0.43
2:B:249:ASP:OD2	2:B:250:TYR:N	2.51	0.43
1:A:164:PHE:HA	1:A:165:PRO:C	2.38	0.43
1:E:1005:ILE:HG21	1:E:1032:SER:HB3	2.00	0.43
1:E:139:ILE:HD11	1:E:141:LEU:HD12	2.00	0.43
2:B:63:VAL:O	2:B:94:ASN:HB2	2.18	0.43
1:E:1001:ILE:CG1	1:E:1002:GLN:N	2.82	0.43
2:F:177:LEU:HB3	10:F:2347:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:253:THR:O	2:H:256:GLN:HB2	2.18	0.43
1:E:864:VAL:O	1:E:868:VAL:HG23	2.19	0.43
2:D:188:ASP:N	2:D:188:ASP:OD2	2.47	0.43
2:B:153:LEU:HD12	2:B:153:LEU:HA	1.84	0.43
1:C:695:VAL:CG1	1:C:700:MET:HB3	2.45	0.43
2:H:199:PHE:HE2	2:H:238:LEU:HB3	1.84	0.43
1:C:17:PRO:HG3	1:C:917:VAL:HG13	2.01	0.43
2:D:116:ARG:O	2:D:120:ARG:HG3	2.18	0.43
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.54	0.43
1:E:235:GLU:HB2	1:E:253:ALA:HA	2.01	0.43
1:A:728:VAL:HG11	1:A:734:LEU:HA	2.00	0.43
1:G:986:ILE:O	1:G:988:PRO:HD3	2.18	0.43
1:C:671:ARG:HG2	1:C:677:ARG:NH1	2.33	0.43
1:A:344:THR:CB	1:A:345:PRO:HD2	2.48	0.43
1:A:1004:ARG:HB3	1:A:1009[B]:GLU:HG3	2.00	0.43
2:D:370:PHE:O	2:D:374:ILE:HG13	2.19	0.43
1:E:358:LYS:HE3	10:E:5353:HOH:O	2.18	0.43
1:A:601:CYS:HA	1:A:618:PHE:CE1	2.53	0.43
2:F:249:ASP:OD2	2:F:250:TYR:N	2.50	0.43
1:A:761:GLU:HB3	1:A:781:HIS:ND1	2.34	0.43
1:E:560:GLU:OE1	1:E:636:LYS:HE3	2.19	0.43
1:G:734:LEU:CD1	1:G:738:PHE:CE2	2.99	0.43
1:A:992:ASN:O	1:A:1000:HIS:HA	2.19	0.43
1:A:793:ALA:HA	1:A:891:LYS:O	2.19	0.43
2:B:268:ILE:HD13	2:B:268:ILE:HG21	1.73	0.43
1:G:128:ASP:CG	1:G:131:ARG:HG3	2.39	0.43
1:C:678:PHE:O	1:C:682:VAL:HG23	2.18	0.43
2:H:322:PRO:CB	2:H:324:ASN:ND2	2.80	0.43
1:C:642:TYR:OH	1:C:865:ALA:HB3	2.18	0.43
1:C:423:LYS:H	1:C:423:LYS:HG3	1.52	0.43
2:H:286:MET:CE	2:H:312:HIS:ND1	2.82	0.43
1:G:1036:TYR:C	1:G:1037:LYS:HG2	2.38	0.43
1:A:1061:LYS:HG2	1:A:1062:VAL:N	2.34	0.43
1:E:5:THR:O	1:E:8:LYS:NZ	2.52	0.43
1:A:711:PRO:HG2	1:A:755:PHE:HD2	1.83	0.43
2:F:229:LEU:N	2:F:229:LEU:HD23	2.33	0.43
1:C:176:GLY:HA3	1:C:377:GLN:HA	2.01	0.43
2:B:244:ASP:O	2:B:247:PRO:HD2	2.19	0.43
2:F:29:GLU:HB3	2:F:51:GLN:HG2	2.00	0.43
2:D:78:GLN:HE21	2:D:78:GLN:CA	2.10	0.42
1:E:563:MET:CE	1:E:635:PRO:HG3	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:998:ARG:CB	1:G:999:PRO:HA	2.47	0.42
1:E:40:GLU:OE2	1:E:330:TYR:OH	2.28	0.42
1:G:426:ARG:HD3	1:G:426:ARG:C	2.39	0.42
1:G:681:ALA:O	1:G:685:LEU:HG	2.19	0.42
1:G:165:PRO:HA	1:G:182:ALA:O	2.19	0.42
1:E:347:SER:O	2:F:296:PRO:HB3	2.19	0.42
1:C:252:PRO:HD3	1:C:352:ILE:HD11	2.01	0.42
1:A:995:HIS:CD2	1:A:995:HIS:H	2.36	0.42
1:G:69:ILE:O	1:G:69:ILE:HG22	2.19	0.42
2:H:324:ASN:O	2:H:342:ARG:HA	2.20	0.42
1:G:1017:THR:CG2	1:G:1018:SER:N	2.80	0.42
2:B:350:PHE:CG	2:B:366:LEU:HD22	2.54	0.42
1:A:559:ARG:NH1	1:A:559:ARG:HG3	2.32	0.42
1:C:419:GLU:HB3	1:C:423:LYS:HE3	2.00	0.42
2:D:6:LEU:O	2:D:132:ILE:HA	2.18	0.42
1:C:637:GLY:HA3	1:C:662:ILE:HG23	2.01	0.42
1:A:237:PHE:CE2	1:A:458:ILE:HD13	2.54	0.42
1:A:375:THR:HG23	1:A:377:GLN:H	1.84	0.42
2:D:326:ARG:O	2:D:340:ILE:HA	2.18	0.42
2:F:231:MET:HE3	2:F:231:MET:HB2	1.85	0.42
1:G:994:VAL:HG22	1:G:1000:HIS:ND1	2.34	0.42
2:F:6:LEU:HD13	2:F:16:HIS:ND1	2.33	0.42
1:E:1004:ARG:NH1	1:E:1009[A]:GLU:OE1	2.45	0.42
1:G:534:ALA:HB1	2:H:120:ARG:HG2	2.01	0.42
2:H:310:GLN:OE1	2:H:312:HIS:NE2	2.53	0.42
2:F:186:LYS:HB2	2:F:189:GLU:OE2	2.20	0.42
1:C:571:ARG:HD3	1:C:574:GLN:HB2	2.02	0.42
1:G:158:VAL:O	1:G:161:ASP:HB3	2.19	0.42
1:E:689:GLN:HG2	1:E:690:PRO:HD2	2.01	0.42
2:B:5:ALA:HB3	2:B:110:ILE:HG13	2.01	0.42
1:C:701:ALA:O	1:C:705:ALA:HB2	2.19	0.42
2:H:158:LEU:HA	2:H:158:LEU:HD23	1.40	0.42
1:C:994:VAL:HG23	1:C:1001:ILE:CD1	2.49	0.42
2:F:170:TRP:HB3	2:F:216:LEU:HD12	2.00	0.42
1:A:958:VAL:HG22	1:A:981:LEU:HD23	2.01	0.42
1:C:793:ALA:HA	1:C:891:LYS:O	2.20	0.42
1:C:1063:ILE:HG13	1:C:1067:GLU:OE2	2.20	0.42
1:A:627:LEU:HA	1:A:627:LEU:HD23	1.84	0.42
1:G:1:MET:HB3	1:G:2:PRO:HD2	2.01	0.42
1:A:698:ILE:CD1	1:A:698:ILE:N	2.80	0.42
1:A:3:LYS:HA	1:A:328:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:904:ASP:HA	1:G:905:PRO:HD3	1.91	0.42
1:C:703:GLU:OE2	1:C:703:GLU:HA	2.19	0.42
1:C:940:LYS:HA	5:C:5038:CL:CL	2.56	0.42
2:F:46:PRO:HA	2:F:76:HIS:CG	2.54	0.42
1:C:991[A]:VAL:HG12	1:C:1004:ARG:HH21	1.83	0.42
1:E:1028:VAL:CG1	1:E:1029:ILE:N	2.82	0.42
2:H:193:HIS:O	2:H:234:ASP:HB2	2.19	0.42
1:A:674:ASP:HB3	1:A:677:ARG:HB2	2.01	0.42
1:C:259:LYS:HD3	2:D:175:TRP:CE3	2.55	0.42
1:E:901:PRO:HD2	5:E:5060:CL:CL	2.57	0.42
2:H:344:ASP:OD2	2:H:344:ASP:N	2.29	0.42
1:E:855:LYS:HA	1:E:855:LYS:HD2	1.77	0.42
2:B:274:LEU:HD23	2:B:274:LEU:HA	1.92	0.42
1:C:919:GLY:HA2	10:C:1219:HOH:O	2.18	0.42
2:H:190:LEU:HA	2:H:190:LEU:HD23	1.82	0.42
1:A:726:GLU:CG	1:A:727:ILE:N	2.79	0.42
1:E:702:VAL:O	1:E:706:LYS:HD3	2.19	0.42
2:F:225:ALA:HA	2:F:258:PHE:CZ	2.54	0.42
1:C:698:ILE:O	1:C:702:VAL:HG23	2.19	0.42
1:G:1055:ASN:HB2	10:G:5826:HOH:O	2.20	0.42
1:E:449:VAL:HG21	1:E:464:VAL:HG12	2.01	0.42
1:A:301:ASN:HA	1:A:302:PRO:HD3	1.88	0.42
1:G:370:ALA:HB2	1:G:900:PHE:HB3	2.00	0.42
1:G:827:ASN:N	1:G:843:ASN:O	2.50	0.42
1:G:736:ARG:HB3	1:G:736:ARG:NH1	2.35	0.42
2:F:195:VAL:HG21	2:F:231:MET:HE1	2.01	0.42
2:H:190:LEU:HA	2:H:191:PRO:HD3	1.92	0.42
2:H:191:PRO:HD2	2:H:213:GLY:O	2.20	0.42
1:E:1:MET:HG3	1:E:2:PRO:HD2	2.01	0.42
1:C:998:ARG:HA	1:C:999:PRO:C	2.40	0.42
1:G:423:LYS:H	1:G:423:LYS:HG3	1.53	0.42
1:C:957:VAL:O	1:C:957:VAL:HG22	2.20	0.42
1:A:814:GLN:CG	1:A:818:PHE:CE2	3.02	0.42
1:C:809:MET:HG2	1:C:837:VAL:HG11	2.01	0.42
1:C:892:GLU:HG3	1:C:893:VAL:N	2.35	0.42
1:A:558:ASP:HB3	1:A:559:ARG:H	1.46	0.42
2:D:208:MET:SD	2:D:355:GLU:HA	2.59	0.42
1:E:688:LYS:HD2	1:E:838:TYR:CE1	2.55	0.42
1:A:5:THR:C	1:A:7:ILE:H	2.23	0.42
2:D:169:SER:HA	2:D:216:LEU:O	2.20	0.42
2:F:164:THR:O	2:F:220:PRO:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:LEU:HD11	1:C:812:GLN:HG2	2.02	0.42
1:C:751:LEU:O	1:C:752:LEU:HD12	2.20	0.42
1:G:40:GLU:HG2	1:G:325:LYS:HE2	2.02	0.42
2:D:350:PHE:HB2	2:D:366:LEU:CD2	2.50	0.42
1:E:765:ASP:OD2	1:E:827:ASN:HB2	2.20	0.42
2:B:170:TRP:HB3	2:B:216:LEU:HD12	2.02	0.42
2:D:317:ASP:OD1	2:D:320:THR:HG23	2.20	0.42
1:C:141:LEU:HD23	1:C:141:LEU:HA	1.89	0.42
1:G:1000:HIS:HD2	1:G:1002:GLN:H	1.66	0.42
1:G:963:LYS:HE3	1:G:1052[B]:MET:HE1	2.02	0.42
1:G:1017:THR:HG21	1:G:1023:ILE:HA	2.01	0.42
1:A:813:VAL:HG22	1:A:828:VAL:CG2	2.48	0.42
1:C:22:GLN:HG3	1:C:26:PHE:HE2	1.84	0.42
2:H:316:VAL:HG12	2:H:337:LEU:HD23	2.02	0.42
1:C:562:ILE:HG21	1:C:589:LEU:HD13	2.02	0.42
1:G:646:THR:HB	1:G:647:PRO:HD3	2.01	0.42
1:C:542:TYR:HE1	1:C:618:PHE:HB2	1.85	0.42
2:D:246:ALA:N	2:D:247:PRO:HD2	2.35	0.42
1:G:775:ILE:HA	1:G:775:ILE:HD13	1.71	0.42
1:G:728:VAL:HG11	1:G:734:LEU:N	2.35	0.41
1:E:695:VAL:CG1	1:E:696:THR:N	2.82	0.41
1:E:698:ILE:N	1:E:698:ILE:HD12	2.35	0.41
1:A:992:ASN:ND2	1:A:996:GLU:CB	2.78	0.41
1:E:1028:VAL:HG13	1:E:1029:ILE:N	2.34	0.41
1:G:947:LEU:HG	1:G:1014:ILE:HG21	2.02	0.41
1:A:835:ASN:HA	1:A:835:ASN:HD22	1.63	0.41
1:G:698:ILE:O	1:G:702:VAL:HG23	2.20	0.41
2:D:178:THR:HG22	2:D:179:GLY:N	2.35	0.41
1:G:361:ARG:HH11	1:G:361:ARG:HG3	1.85	0.41
1:A:805:ILE:HD12	1:A:832:VAL:HG11	2.01	0.41
1:G:700:MET:O	1:G:704:LYS:HB2	2.21	0.41
1:C:734:LEU:HD11	1:C:738:PHE:HE2	1.74	0.41
1:E:702:VAL:CG1	1:E:731:GLU:HG3	2.49	0.41
1:A:990:LEU:HG	1:A:991:VAL:N	2.36	0.41
2:D:208:MET:O	2:D:211:ASP:HB2	2.19	0.41
1:E:655[B]:GLU:HG2	10:E:5790:HOH:O	2.19	0.41
1:E:1036:TYR:C	1:E:1037:LYS:HG2	2.40	0.41
1:A:129:ARG:HB3	1:A:205:LEU:HD22	2.02	0.41
2:D:254:ALA:O	2:D:257:LYS:HB2	2.19	0.41
1:G:102:LEU:HA	1:G:102:LEU:HD23	1.95	0.41
1:G:695:VAL:HG11	1:G:701:ALA:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:MET:CE	2:B:312:HIS:CE1	3.04	0.41
1:G:40:GLU:CG	1:G:325:LYS:HE2	2.51	0.41
1:C:167:ILE:CD1	1:C:167:ILE:N	2.83	0.41
2:D:364:ALA:N	2:D:365:PRO:CD	2.82	0.41
2:F:251:ALA:O	2:F:255:ILE:HD12	2.21	0.41
2:H:190:LEU:HD13	2:H:215:ARG:HA	2.01	0.41
1:G:1001:ILE:CD1	1:G:1002:GLN:N	2.74	0.41
1:G:254:GLN:NE2	2:H:57:TYR:OH	2.53	0.41
2:H:279:SER:OG	2:H:342:ARG:HD3	2.19	0.41
1:C:670:ASP:HB3	1:C:677:ARG:NH2	2.35	0.41
1:A:681:ALA:HA	1:A:684:ARG:HB3	2.02	0.41
1:C:1027:ARG:HH11	1:C:1027:ARG:HG3	1.85	0.41
2:D:344:ASP:O	2:D:345:LYS:HG2	2.21	0.41
1:A:965:LEU:HD23	1:A:965:LEU:HA	1.68	0.41
1:G:885:PRO:HA	1:G:886:PRO:HD3	1.89	0.41
2:F:357:SER:HA	2:F:358:PRO:HA	1.89	0.41
1:C:520:TYR:O	1:C:521:ASP:HB3	2.20	0.41
1:A:833:LYS:O	1:A:836:GLU:HB2	2.20	0.41
1:A:695:VAL:HG11	1:A:701:ALA:CA	2.51	0.41
1:C:805:ILE:HG22	1:C:806:GLN:N	2.36	0.41
1:A:941:LYS:HE3	10:A:5890:HOH:O	2.20	0.41
1:E:781:HIS:CE1	1:E:789:SER:HA	2.55	0.41
2:D:87:LEU:HB2	10:D:1948:HOH:O	2.20	0.41
2:D:123:ARG:O	2:D:287:LYS:HE2	2.21	0.41
1:A:159:ALA:HB2	1:A:188:PHE:CZ	2.56	0.41
1:G:5:THR:C	1:G:7:ILE:H	2.22	0.41
1:C:493:LYS:HD2	1:C:493:LYS:HA	1.83	0.41
1:C:516:LEU:HA	1:C:516:LEU:HD12	1.75	0.41
2:D:227:ASP:O	2:D:230:LYS:HB2	2.21	0.41
1:C:761:GLU:HB3	1:C:781:HIS:ND1	2.36	0.41
2:D:46:PRO:HA	2:D:76:HIS:CD2	2.56	0.41
2:B:277:LEU:HD23	2:B:277:LEU:HA	1.95	0.41
2:H:120:ARG:HD2	10:H:3737:HOH:O	2.21	0.41
2:D:158:LEU:HA	2:D:158:LEU:HD23	1.92	0.41
1:A:289:ASN:OD1	1:A:290:PRO:HD2	2.20	0.41
1:E:671:ARG:NH2	1:E:819:GLU:O	2.54	0.41
1:A:858:GLY:HA2	1:A:1069:HIS:CE1	2.55	0.41
2:F:325:LEU:HD23	2:F:325:LEU:HA	1.82	0.41
2:D:362:ASP:OD2	2:D:362:ASP:N	2.53	0.41
1:E:447:LEU:HD23	1:E:447:LEU:HA	1.98	0.41
2:B:158:LEU:HA	2:B:158:LEU:HD23	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:HH11	1:A:104:ARG:HG3	1.85	0.41
1:E:213:TRP:CZ2	1:E:289:ASN:HB2	2.56	0.41
1:G:805:ILE:CD1	1:G:832:VAL:HG13	2.51	0.41
1:C:220:VAL:HG12	1:C:221:VAL:N	2.36	0.41
2:H:23:THR:HG22	2:H:24:GLY:N	2.36	0.41
1:E:775:ILE:HD13	1:E:775:ILE:HA	1.90	0.41
1:G:1027[B]:ARG:HG2	1:G:1031:ARG:HG3	2.03	0.41
1:C:730:ASP:OD2	1:C:733:ASP:HB2	2.21	0.41
1:A:1:MET:CB	1:A:224:LYS:HZ1	2.27	0.41
1:A:702:VAL:O	1:A:706:LYS:HD3	2.21	0.41
2:H:29:GLU:OE1	2:H:285:LYS:NZ	2.39	0.41
1:A:3:LYS:HB3	1:A:330:TYR:CE1	2.55	0.41
1:G:1014:ILE:O	1:G:1014:ILE:HG23	2.21	0.41
2:H:142:LEU:HD12	2:H:142:LEU:C	2.40	0.41
2:H:168:TYR:N	2:H:168:TYR:CD1	2.88	0.41
2:H:302:LYS:HB2	2:H:304:VAL:HG22	2.02	0.41
2:H:299:ASP:HA	2:H:329:HIS:CD2	2.55	0.41
2:H:45:ASP:HB3	2:H:48:TYR:HD2	1.85	0.41
2:D:354:PRO:HB2	2:D:367:PHE:CE2	2.56	0.41
2:D:204:ASN:O	2:D:208:MET:HG3	2.21	0.41
1:G:82:ARG:N	1:G:83:PRO:CD	2.84	0.41
1:C:513:ILE:HA	1:C:513:ILE:HD13	1.86	0.41
1:G:1032:SER:O	1:G:1036:TYR:HD1	2.03	0.41
1:C:28:TYR:CZ	1:C:313:LYS:HE3	2.56	0.41
9:A:5094:NET:H63	9:A:5094:NET:H31	1.69	0.41
9:A:5094:NET:H82	9:A:5094:NET:H52	1.80	0.41
1:G:121:ASP:O	1:G:125:LYS:HB2	2.20	0.41
1:G:710:TYR:HB3	1:G:729:TYR:O	2.21	0.41
1:G:363:ASN:OD1	1:G:381:VAL:HG21	2.20	0.41
1:A:17:PRO:HG3	1:A:917:VAL:HG13	2.03	0.41
1:G:654:LEU:O	1:G:659:VAL:HB	2.21	0.41
1:G:708:ILE:HG23	1:G:754:HIS:HB2	2.03	0.41
1:G:734:LEU:CD1	1:G:738:PHE:CD2	3.04	0.41
1:A:150:HIS:NE2	1:A:203:GLU:HG3	2.36	0.41
1:E:1002:GLN:O	1:E:1006:LYS:HB3	2.20	0.41
2:D:266:PHE:HA	2:D:348:PHE:O	2.21	0.41
1:A:331:THR:O	1:A:334:GLU:HB2	2.21	0.41
1:E:891:LYS:HG2	1:E:892:GLU:N	2.36	0.41
2:B:25:SER:HA	2:B:132:ILE:O	2.20	0.41
2:D:327:VAL:HG13	2:D:337:LEU:CD1	2.50	0.41
1:G:799:TYR:N	1:G:799:TYR:CD2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:181:LEU:HD23	2:H:181:LEU:HA	1.90	0.41
2:H:7:LEU:HD23	2:H:15:PHE:CD2	2.56	0.40
1:C:714:VAL:CG2	1:C:728:VAL:CG2	2.99	0.40
1:A:697:ALA:O	1:A:700:MET:HB3	2.21	0.40
1:A:954:LYS:HB3	1:A:980:VAL:HG21	2.03	0.40
1:C:805:ILE:CD1	1:C:837:VAL:CG2	3.00	0.40
1:C:904:ASP:OD1	1:C:906:LEU:HD22	2.21	0.40
2:H:234:ASP:HB3	2:H:374:ILE:CG2	2.51	0.40
1:G:485:ASN:OD1	1:G:487:ASP:HB2	2.21	0.40
1:A:165:PRO:HB3	1:A:183:TYR:CD1	2.56	0.40
1:A:962:ALA:O	1:A:965:LEU:HB2	2.21	0.40
2:F:98:LEU:O	2:F:102:LEU:HG	2.20	0.40
2:H:326:ARG:O	2:H:340:ILE:HA	2.21	0.40
1:E:711:PRO:HG2	1:E:755:PHE:HD2	1.86	0.40
1:C:339:ILE:HD11	1:C:529:VAL:HG12	2.03	0.40
1:C:250:VAL:HA	1:C:356:VAL:O	2.22	0.40
1:E:237:PHE:HB3	1:E:248:ILE:O	2.22	0.40
1:E:266:ASN:HA	1:E:266:ASN:HD22	1.60	0.40
1:A:493:LYS:HA	1:A:493:LYS:HD2	1.80	0.40
2:F:158:LEU:HD12	2:F:243:GLY:N	2.36	0.40
1:G:1001:ILE:HD12	1:G:1002:GLN:H	1.81	0.40
2:B:46:PRO:HA	2:B:76:HIS:CB	2.50	0.40
1:A:344:THR:CB	1:A:345:PRO:CD	3.00	0.40
2:F:212:ARG:NH1	2:F:212:ARG:CG	2.81	0.40
2:H:81:VAL:HG11	2:H:113:ILE:HD11	2.03	0.40
1:C:344:THR:HB	1:C:345:PRO:CD	2.51	0.40
1:G:426:ARG:NH2	10:G:5760:HOH:O	2.49	0.40
1:E:36:ALA:O	1:E:39:GLU:HB2	2.21	0.40
1:G:915:GLY:HA2	10:G:5183:HOH:O	2.21	0.40
1:C:895:LEU:HA	1:C:896:PRO:HD3	1.91	0.40
1:G:375:THR:HG23	1:G:377:GLN:H	1.86	0.40
1:G:839:LEU:HD12	1:G:839:LEU:HA	1.69	0.40
2:B:187:GLU:CG	2:B:215:ARG:HD2	2.16	0.40
2:H:132:ILE:CG2	2:H:133:ILE:N	2.84	0.40
1:G:858:GLY:O	1:G:860:PRO:HD3	2.22	0.40
1:G:860:PRO:O	1:G:864:VAL:HG23	2.22	0.40
1:G:712:LEU:O	1:G:727:ILE:HA	2.22	0.40
1:E:167:ILE:N	1:E:167:ILE:HD12	2.37	0.40
2:D:237:PHE:CZ	2:D:268:ILE:HD12	2.56	0.40
1:E:159:ALA:HB2	1:E:188:PHE:CE2	2.56	0.40
2:B:157:ASP:CG	2:B:160:LYS:HG2	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:ALA:HB2	1:C:510:GLU:HA	2.02	0.40
1:A:9:SER:OG	1:A:83:PRO:HA	2.21	0.40
2:B:197:TYR:HA	2:B:219:VAL:HG22	2.02	0.40
1:G:733:ASP:HA	1:G:736:ARG:NH1	2.29	0.40
1:G:726:GLU:OE1	1:G:1020:ARG:HD3	2.21	0.40
1:C:318:PRO:HB2	1:C:321:LYS:HB2	2.02	0.40
1:G:963:LYS:HE3	1:G:1052[B]:MET:CE	2.52	0.40
1:C:708:ILE:HG21	1:C:712:LEU:HD11	2.03	0.40
1:E:509:ARG:HH22	1:E:515:LYS:HZ3	1.66	0.40
1:G:51:PRO:HG2	1:G:916:GLU:OE2	2.21	0.40
1:A:475:LYS:HE2	1:A:488:PHE:CE2	2.56	0.40
1:G:236:ASN:N	1:G:236:ASN:HD22	2.20	0.40
1:E:750:VAL:O	1:E:750:VAL:HG12	2.22	0.40
2:H:379:LYS:HE2	2:H:379:LYS:HB3	1.65	0.40
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.88	0.40
1:C:714:VAL:HG21	1:C:728:VAL:CG2	2.52	0.40
1:G:1021:ARG:NH1	1:G:1021:ARG:CG	2.79	0.40
1:E:693:ALA:HB3	1:E:708:ILE:HD11	2.02	0.40
1:G:481:ILE:HG13	1:G:481:ILE:O	2.21	0.40
1:E:318:PRO:HG3	1:E:610:TYR:OH	2.22	0.40
1:C:571:ARG:HD3	1:C:571:ARG:N	2.36	0.40
1:A:441:ASP:OD2	1:A:444:ARG:NH1	2.49	0.40
2:B:341:HIS:CD2	2:B:348:PHE:HB3	2.57	0.40
1:A:820:LEU:O	1:A:821:GLN:HB2	2.21	0.40
1:A:840:ILE:O	1:A:841:GLU:HB3	2.22	0.40
1:G:672:ALA:CB	1:G:844:PRO:HG3	2.52	0.40
1:A:115:MET:HG2	1:A:118:ALA:O	2.21	0.40
1:C:627:LEU:HD23	1:C:627:LEU:HA	1.87	0.40
1:A:222:ARG:HD3	1:A:277:VAL:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1055/1073 (98%)	1010 (96%)	43 (4%)	2 (0%)	52	48
1	C	1055/1073 (98%)	999 (95%)	53 (5%)	3 (0%)	46	41
1	E	1058/1073 (99%)	1013 (96%)	42 (4%)	3 (0%)	46	41
1	G	1055/1073 (98%)	1000 (95%)	51 (5%)	4 (0%)	39	33
2	B	376/382 (98%)	357 (95%)	19 (5%)	0	100	100
2	D	377/382 (99%)	364 (97%)	13 (3%)	0	100	100
2	F	376/382 (98%)	361 (96%)	15 (4%)	0	100	100
2	H	377/382 (99%)	367 (97%)	10 (3%)	0	100	100
All	All	5729/5820 (98%)	5471 (96%)	246 (4%)	12 (0%)	52	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	954	LYS
1	G	739	GLN
1	A	558	ASP
1	C	739	GLN
1	E	738	PHE
1	G	873	SER
1	A	975	HIS
1	C	2	PRO
1	E	675	ARG
1	G	2	PRO
1	G	788	HIS
1	C	698	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	868/878 (99%)	810 (93%)	58 (7%)	20	14
1	C	868/878 (99%)	798 (92%)	70 (8%)	15	9
1	E	871/878 (99%)	814 (94%)	57 (6%)	21	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	868/878 (99%)	806 (93%)	62 (7%)	18	12
2	B	307/309 (99%)	284 (92%)	23 (8%)	17	11
2	D	308/309 (100%)	285 (92%)	23 (8%)	17	11
2	F	307/309 (99%)	288 (94%)	19 (6%)	23	16
2	H	308/309 (100%)	283 (92%)	25 (8%)	15	9
All	All	4705/4748 (99%)	4368 (93%)	337 (7%)	18	12

All (337) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	46	LEU
1	A	103	GLU
1	A	174	MET
1	A	185	ARG
1	A	202	LYS
1	A	297	VAL
1	A	299	GLU
1	A	326	LEU
1	A	343	ARG
1	A	358	LYS
1	A	363	ASN
1	A	426	ARG
1	A	542	TYR
1	A	548	GLU
1	A	549	GLU
1	A	554	ASN
1	A	558	ASP
1	A	559	ARG
1	A	571	ARG
1	A	591	GLU
1	A	652	ARG
1	A	671	ARG
1	A	674	ASP
1	A	675	ARG
1	A	696	THR
1	A	702	VAL
1	A	704	LYS
1	A	706	LYS
1	A	712	LEU

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Mol	Chain	Res	Type
1	A	733	ASP
1	A	734	LEU
1	A	735	ARG
1	A	751	LEU
1	A	752	LEU
1	A	753	ASP
1	A	757	ASP
1	A	763	ASP
1	A	784	GLN
1	A	805	ILE
1	A	835	ASN
1	A	845	ARG
1	A	855	LYS
1	A	881	LYS
1	A	891	LYS
1	A	906	LEU
1	A	912	ARG
1	A	922	ARG
1	A	940	LYS
1	A	950	ARG
1	A	951	GLU
1	A	955	GLU
1	A	992	ASN
1	A	1020	ARG
1	A	1021	ARG
1	A	1026	SER
1	A	1072	ILE
1	A	1073	LYS
2	B	2	ILE
2	B	6	LEU
2	B	35	SER
2	B	50	ARG
2	B	87	LEU
2	B	123	ARG
2	B	153	LEU
2	B	154	ASN
2	B	166	GLU
2	B	186	LYS
2	B	192	PHE
2	B	215	ARG
2	B	222	GLN
2	B	257	LYS

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Mol	Chain	Res	Type
2	B	282	LYS
2	B	304	VAL
2	B	306	MET
2	B	324	ASN
2	B	332	LEU
2	B	333	PHE
2	B	357	SER
2	B	376	GLN
2	B	379	LYS
1	C	4	ARG
1	C	38	ARG
1	C	46	LEU
1	C	55	MET
1	C	68	PRO
1	C	103	GLU
1	C	174	MET
1	C	185	ARG
1	C	202	LYS
1	C	224	LYS
1	C	299	GLU
1	C	313	LYS
1	C	321	LYS
1	C	326	LEU
1	C	339	ILE
1	C	343	ARG
1	C	358	LYS
1	C	363	ASN
1	C	412	LYS
1	C	414	SER
1	C	422	THR
1	C	426	ARG
1	C	428	LEU
1	C	481	ILE
1	C	509	ARG
1	C	548	GLU
1	C	559	ARG
1	C	571	ARG
1	C	591	GLU
1	C	632	ILE
1	C	634	LYS
1	C	648	LEU
1	C	652	ARG

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Mol	Chain	Res	Type
1	C	665	SER
1	C	671	ARG
1	C	675	ARG
1	C	688	LYS
1	C	696	THR
1	C	706	LYS
1	C	728	VAL
1	C	733	ASP
1	C	735	ARG
1	C	751	LEU
1	C	757	ASP
1	C	763	ASP
1	C	784	GLN
1	C	800	THR
1	C	805	ILE
1	C	815	LYS
1	C	845	ARG
1	C	855	LYS
1	C	891	LYS
1	C	906	LEU
1	C	912	ARG
1	C	940	LYS
1	C	950	ARG
1	C	951	GLU
1	C	955	GLU
1	C	956	ARG
1	C	1003	ASP
1	C	1006	LYS
1	C	1009[A]	GLU
1	C	1009[B]	GLU
1	C	1018	SER
1	C	1020	ARG
1	C	1021	ARG
1	C	1031	ARG
1	C	1061	LYS
1	C	1072	ILE
1	C	1073	LYS
2	D	2	ILE
2	D	50	ARG
2	D	58	PRO
2	D	78	GLN
2	D	87	LEU

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Mol	Chain	Res	Type
2	D	153	LEU
2	D	154	ASN
2	D	166	GLU
2	D	183	GLU
2	D	191	PRO
2	D	215	ARG
2	D	222	GLN
2	D	232	ASN
2	D	257	LYS
2	D	282	LYS
2	D	306	MET
2	D	324	ASN
2	D	332	LEU
2	D	366	LEU
2	D	372[A]	GLU
2	D	372[B]	GLU
2	D	379	LYS
2	D	380	THR
1	E	1	MET
1	E	5	THR
1	E	46	LEU
1	E	55	MET
1	E	174	MET
1	E	236	ASN
1	E	275	ILE
1	E	317	PHE
1	E	321	LYS
1	E	343	ARG
1	E	363	ASN
1	E	412	LYS
1	E	426	ARG
1	E	429	LYS
1	E	509	ARG
1	E	542	TYR
1	E	548	GLU
1	E	556	SER
1	E	559	ARG
1	E	571	ARG
1	E	591	GLU
1	E	634	LYS
1	E	675	ARG
1	E	688	LYS

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Mol	Chain	Res	Type
1	E	690	PRO
1	E	696	THR
1	E	698	ILE
1	E	702	VAL
1	E	706	LYS
1	E	712	LEU
1	E	733	ASP
1	E	734	LEU
1	E	735	ARG
1	E	750	VAL
1	E	751	LEU
1	E	752	LEU
1	E	784	GLN
1	E	795	SER
1	E	805	ILE
1	E	811	GLN
1	E	845	ARG
1	E	849	THR
1	E	855	LYS
1	E	881	LYS
1	E	906	LEU
1	E	912	ARG
1	E	940	LYS
1	E	950	ARG
1	E	951	GLU
1	E	956	ARG
1	E	967	GLN
1	E	998	ARG
1	E	1020	ARG
1	E	1021	ARG
1	E	1027	ARG
1	E	1031	ARG
1	E	1073	LYS
2	F	2	ILE
2	F	87	LEU
2	F	106	ASN
2	F	153	LEU
2	F	154	ASN
2	F	166	GLU
2	F	183	GLU
2	F	186	LYS
2	F	192	PHE

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Mol	Chain	Res	Type
2	F	215	ARG
2	F	239	SER
2	F	261	THR
2	F	282	LYS
2	F	306	MET
2	F	324	ASN
2	F	331	SER
2	F	332	LEU
2	F	366	LEU
2	F	379	LYS
1	G	1	MET
1	G	4	ARG
1	G	8	LYS
1	G	46	LEU
1	G	55	MET
1	G	76	LYS
1	G	145	ARG
1	G	146	SER
1	G	174	MET
1	G	185	ARG
1	G	236	ASN
1	G	307	SER
1	G	321	LYS
1	G	358	LYS
1	G	416	ASP
1	G	426	ARG
1	G	481	ILE
1	G	482	THR
1	G	518[A]	ASP
1	G	518[B]	ASP
1	G	542	TYR
1	G	548	GLU
1	G	559	ARG
1	G	571	ARG
1	G	631	ARG
1	G	652	ARG
1	G	660	PRO
1	G	671	ARG
1	G	673	GLU
1	G	675	ARG
1	G	684	ARG
1	G	688	LYS

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Mol	Chain	Res	Type
1	G	692	ASN
1	G	696	THR
1	G	706	LYS
1	G	712	LEU
1	G	714	VAL
1	G	733	ASP
1	G	734	LEU
1	G	735	ARG
1	G	752	LEU
1	G	753	ASP
1	G	763	ASP
1	G	784	GLN
1	G	805	ILE
1	G	815	LYS
1	G	845	ARG
1	G	849	THR
1	G	855	LYS
1	G	906	LEU
1	G	912	ARG
1	G	940	LYS
1	G	950	ARG
1	G	951	GLU
1	G	956	ARG
1	G	966	LYS
1	G	967	GLN
1	G	1018	SER
1	G	1020	ARG
1	G	1021	ARG
1	G	1031	ARG
1	G	1073	LYS
2	H	6	LEU
2	H	7	LEU
2	H	50	ARG
2	H	73	SER
2	H	87	LEU
2	H	125	LYS
2	H	153	LEU
2	H	154	ASN
2	H	166	GLU
2	H	169	SER
2	H	183	GLU
2	H	192	PHE

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Mol	Chain	Res	Type
2	H	216	LEU
2	H	222	GLN
2	H	257	LYS
2	H	279	SER
2	H	282	LYS
2	H	306	MET
2	H	321	LEU
2	H	324	ASN
2	H	332	LEU
2	H	340	ILE
2	H	366	LEU
2	H	376	GLN
2	H	379	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	679	GLN
1	A	689	GLN
1	A	784	GLN
1	A	803	GLN
1	A	812	GLN
1	A	814	GLN
1	A	835	ASN
1	A	936	ASN
1	A	987	ASN
1	A	992	ASN
1	A	995	HIS
1	A	1000	HIS
1	A	1035	GLN
1	A	1055	ASN
1	A	1071	GLN
2	B	51	GLN
2	B	154	ASN
2	B	222	GLN
2	B	324	ASN
2	B	351	GLN
1	C	105	GLN
1	C	266	ASN
1	C	457	ASN
1	C	679	GLN

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Mol	Chain	Res	Type
1	C	689	GLN
1	C	784	GLN
1	C	803	GLN
1	C	812	GLN
1	C	814	GLN
1	C	936	ASN
1	C	942	HIS
1	C	987	ASN
1	C	992	ASN
1	C	1000	HIS
1	C	1035	GLN
1	C	1055	ASN
1	C	1071	GLN
2	D	51	GLN
2	D	78	GLN
2	D	154	ASN
2	D	222	GLN
2	D	324	ASN
2	D	351	GLN
1	E	105	GLN
1	E	266	ASN
1	E	457	ASN
1	E	689	GLN
1	E	784	GLN
1	E	803	GLN
1	E	812	GLN
1	E	814	GLN
1	E	936	ASN
1	E	942	HIS
1	E	992	ASN
1	E	1000	HIS
1	E	1015	ASN
1	E	1035	GLN
2	F	51	GLN
2	F	78	GLN
2	F	154	ASN
2	F	324	ASN
2	F	351	GLN
1	G	105	GLN
1	G	266	ASN
1	G	457	ASN
1	G	645	GLN

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Mol	Chain	Res	Type
1	G	679	GLN
1	G	689	GLN
1	G	692	ASN
1	G	784	GLN
1	G	803	GLN
1	G	814	GLN
1	G	835	ASN
1	G	992	ASN
1	G	1000	HIS
1	G	1035	GLN
1	G	1055	ASN
1	G	1071	GLN
2	H	51	GLN
2	H	78	GLN
2	H	154	ASN
2	H	222	GLN
2	H	324	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CYG	B	269	2	10,14,15	2.73	2 (20%)	6,17,19	9.27	2 (33%)
2	CYG	D	269	2	10,14,15	2.73	2 (20%)	6,17,19	9.25	2 (33%)
2	CYG	F	269	2	10,14,15	2.74	2 (20%)	6,17,19	9.26	2 (33%)
2	CYG	H	269	2	10,14,15	2.76	2 (20%)	6,17,19	9.27	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CYG	B	269	2	-	0/10/16/18	0/0/0/0
2	CYG	D	269	2	-	0/10/16/18	0/0/0/0
2	CYG	F	269	2	-	0/10/16/18	0/0/0/0
2	CYG	H	269	2	-	0/10/16/18	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	269	CYG	CD1-SG	-4.26	1.67	1.76
2	F	269	CYG	CD1-SG	-4.24	1.67	1.76
2	B	269	CYG	CD1-SG	-4.23	1.67	1.76
2	D	269	CYG	CD1-SG	-4.22	1.67	1.76
2	B	269	CYG	OE2-CD1	7.15	1.32	1.21
2	D	269	CYG	OE2-CD1	7.17	1.32	1.21
2	F	269	CYG	OE2-CD1	7.17	1.32	1.21
2	H	269	CYG	OE2-CD1	7.21	1.32	1.21

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	269	CYG	OE2-CD1-CG1	-17.52	111.88	123.94
2	B	269	CYG	OE2-CD1-CG1	-17.52	111.89	123.94
2	F	269	CYG	OE2-CD1-CG1	-17.51	111.89	123.94
2	D	269	CYG	OE2-CD1-CG1	-17.46	111.92	123.94
2	D	269	CYG	OE2-CD1-SG	-14.22	111.55	122.83
2	B	269	CYG	OE2-CD1-SG	-14.21	111.56	122.83
2	H	269	CYG	OE2-CD1-SG	-14.20	111.57	122.83
2	F	269	CYG	OE2-CD1-SG	-14.19	111.57	122.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	269	CYG	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 95 ligands modelled in this entry, 74 are monoatomic - leaving 21 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$
7	ADP	A	5000	3	22,29,29	1.31	4 (18%)	27,45,45	1.08	2 (7%)
6	PO4	A	5005	3,4	4,4,4	1.38	0	6,6,6	0.31	0
7	ADP	A	5006	3,4	22,29,29	1.13	2 (9%)	27,45,45	0.84	0
8	ORN	A	5010	-	5,8,8	0.59	0	3,9,9	1.02	0
9	NET	A	5094	-	8,8,8	0.54	0	10,10,10	0.65	0
7	ADP	C	5023	3	22,29,29	1.34	5 (22%)	27,45,45	0.87	1 (3%)
6	PO4	C	5028	3,4	4,4,4	1.60	1 (25%)	6,6,6	0.31	0
7	ADP	C	5029	3,4	22,29,29	1.20	2 (9%)	27,45,45	1.07	3 (11%)
8	ORN	C	5033	-	5,8,8	0.68	0	3,9,9	0.38	0
9	NET	C	5034	-	8,8,8	0.67	0	10,10,10	0.48	0
7	ADP	E	5046	3	22,29,29	1.21	3 (13%)	27,45,45	0.98	0
6	PO4	E	5051	3,4	4,4,4	1.92	2 (50%)	6,6,6	0.30	0
7	ADP	E	5052	3,4	22,29,29	1.06	3 (13%)	27,45,45	1.08	3 (11%)
8	ORN	E	5056	-	5,8,8	0.67	0	3,9,9	0.64	0
9	NET	E	5057	-	8,8,8	0.77	0	10,10,10	0.36	0
6	PO4	E	5070	-	4,4,4	1.34	0	6,6,6	0.31	0
7	ADP	G	5071	3	22,29,29	1.37	4 (18%)	27,45,45	1.41	3 (11%)
6	PO4	G	5076	3,4	4,4,4	1.46	1 (25%)	6,6,6	0.30	0
7	ADP	G	5077	3,4	22,29,29	1.25	4 (18%)	27,45,45	1.15	3 (11%)
8	ORN	G	5081	-	5,8,8	0.47	0	3,9,9	0.30	0
9	NET	G	5082	-	8,8,8	0.60	0	10,10,10	0.49	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
7	ADP	A	5000	3	-	0/12/32/32	0/3/3/3
6	PO4	A	5005	3,4	-	0/0/0/0	0/0/0/0
7	ADP	A	5006	3,4	-	0/12/32/32	0/3/3/3
8	ORN	A	5010	-	-	0/4/8/8	0/0/0/0
9	NET	A	5094	-	-	0/12/12/12	0/0/0/0
7	ADP	C	5023	3	-	0/12/32/32	0/3/3/3
6	PO4	C	5028	3,4	-	0/0/0/0	0/0/0/0
7	ADP	C	5029	3,4	-	0/12/32/32	0/3/3/3
8	ORN	C	5033	-	-	0/4/8/8	0/0/0/0
9	NET	C	5034	-	-	0/12/12/12	0/0/0/0
7	ADP	E	5046	3	-	0/12/32/32	0/3/3/3
6	PO4	E	5051	3,4	-	0/0/0/0	0/0/0/0
7	ADP	E	5052	3,4	-	0/12/32/32	0/3/3/3
8	ORN	E	5056	-	-	0/4/8/8	0/0/0/0
9	NET	E	5057	-	-	0/12/12/12	0/0/0/0
6	PO4	E	5070	-	-	0/0/0/0	0/0/0/0
7	ADP	G	5071	3	-	0/12/32/32	0/3/3/3
6	PO4	G	5076	3,4	-	0/0/0/0	0/0/0/0
7	ADP	G	5077	3,4	-	0/12/32/32	0/3/3/3
8	ORN	G	5081	-	-	0/4/8/8	0/0/0/0
9	NET	G	5082	-	-	0/12/12/12	0/0/0/0

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5000	ADP	O4'-C1'	-3.86	1.36	1.41
7	E	5046	ADP	O4'-C1'	-3.24	1.37	1.41
6	E	5051	PO4	P-O3	-2.67	1.43	1.53
7	C	5023	ADP	O4'-C1'	-2.66	1.37	1.41
7	E	5052	ADP	O4'-C1'	-2.57	1.38	1.41
7	C	5023	ADP	PA-O2A	-2.50	1.44	1.54
7	G	5071	ADP	O4'-C1'	-2.47	1.38	1.41
7	G	5077	ADP	O4'-C1'	-2.42	1.38	1.41
6	G	5076	PO4	P-O2	-2.18	1.45	1.53
7	C	5023	ADP	PB-O2B	-2.13	1.47	1.54
7	A	5006	ADP	O4'-C1'	-2.12	1.38	1.41
7	A	5000	ADP	PA-O2A	-2.05	1.46	1.54
6	E	5051	PO4	P-O2	-2.03	1.46	1.53
6	C	5028	PO4	P-O2	-2.00	1.46	1.53
7	E	5046	ADP	C2-N1	2.02	1.37	1.33
7	E	5052	ADP	O3'-C3'	2.17	1.48	1.43
7	G	5077	ADP	O3'-C3'	2.20	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5071	ADP	O2'-C2'	2.21	1.48	1.43
7	E	5046	ADP	O3'-C3'	2.22	1.48	1.43
7	A	5000	ADP	C2-N1	2.23	1.38	1.33
7	G	5077	ADP	C2-N1	2.26	1.38	1.33
7	A	5000	ADP	O3'-C3'	2.29	1.48	1.43
7	A	5006	ADP	O3'-C3'	2.36	1.48	1.43
7	E	5052	ADP	C2-N1	2.36	1.38	1.33
7	C	5023	ADP	O2'-C2'	2.37	1.48	1.43
7	C	5029	ADP	O2'-C2'	2.57	1.49	1.43
7	C	5023	ADP	C2-N1	2.65	1.38	1.33
7	G	5077	ADP	O2'-C2'	2.94	1.50	1.43
7	G	5071	ADP	C2-N1	3.07	1.39	1.33
7	G	5071	ADP	O3'-C3'	3.55	1.51	1.43
7	C	5029	ADP	O3'-C3'	3.76	1.52	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	5000	ADP	C1'-N9-C4	-2.49	123.19	126.94
7	E	5052	ADP	C2'-C3'-C4'	-2.26	97.96	102.61
7	G	5071	ADP	O3B-PB-O3A	-2.07	95.68	105.09
7	A	5000	ADP	N6-C6-N1	2.00	123.50	119.20
7	C	5023	ADP	O3'-C3'-C2'	2.07	118.55	111.83
7	C	5029	ADP	O2'-C2'-C3'	2.09	118.61	111.83
7	G	5077	ADP	O3'-C3'-C2'	2.19	118.95	111.83
7	E	5052	ADP	O3'-C3'-C2'	2.21	119.03	111.83
7	C	5029	ADP	O3'-C3'-C2'	2.26	119.19	111.83
7	C	5029	ADP	O2A-PA-O3A	2.37	115.83	105.09
7	G	5077	ADP	O2'-C2'-C3'	2.43	119.75	111.83
7	E	5052	ADP	O2A-PA-O3A	2.45	116.22	105.09
7	G	5077	ADP	O3B-PB-O3A	2.48	116.35	105.09
7	G	5071	ADP	O3'-C3'-C2'	3.16	122.10	111.83
7	G	5071	ADP	O2'-C2'-C3'	3.91	124.54	111.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	5094	NET	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	5033	ORN	2	0
7	E	5052	ADP	1	0
8	E	5056	ORN	3	0
9	E	5057	NET	1	0
7	G	5071	ADP	1	0
7	G	5077	ADP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.