



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 03:05 am BST

PDB ID : 1BXR  
Title : STRUCTURE OF CARBAMOYL PHOSPHATE SYNTHETASE COM-  
PLEXED WITH THE ATP ANALOG AMPPNP  
Authors : Thoden, J.B.; Wesenberg, G.; Raushel, F.M.; Holden, H.M.  
Deposited on : 1998-10-08  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

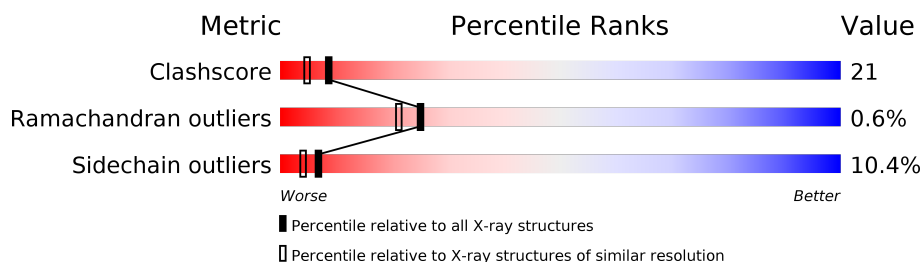
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	
1	C	1073	
1	E	1073	
1	G	1073	
2	B	382	
2	D	382	
2	F	382	
2	H	382	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CL	E	2980	-	-	X	-
8	NET	A	1086	-	-	X	-
8	NET	E	2950	-	X	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 48307 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 SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1073	Total	C	N	O	S	0	4	0
			8288	5203	1445	1594	46			
1	C	1073	Total	C	N	O	S	0	0	0
			8268	5190	1441	1592	45			
1	E	1073	Total	C	N	O	S	0	3	0
			8284	5199	1445	1595	45			
1	G	1073	Total	C	N	O	S	0	2	0
			8279	5196	1445	1593	45			

- Molecule 2 is a protein called CARBAMOYL-PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			
2	D	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			
2	F	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			
2	H	379	Total	C	N	O	S	0	0	0
			2895	1825	509	551	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	183	GLN	GLU	CONFLICT	UNP P0A6F1
D	183	GLN	GLU	CONFLICT	UNP P0A6F1
F	183	GLN	GLU	CONFLICT	UNP P0A6F1
H	183	GLN	GLU	CONFLICT	UNP P0A6F1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	3	Total Mn 3 3	0	0
3	A	3	Total Mn 3 3	0	0
3	C	4	Total Mn 4 4	0	0
3	E	3	Total Mn 3 3	0	0

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

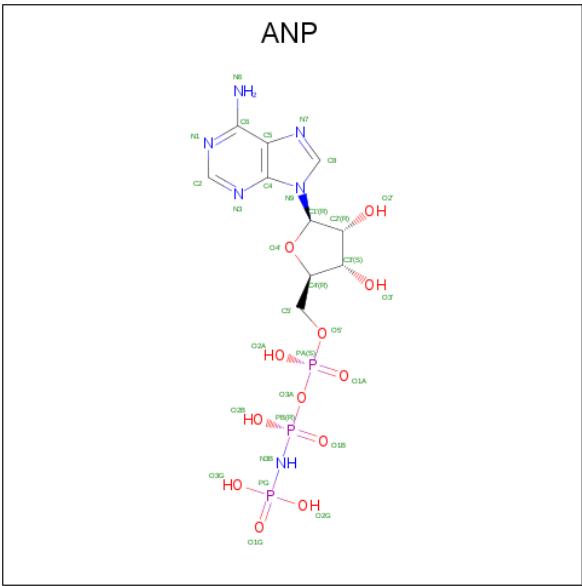
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	4	Total K 4 4	0	0
4	D	1	Total K 1 1	0	0
4	E	5	Total K 5 5	0	0
4	H	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	4	Total K 4 4	0	0
4	A	3	Total K 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	4	Total Cl 4 4	0	0
5	D	1	Total Cl 1 1	0	0
5	E	2	Total Cl 2 2	0	0
5	B	1	Total Cl 1 1	0	0
5	C	3	Total Cl 3 3	0	0
5	A	3	Total Cl 3 3	0	0

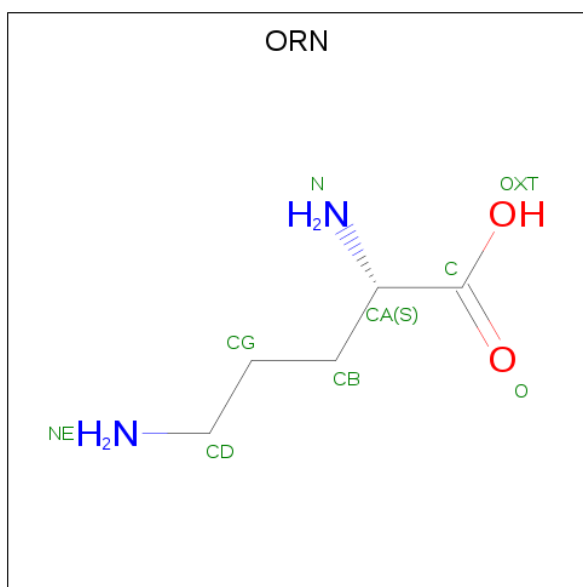
- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



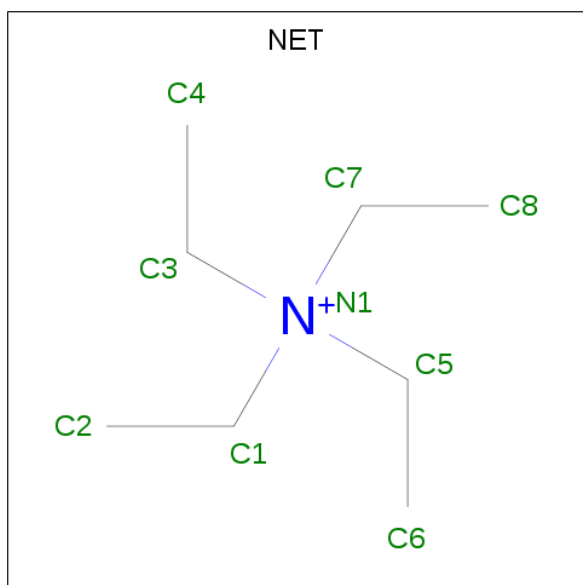
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is L-ornithine (three-letter code: ORN) (formula: C<sub>5</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>).



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

- Molecule 8 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula:  $C_8H_{20}N$ ).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	677	Total O 677 677	0	0
9	B	169	Total O 169 169	0	0
9	C	624	Total O 624 624	0	0
9	D	234	Total O 234 234	0	0
9	E	650	Total O 650 650	0	0
9	F	193	Total O 193 193	0	0
9	G	530	Total O 530 530	0	0
9	H	165	Total O 165 165	0	0

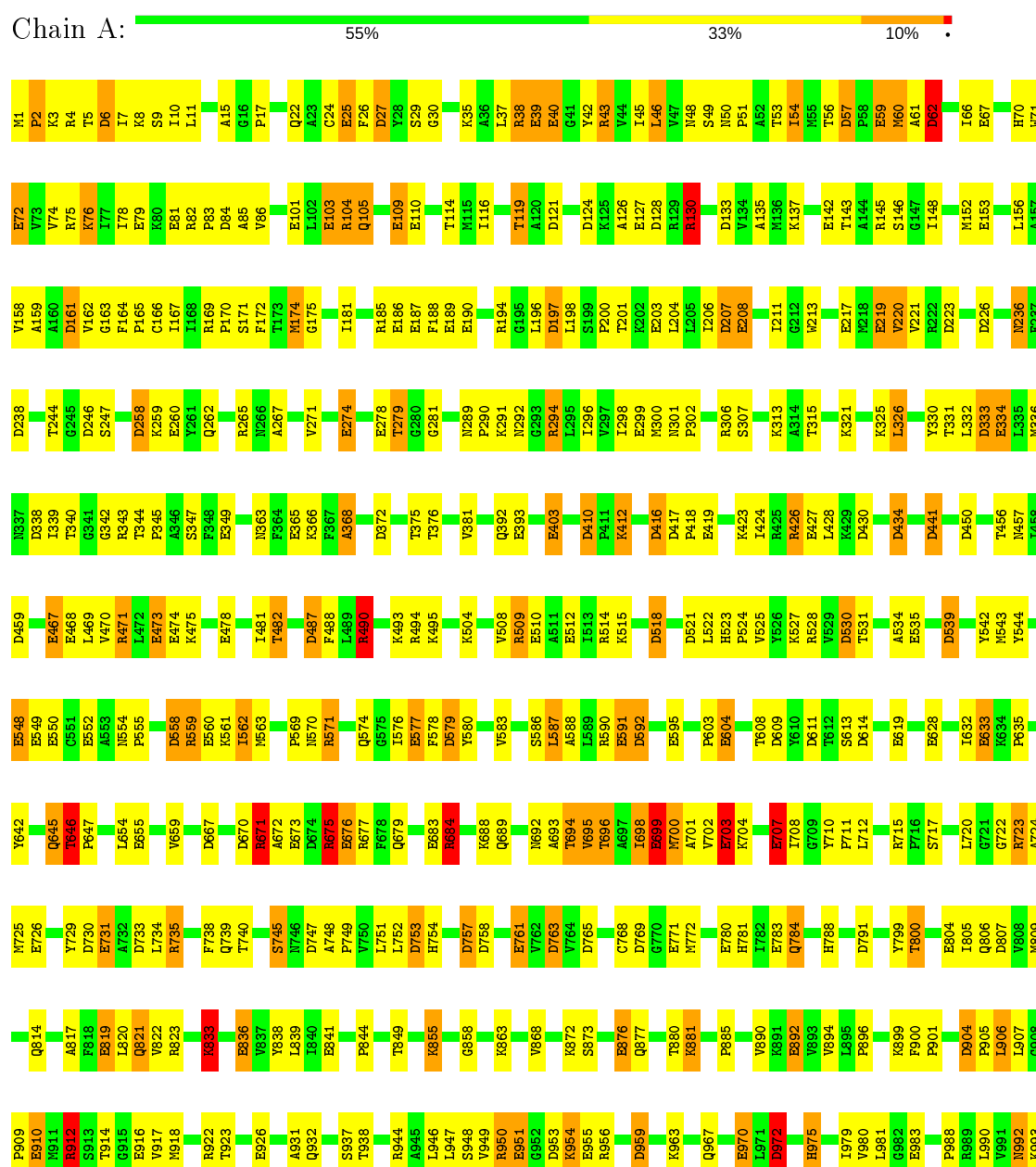


### 3 Residue-property plots

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

Note EDS was not executed.

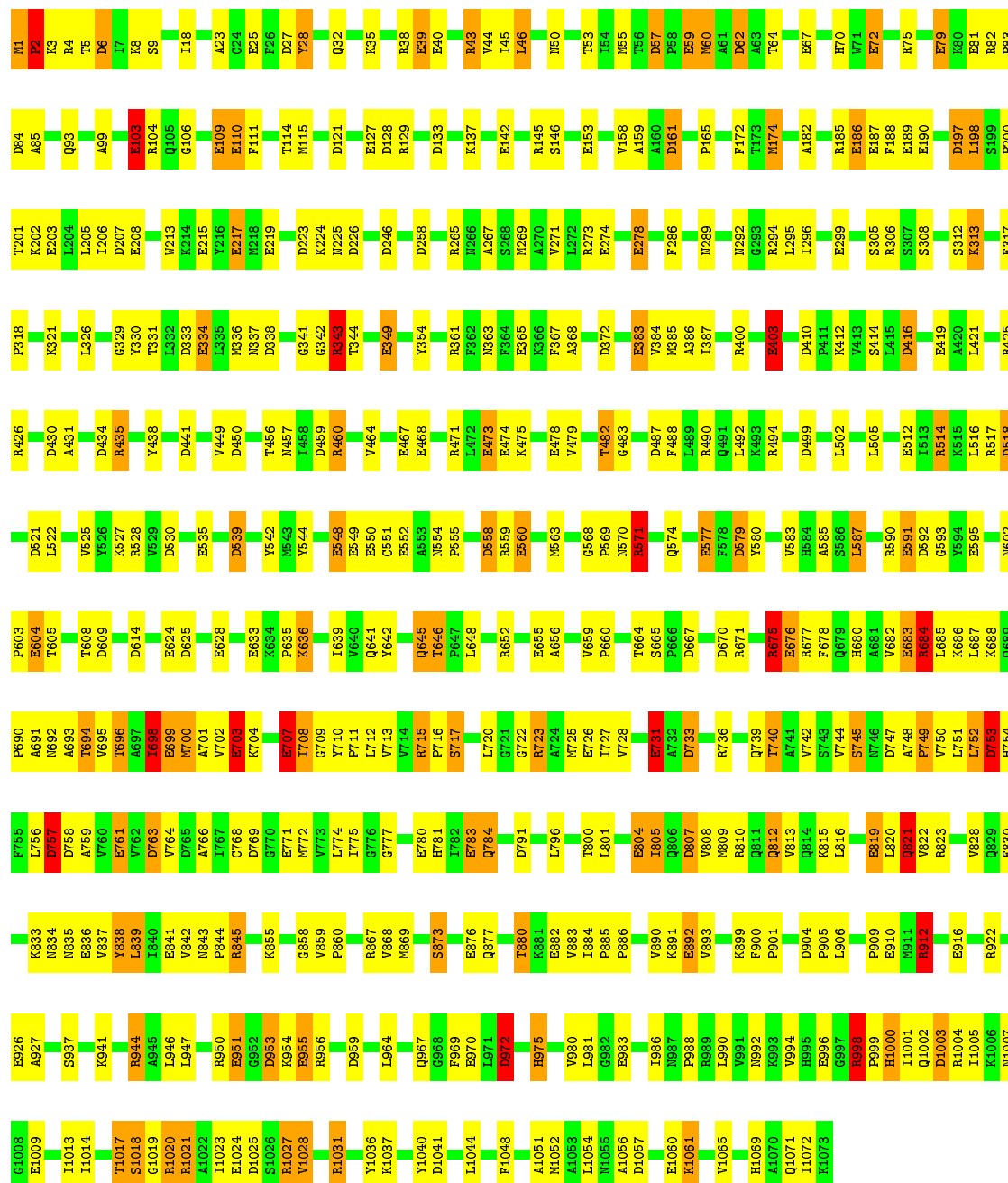
#### • Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE





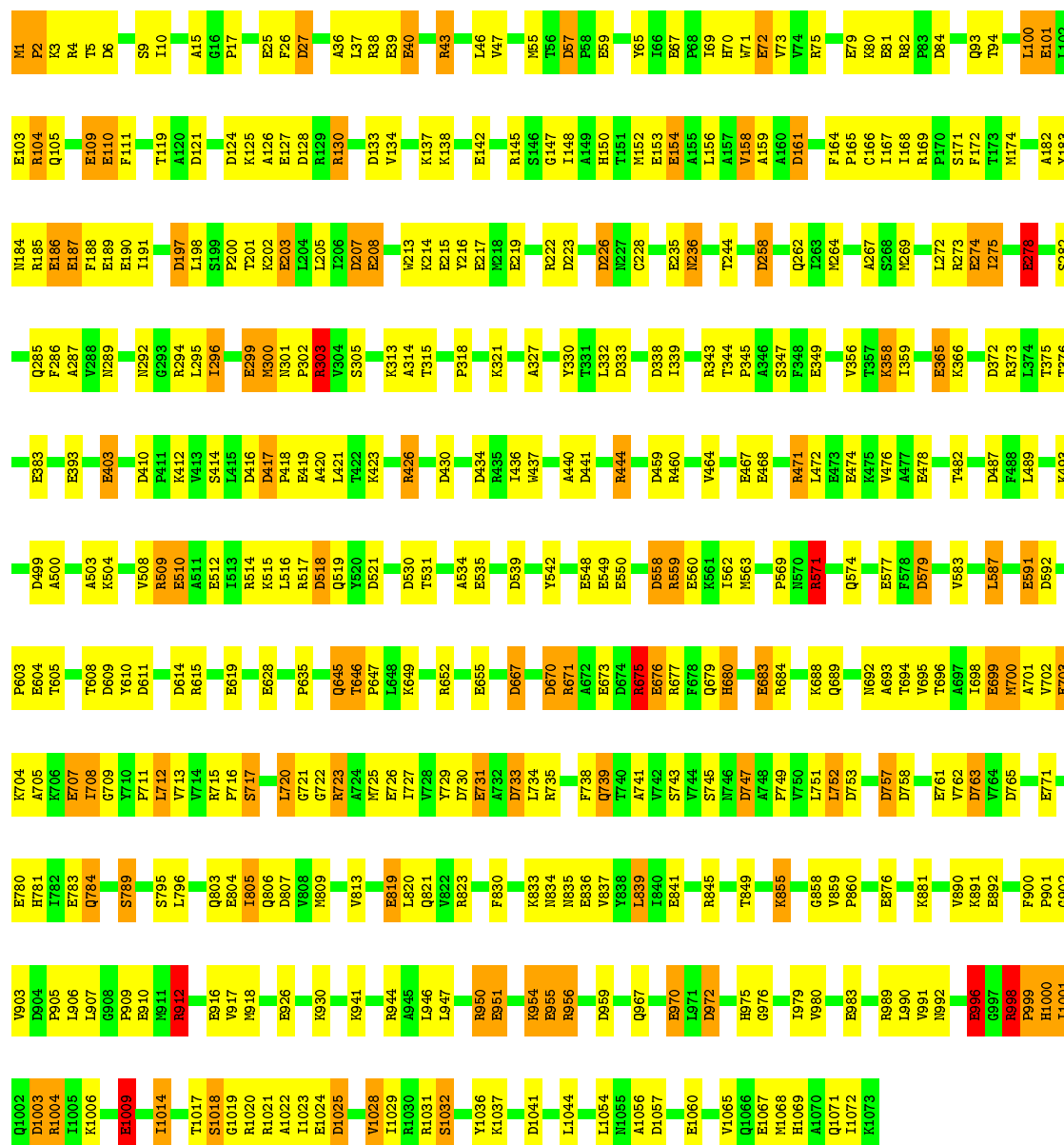
• Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE

Chain C: 57% 33% 8%



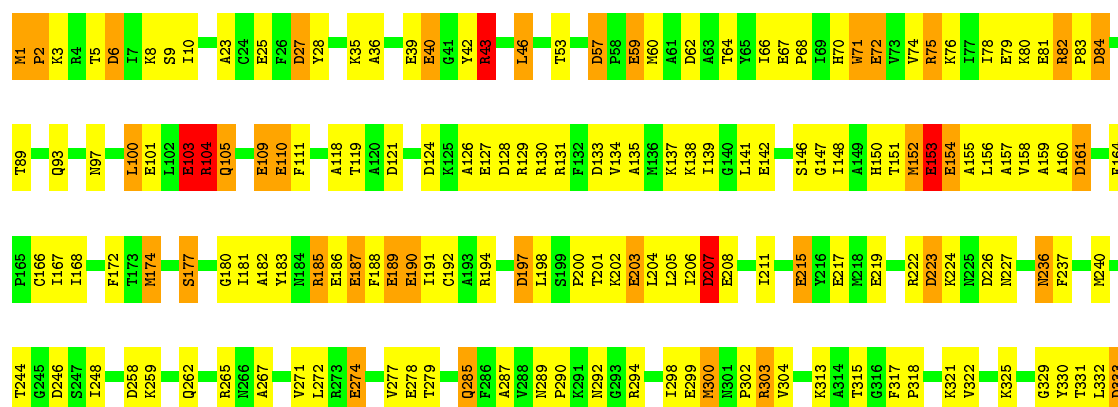
• Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE

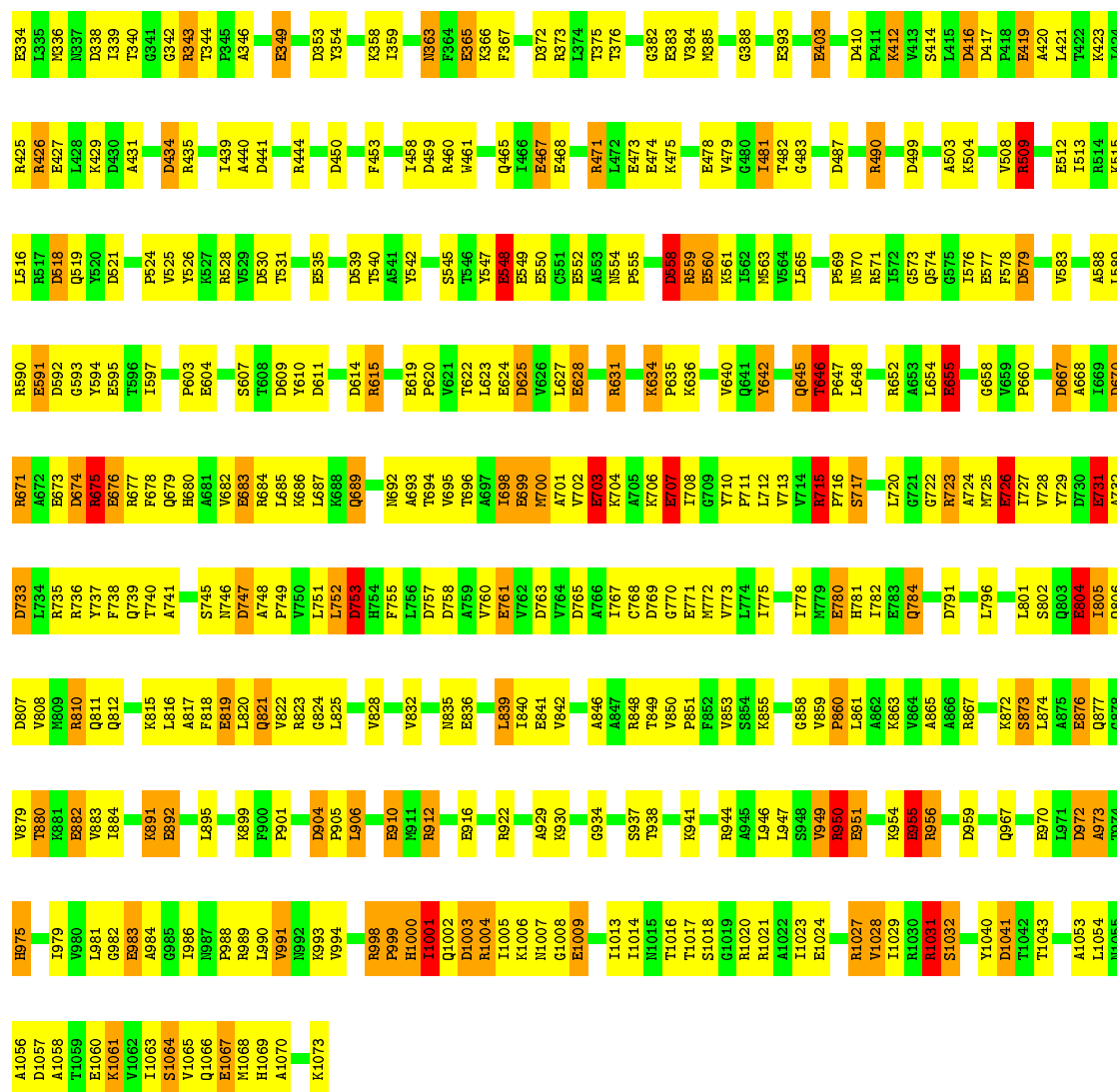
Chain E: 60% 31% 9%



- Molecule 1: CARBAMOYL-PHOSPHATE SYNTHASE

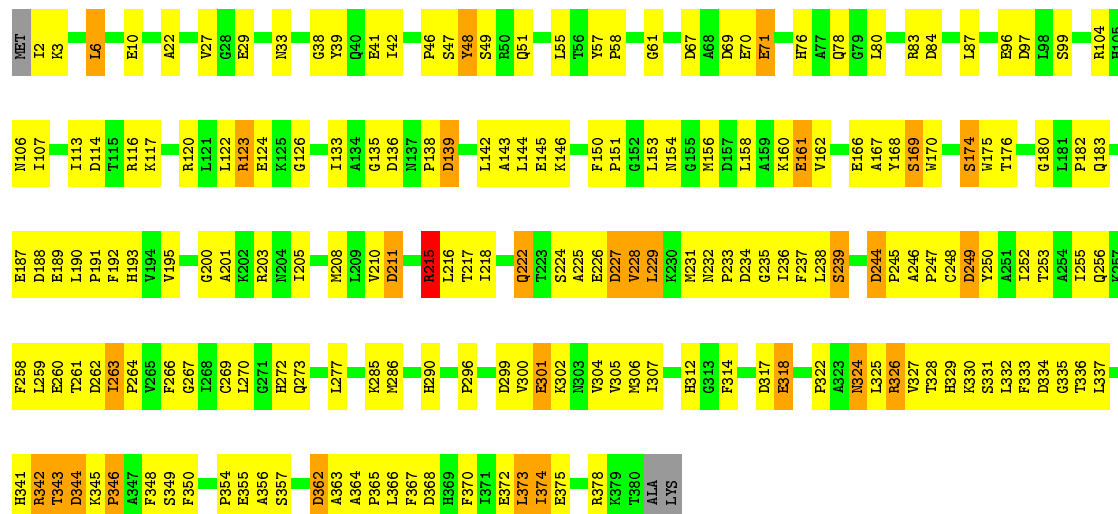
Chain G:  48% 39% 11%



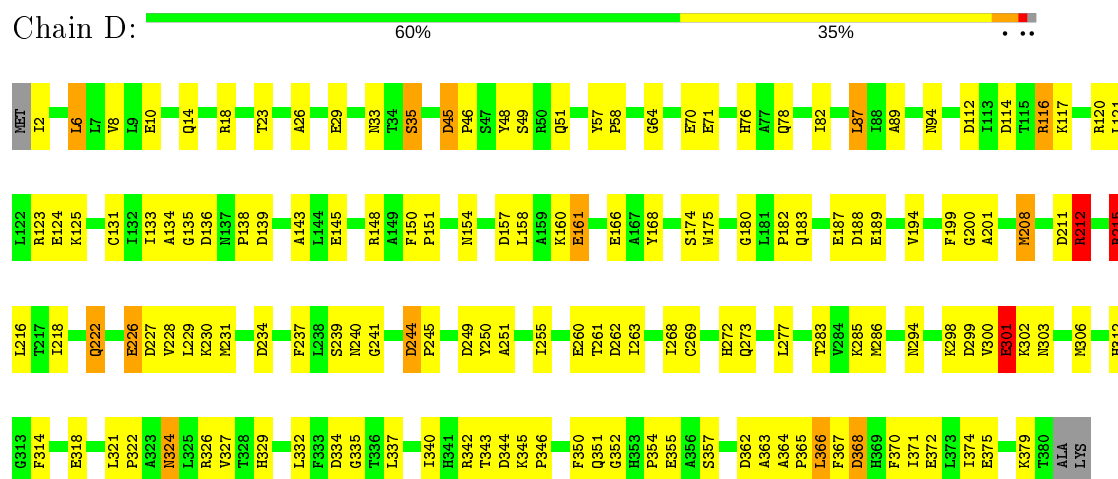


- Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

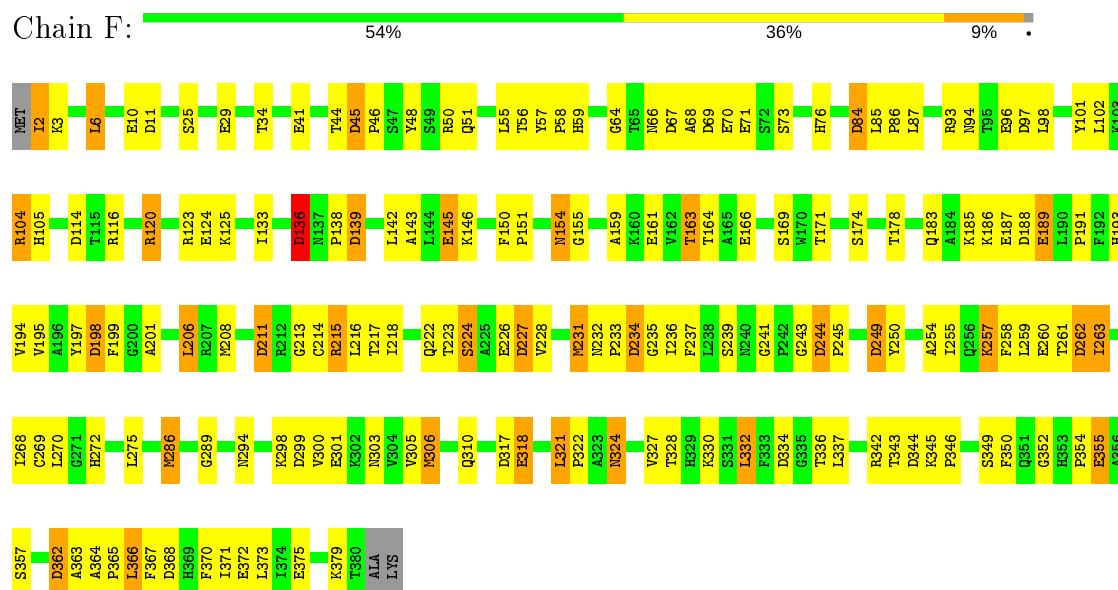
Chain B:  49% 43% 7%



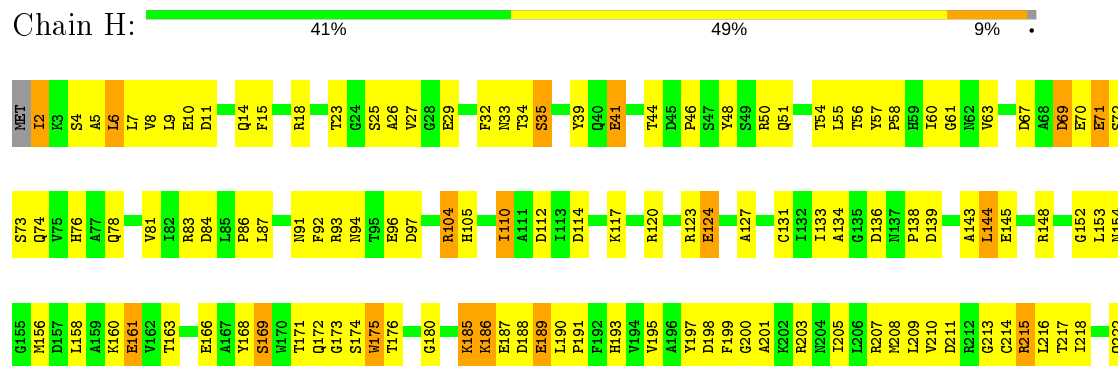
• Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE

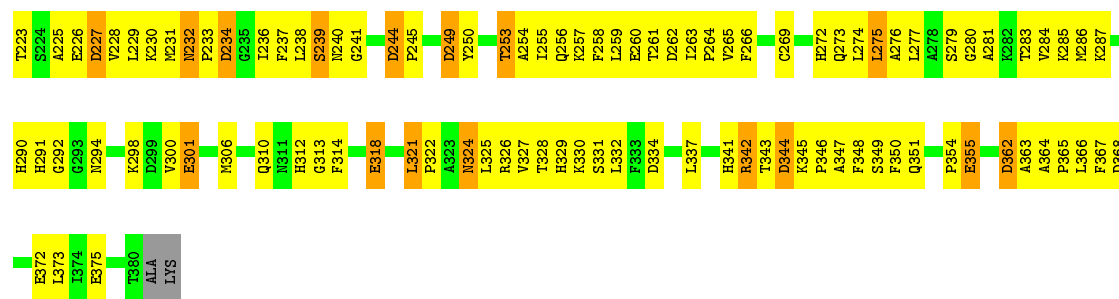


• Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE



• Molecule 2: CARBAMOYL-PHOSPHATE SYNTHASE





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.90Å 164.50Å 332.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10	Depositor
% Data completeness (in resolution range)	93.0 (30.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	TNT 5E	Depositor
R, $R_{free}$	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48307	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	1.01	83/8435 (1.0%)	1.41	129/11407 (1.1%)
1	C	1.01	81/8399 (1.0%)	1.38	129/11361 (1.1%)
1	E	1.01	82/8427 (1.0%)	1.38	122/11398 (1.1%)
1	G	1.02	82/8418 (1.0%)	1.39	140/11386 (1.2%)
2	B	0.87	19/2957 (0.6%)	1.28	33/4016 (0.8%)
2	D	0.91	16/2957 (0.5%)	1.31	38/4016 (0.9%)
2	F	0.89	19/2957 (0.6%)	1.28	41/4016 (1.0%)
2	H	0.89	19/2957 (0.6%)	1.30	33/4016 (0.8%)
All	All	0.98	401/45507 (0.9%)	1.36	665/61616 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
2	F	1	0
All	All	1	1

All (401) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	GLU	CD-OE1	9.89	1.36	1.25
2	H	10	GLU	CD-OE1	9.59	1.36	1.25
1	G	153	GLU	CD-OE1	8.90	1.35	1.25
1	C	110	GLU	CD-OE1	8.43	1.34	1.25
1	G	103	GLU	CD-OE1	8.38	1.34	1.25
1	C	383	GLU	CD-OE1	8.29	1.34	1.25
1	G	512	GLU	CD-OE1	8.27	1.34	1.25
1	A	804	GLU	CD-OE1	8.25	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	631	ARG	CZ-NH1	8.14	1.43	1.33
1	A	419	GLU	CD-OE1	8.10	1.34	1.25
1	E	468	GLU	CD-OE1	7.95	1.34	1.25
1	C	683	GLU	CD-OE1	7.85	1.34	1.25
1	G	59	GLU	CD-OE2	7.82	1.34	1.25
1	C	655	GLU	CD-OE2	7.81	1.34	1.25
1	G	951	GLU	CD-OE1	7.66	1.34	1.25
1	C	109	GLU	CD-OE2	7.62	1.34	1.25
1	A	577	GLU	CD-OE1	7.48	1.33	1.25
1	A	910	GLU	CD-OE2	7.45	1.33	1.25
1	C	190	GLU	CD-OE1	7.44	1.33	1.25
1	A	591	GLU	CD-OE1	7.40	1.33	1.25
1	G	72	GLU	CD-OE2	7.39	1.33	1.25
1	G	1024	GLU	CD-OE1	7.39	1.33	1.25
1	C	577	GLU	CD-OE1	7.33	1.33	1.25
1	E	999	PRO	N-CD	7.26	1.58	1.47
1	E	278	GLU	CD-OE2	7.24	1.33	1.25
1	C	278	GLU	CD-OE2	7.16	1.33	1.25
1	E	591	GLU	CD-OE2	7.14	1.33	1.25
1	E	365	GLU	CD-OE1	7.12	1.33	1.25
1	C	334	GLU	CD-OE2	7.11	1.33	1.25
1	G	604	GLU	CD-OE1	7.10	1.33	1.25
1	C	219	GLU	CD-OE1	7.10	1.33	1.25
1	E	999	PRO	N-CA	-7.08	1.35	1.47
1	E	219	GLU	CD-OE1	7.06	1.33	1.25
1	C	217	GLU	CD-OE2	7.03	1.33	1.25
1	G	1009	GLU	CD-OE2	7.02	1.33	1.25
1	G	726	GLU	CD-OE1	7.02	1.33	1.25
2	H	226	GLU	CD-OE1	7.00	1.33	1.25
1	A	996	GLU	CD-OE2	6.99	1.33	1.25
1	G	474	GLU	CD-OE1	6.97	1.33	1.25
1	C	127	GLU	CD-OE1	6.92	1.33	1.25
1	A	833	LYS	CE-NZ	-6.91	1.31	1.49
1	A	190	GLU	CD-OE1	6.88	1.33	1.25
1	G	154	GLU	CD-OE1	6.87	1.33	1.25
1	C	1009	GLU	CD-OE2	6.82	1.33	1.25
1	C	110	GLU	CD-OE2	-6.80	1.18	1.25
1	A	983	GLU	CD-OE1	6.79	1.33	1.25
1	A	110	GLU	CD-OE1	6.78	1.33	1.25
1	G	186	GLU	CD-OE2	6.76	1.33	1.25
1	G	190	GLU	CD-OE1	6.76	1.33	1.25
1	G	683	GLU	CD-OE1	6.74	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	951	GLU	CD-OE1	6.73	1.33	1.25
2	F	166	GLU	CD-OE1	6.73	1.33	1.25
1	G	916	GLU	CD-OE2	6.71	1.33	1.25
1	C	1024	GLU	CD-OE1	6.70	1.33	1.25
1	A	628	GLU	CD-OE1	6.69	1.33	1.25
2	H	145	GLU	CD-OE1	6.69	1.33	1.25
2	H	166	GLU	CD-OE2	6.67	1.32	1.25
2	H	71	GLU	CD-OE2	6.64	1.32	1.25
1	A	427	GLU	CD-OE2	6.60	1.32	1.25
1	A	260	GLU	CD-OE2	6.59	1.32	1.25
1	A	153	GLU	CD-OE1	6.59	1.32	1.25
1	A	676	GLU	CD-OE2	6.55	1.32	1.25
2	H	372	GLU	CD-OE1	6.55	1.32	1.25
1	A	279	THR	C-O	-6.54	1.10	1.23
1	E	153	GLU	CD-OE1	6.54	1.32	1.25
1	A	1024	GLU	CD-OE1	6.54	1.32	1.25
1	G	707	GLU	CD-OE1	6.53	1.32	1.25
1	A	474	GLU	CD-OE1	6.53	1.32	1.25
1	E	59	GLU	CD-OE1	6.53	1.32	1.25
1	C	771	GLU	CD-OE2	6.52	1.32	1.25
1	A	876	GLU	CD-OE2	6.52	1.32	1.25
1	C	349	GLU	CD-OE2	6.52	1.32	1.25
1	E	655	GLU	CD-OE1	6.49	1.32	1.25
1	E	780	GLU	CD-OE1	6.47	1.32	1.25
1	E	619	GLU	CD-OE1	6.45	1.32	1.25
1	A	1067	GLU	CD-OE1	6.44	1.32	1.25
1	G	761	GLU	CD-OE1	6.44	1.32	1.25
1	E	876	GLU	CD-OE2	6.43	1.32	1.25
1	C	549	GLU	CD-OE2	6.43	1.32	1.25
2	F	355	GLU	CD-OE1	6.42	1.32	1.25
1	G	110	GLU	CD-OE1	6.42	1.32	1.25
1	C	186	GLU	CD-OE2	6.42	1.32	1.25
1	E	403	GLU	CD-OE2	6.42	1.32	1.25
2	D	189	GLU	CD-OE2	6.41	1.32	1.25
1	E	1024	GLU	CD-OE1	6.41	1.32	1.25
1	A	955	GLU	CD-OE1	6.41	1.32	1.25
1	C	512	GLU	CD-OE1	6.41	1.32	1.25
1	G	478	GLU	CD-OE1	6.41	1.32	1.25
1	C	299	GLU	CD-OE2	6.39	1.32	1.25
2	B	260	GLU	CD-OE2	6.38	1.32	1.25
1	G	628	GLU	CD-OE1	6.37	1.32	1.25
2	B	145	GLU	CD-OE1	6.37	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	318	GLU	CD-OE2	6.37	1.32	1.25
1	G	804	GLU	CD-OE2	6.36	1.32	1.25
2	B	301	GLU	CD-OE1	6.35	1.32	1.25
1	G	109	GLU	CD-OE2	6.35	1.32	1.25
1	A	186	GLU	CD-OE2	6.33	1.32	1.25
2	F	71	GLU	CD-OE2	6.33	1.32	1.25
1	A	731	GLU	CD-OE1	6.32	1.32	1.25
1	C	334	GLU	CD-OE1	-6.32	1.18	1.25
2	D	226	GLU	CD-OE1	6.32	1.32	1.25
1	C	731	GLU	CD-OE1	6.32	1.32	1.25
1	A	103	GLU	CD-OE1	6.32	1.32	1.25
1	E	535	GLU	CD-OE1	6.32	1.32	1.25
1	E	110	GLU	CD-OE1	6.30	1.32	1.25
1	A	819	GLU	CD-OE1	6.30	1.32	1.25
2	B	372	GLU	CD-OE1	6.29	1.32	1.25
2	D	372	GLU	CD-OE1	6.29	1.32	1.25
2	D	70	GLU	CD-OE1	6.29	1.32	1.25
1	E	215	GLU	CD-OE1	6.28	1.32	1.25
1	G	731	GLU	CD-OE1	6.28	1.32	1.25
1	G	59	GLU	CD-OE1	-6.27	1.18	1.25
1	E	549	GLU	CD-OE2	6.27	1.32	1.25
2	B	166	GLU	CD-OE2	6.26	1.32	1.25
1	C	804	GLU	CD-OE1	6.26	1.32	1.25
1	E	673	GLU	CD-OE1	6.26	1.32	1.25
1	G	876	GLU	CD-OE2	6.25	1.32	1.25
1	E	103	GLU	CD-OE1	6.24	1.32	1.25
1	E	217	GLU	CD-OE2	6.24	1.32	1.25
1	A	699	GLU	CD-OE2	-6.23	1.18	1.25
2	F	41	GLU	CD-OE1	6.22	1.32	1.25
1	G	703	GLU	CD-OE1	6.21	1.32	1.25
1	G	535	GLU	CD-OE1	6.21	1.32	1.25
1	A	127	GLU	CD-OE1	6.21	1.32	1.25
1	A	535	GLU	CD-OE1	6.20	1.32	1.25
1	C	468	GLU	CD-OE1	6.19	1.32	1.25
1	A	951	GLU	CD-OE1	6.18	1.32	1.25
1	C	676	GLU	CD-OE2	6.18	1.32	1.25
1	C	951	GLU	CD-OE1	6.18	1.32	1.25
1	G	771	GLU	CD-OE2	6.18	1.32	1.25
1	E	955	GLU	CD-OE2	6.17	1.32	1.25
1	C	419	GLU	CD-OE1	6.17	1.32	1.25
1	E	804	GLU	CD-OE1	6.15	1.32	1.25
2	H	375	GLU	CD-OE2	6.15	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	676	GLU	CD-OE2	6.14	1.32	1.25
2	B	187	GLU	CD-OE1	6.14	1.32	1.25
1	E	707	GLU	CD-OE1	6.13	1.32	1.25
1	C	203	GLU	CD-OE2	6.13	1.32	1.25
1	C	783	GLU	CD-OE1	6.13	1.32	1.25
1	C	703	GLU	CD-OE1	6.12	1.32	1.25
2	F	375	GLU	CD-OE2	6.12	1.32	1.25
1	E	703	GLU	CD-OE2	6.12	1.32	1.25
1	C	473	GLU	CD-OE1	6.12	1.32	1.25
2	F	226	GLU	CD-OE1	6.12	1.32	1.25
2	H	161	GLU	CD-OE2	6.11	1.32	1.25
2	D	318	GLU	CD-OE2	6.11	1.32	1.25
2	B	189	GLU	CD-OE2	6.11	1.32	1.25
1	A	1060	GLU	CD-OE2	6.11	1.32	1.25
1	G	560	GLU	CD-OE1	6.11	1.32	1.25
1	A	549	GLU	CD-OE2	6.09	1.32	1.25
1	E	190	GLU	CD-OE1	6.08	1.32	1.25
1	C	79	GLU	CD-OE2	6.08	1.32	1.25
1	A	699	GLU	CD-OE1	6.07	1.32	1.25
1	C	153	GLU	CD-OE1	6.06	1.32	1.25
1	C	59	GLU	CD-OE1	6.06	1.32	1.25
1	E	109	GLU	CD-OE2	6.06	1.32	1.25
2	F	301	GLU	CD-OE1	6.06	1.32	1.25
1	E	970	GLU	CD-OE1	6.05	1.32	1.25
1	E	208	GLU	CD-OE1	6.05	1.32	1.25
1	C	474	GLU	CD-OE1	6.05	1.32	1.25
1	C	403	GLU	CD-OE2	6.04	1.32	1.25
1	C	882	GLU	CD-OE2	6.04	1.32	1.25
1	C	916	GLU	CD-OE2	6.04	1.32	1.25
1	A	478	GLU	CD-OE1	6.04	1.32	1.25
1	E	683	GLU	CD-OE1	6.03	1.32	1.25
2	F	96	GLU	CD-OE2	6.02	1.32	1.25
2	B	318	GLU	CD-OE2	6.02	1.32	1.25
1	G	1067	GLU	CD-OE1	6.02	1.32	1.25
1	A	560	GLU	CD-OE2	6.02	1.32	1.25
1	E	101	GLU	CD-OE1	6.01	1.32	1.25
1	C	103	GLU	CD-OE1	6.00	1.32	1.25
1	C	628	GLU	CD-OE1	6.00	1.32	1.25
1	A	683	GLU	CD-OE1	6.00	1.32	1.25
2	D	71	GLU	CD-OE2	6.00	1.32	1.25
1	G	79	GLU	CD-OE2	6.00	1.32	1.25
1	G	591	GLU	CD-OE1	6.00	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	GLU	CD-OE2	6.00	1.32	1.25
1	A	278	GLU	CD-OE2	5.99	1.32	1.25
1	E	349	GLU	CD-OE2	5.99	1.32	1.25
1	E	731	GLU	CD-OE2	5.99	1.32	1.25
1	A	595	GLU	CD-OE1	5.99	1.32	1.25
1	C	955	GLU	CD-OE1	5.99	1.32	1.25
1	E	72	GLU	CD-OE2	5.98	1.32	1.25
1	G	278	GLU	CD-OE2	5.98	1.32	1.25
1	A	703	GLU	CD-OE1	5.98	1.32	1.25
1	C	892	GLU	CD-OE1	5.93	1.32	1.25
2	H	355	GLU	CD-OE1	5.92	1.32	1.25
2	F	187	GLU	CD-OE1	5.92	1.32	1.25
1	G	215	GLU	CD-OE1	5.92	1.32	1.25
1	G	103	GLU	CD-OE2	-5.91	1.19	1.25
1	E	771	GLU	CD-OE2	5.91	1.32	1.25
1	E	819	GLU	CD-OE1	5.91	1.32	1.25
2	H	301	GLU	CD-OE1	5.90	1.32	1.25
1	C	836	GLU	CD-OE2	5.90	1.32	1.25
1	G	836	GLU	CD-OE1	5.90	1.32	1.25
1	C	365	GLU	CD-OE1	5.90	1.32	1.25
1	G	365	GLU	CD-OE1	5.90	1.32	1.25
1	C	535	GLU	CD-OE1	5.88	1.32	1.25
1	G	819	GLU	CD-OE1	5.88	1.32	1.25
1	G	208	GLU	CD-OE1	5.86	1.32	1.25
1	E	127	GLU	CD-OE1	5.86	1.32	1.25
1	G	676	GLU	CD-OE2	5.85	1.32	1.25
2	B	124	GLU	CD-OE1	5.85	1.32	1.25
2	F	145	GLU	CD-OE1	5.84	1.32	1.25
1	E	726	GLU	CD-OE1	5.84	1.32	1.25
1	E	836	GLU	CD-OE1	5.83	1.32	1.25
1	G	549	GLU	CD-OE2	5.83	1.32	1.25
2	B	226	GLU	CD-OE1	5.83	1.32	1.25
1	C	478	GLU	CD-OE1	5.83	1.32	1.25
1	C	926	GLU	CD-OE1	5.82	1.32	1.25
1	A	79	GLU	CD-OE2	5.82	1.32	1.25
2	F	124	GLU	CD-OE1	5.82	1.32	1.25
1	A	109	GLU	CD-OE2	5.82	1.32	1.25
1	C	699	GLU	CD-OE2	5.81	1.32	1.25
1	C	67	GLU	CD-OE1	5.81	1.32	1.25
2	D	10	GLU	CD-OE1	5.80	1.32	1.25
1	E	474	GLU	CD-OE1	5.80	1.32	1.25
1	A	334	GLU	CD-OE2	5.80	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	GLU	CD-OE1	5.80	1.32	1.25
2	H	70	GLU	CD-OE1	5.80	1.32	1.25
1	A	633	GLU	CD-OE1	5.79	1.32	1.25
1	C	624	GLU	CD-OE1	5.79	1.32	1.25
2	H	10	GLU	CD-OE2	-5.78	1.19	1.25
1	G	983	GLU	CD-OE1	5.78	1.32	1.25
1	A	707	GLU	CD-OE2	5.77	1.32	1.25
2	B	355	GLU	CD-OE1	5.77	1.31	1.25
1	A	510	GLU	CD-OE1	5.76	1.31	1.25
1	C	996	GLU	CD-OE2	5.76	1.31	1.25
1	G	393	GLU	CD-OE1	5.76	1.31	1.25
1	E	699	GLU	CD-OE1	5.74	1.31	1.25
1	A	836	GLU	CD-OE1	5.74	1.31	1.25
1	C	1060	GLU	CD-OE2	5.73	1.31	1.25
1	E	79	GLU	CD-OE2	5.73	1.31	1.25
2	B	161	GLU	CD-OE2	5.72	1.31	1.25
1	G	274	GLU	CD-OE1	5.72	1.31	1.25
1	E	560	GLU	CD-OE2	5.72	1.31	1.25
1	C	560	GLU	CD-OE1	5.72	1.31	1.25
1	A	726	GLU	CD-OE1	5.72	1.31	1.25
1	E	186	GLU	CD-OE2	5.72	1.31	1.25
1	C	707	GLU	CD-OE1	5.72	1.31	1.25
1	G	673	GLU	CD-OE1	5.71	1.31	1.25
1	E	467	GLU	CD-OE1	5.71	1.31	1.25
2	H	96	GLU	CD-OE2	5.71	1.31	1.25
1	E	39	GLU	CD-OE1	5.71	1.31	1.25
1	G	882	GLU	CD-OE2	5.71	1.31	1.25
1	E	142	GLU	CD-OE2	5.70	1.31	1.25
1	C	604	GLU	CD-OE1	5.70	1.31	1.25
1	C	983	GLU	CD-OE1	5.69	1.31	1.25
1	E	783	GLU	CD-OE1	5.68	1.31	1.25
1	E	419	GLU	CD-OE1	5.67	1.31	1.25
1	G	577	GLU	CD-OE1	5.67	1.31	1.25
1	A	780	GLU	CD-OE1	5.67	1.31	1.25
1	A	771	GLU	CD-OE1	5.67	1.31	1.25
1	C	726	GLU	CD-OE1	5.66	1.31	1.25
1	E	478	GLU	CD-OE1	5.66	1.31	1.25
1	G	699	GLU	CD-OE1	5.65	1.31	1.25
2	D	375	GLU	CD-OE2	5.65	1.31	1.25
1	A	619	GLU	CD-OE1	5.65	1.31	1.25
1	G	955	GLU	CD-OE1	5.65	1.31	1.25
2	H	189	GLU	CD-OE2	5.64	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	127	GLU	CD-OE1	5.64	1.31	1.25
1	A	926	GLU	CD-OE1	5.64	1.31	1.25
1	E	203	GLU	CD-OE1	5.64	1.31	1.25
1	C	467	GLU	CD-OE1	5.63	1.31	1.25
1	G	39	GLU	CD-OE1	5.63	1.31	1.25
2	B	70	GLU	CD-OE1	5.62	1.31	1.25
2	D	187	GLU	CD-OE1	5.62	1.31	1.25
1	G	187	GLU	CD-OE2	5.61	1.31	1.25
1	C	780	GLU	CD-OE1	5.61	1.31	1.25
2	F	189	GLU	CD-OE2	5.60	1.31	1.25
2	H	318	GLU	CD-OE2	5.60	1.31	1.25
1	G	189	GLU	CD-OE2	5.59	1.31	1.25
1	G	595	GLU	CD-OE1	5.59	1.31	1.25
1	A	512	GLU	CD-OE2	5.59	1.31	1.25
1	C	819	GLU	CD-OE1	5.59	1.31	1.25
1	C	39	GLU	CD-OE1	5.58	1.31	1.25
1	G	892	GLU	CD-OE2	5.58	1.31	1.25
2	D	166	GLU	CD-OE2	5.58	1.31	1.25
2	D	260	GLU	CD-OE2	5.57	1.31	1.25
1	A	187	GLU	CD-OE2	5.57	1.31	1.25
1	E	577	GLU	CD-OE1	5.56	1.31	1.25
1	A	761	GLU	CD-OE1	5.56	1.31	1.25
1	C	274	GLU	CD-OE1	5.56	1.31	1.25
1	C	591	GLU	CD-OE2	5.56	1.31	1.25
1	A	604	GLU	CD-OE1	5.56	1.31	1.25
1	C	187	GLU	CD-OE2	5.55	1.31	1.25
1	C	72	GLU	CD-OE2	5.55	1.31	1.25
1	E	189	GLU	CD-OE2	5.54	1.31	1.25
1	G	349	GLU	CD-OE2	5.54	1.31	1.25
2	F	161	GLU	CD-OE2	5.53	1.31	1.25
2	B	29	GLU	CD-OE2	5.53	1.31	1.25
1	E	758	ASP	CG-OD1	5.53	1.38	1.25
1	A	970	GLU	CD-OE1	5.53	1.31	1.25
1	E	154	GLU	CD-OE1	5.53	1.31	1.25
1	E	604	GLU	CD-OE1	5.52	1.31	1.25
2	H	124	GLU	CD-OE1	5.52	1.31	1.25
1	G	203	GLU	CD-OE2	5.52	1.31	1.25
1	G	780	GLU	CD-OE1	5.52	1.31	1.25
1	C	595	GLU	CD-OE1	5.51	1.31	1.25
1	C	970	GLU	CD-OE1	5.51	1.31	1.25
1	E	550	GLU	CD-OE1	5.50	1.31	1.25
1	A	40	GLU	CD-OE1	5.50	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	983	GLU	CD-OE1	5.50	1.31	1.25
1	A	655	GLU	CD-OE2	5.49	1.31	1.25
1	G	383	GLU	CD-OE1	5.48	1.31	1.25
1	A	393	GLU	CD-OE1	5.47	1.31	1.25
2	D	124	GLU	CD-OE1	5.47	1.31	1.25
1	G	655	GLU	CD-OE2	5.47	1.31	1.25
1	G	548	GLU	CD-OE1	5.46	1.31	1.25
1	E	235	GLU	CD-OE1	5.45	1.31	1.25
1	A	365	GLU	CD-OE1	5.44	1.31	1.25
2	F	70	GLU	CD-OE1	5.44	1.31	1.25
1	A	349	GLU	CD-OE2	5.43	1.31	1.25
2	H	187	GLU	CD-OE1	5.43	1.31	1.25
1	A	783	GLU	CD-OE1	5.43	1.31	1.25
2	B	375	GLU	CD-OE2	5.42	1.31	1.25
1	G	552	GLU	CD-OE2	5.42	1.31	1.25
1	A	142	GLU	CD-OE2	5.41	1.31	1.25
1	E	1060	GLU	CD-OE2	5.41	1.31	1.25
1	A	467	GLU	CD-OE1	5.41	1.31	1.25
1	G	403	GLU	CD-OE2	5.41	1.31	1.25
1	A	673	GLU	CD-OE1	5.40	1.31	1.25
1	G	334	GLU	CD-OE2	5.40	1.31	1.25
1	A	996	GLU	CD-OE1	-5.39	1.19	1.25
2	B	10	GLU	CD-OE1	5.39	1.31	1.25
1	E	1009[A]	GLU	CD-OE2	-5.38	1.19	1.25
1	E	1009[B]	GLU	CD-OE2	-5.38	1.19	1.25
2	F	260	GLU	CD-OE2	5.38	1.31	1.25
1	E	510	GLU	CD-OE1	5.38	1.31	1.25
1	A	550	GLU	CD-OE1	5.38	1.31	1.25
1	G	427	GLU	CD-OE2	5.37	1.31	1.25
1	E	393	GLU	CD-OE1	5.37	1.31	1.25
2	B	41	GLU	CD-OE1	5.37	1.31	1.25
1	C	876	GLU	CD-OE2	5.37	1.31	1.25
1	C	910	GLU	CD-OE2	5.36	1.31	1.25
1	A	15	ALA	C-O	-5.36	1.13	1.23
1	C	761	GLU	CD-OE1	5.36	1.31	1.25
1	G	910	GLU	CD-OE2	5.36	1.31	1.25
2	F	29	GLU	CD-OE1	5.35	1.31	1.25
1	A	473	GLU	CD-OE1	5.35	1.31	1.25
2	F	262	ASP	CG-OD2	5.34	1.37	1.25
1	E	761	GLU	CD-OE1	5.34	1.31	1.25
2	D	29	GLU	CD-OE1	5.34	1.31	1.25
1	C	208	GLU	CD-OE1	5.33	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	40	GLU	CD-OE1	5.33	1.31	1.25
1	E	996	GLU	CD-OE2	5.33	1.31	1.25
2	F	10	GLU	CD-OE2	5.33	1.31	1.25
1	G	217	GLU	CD-OE2	5.33	1.31	1.25
1	C	552	GLU	CD-OE2	5.32	1.31	1.25
2	H	260	GLU	CD-OE2	5.32	1.31	1.25
1	C	655	GLU	CD-OE1	-5.32	1.19	1.25
1	C	278	GLU	CD-OE1	-5.31	1.19	1.25
2	D	145	GLU	CD-OE2	5.30	1.31	1.25
1	A	1009	GLU	CD-OE1	5.29	1.31	1.25
2	B	71	GLU	CD-OE2	5.29	1.31	1.25
1	C	40	GLU	CD-OE1	5.28	1.31	1.25
1	E	274	GLU	CD-OE1	5.28	1.31	1.25
1	E	512	GLU	CD-OE1	5.28	1.31	1.25
1	G	726	GLU	CD-OE2	-5.27	1.19	1.25
1	A	67	GLU	CD-OE1	5.26	1.31	1.25
1	A	189	GLU	CD-OE2	5.26	1.31	1.25
1	A	274	GLU	CD-OE1	5.26	1.31	1.25
1	G	550	GLU	CD-OE1	5.25	1.31	1.25
1	G	419	GLU	CD-OE2	5.24	1.31	1.25
1	A	203	GLU	CD-OE2	5.24	1.31	1.25
1	G	473	GLU	CD-OE1	5.23	1.31	1.25
1	A	916	GLU	CD-OE2	5.22	1.31	1.25
1	G	219	GLU	CD-OE1	5.22	1.31	1.25
2	H	41	GLU	CD-OE1	5.21	1.31	1.25
2	B	96	GLU	CD-OE2	5.20	1.31	1.25
1	E	67	GLU	CD-OE1	5.20	1.31	1.25
1	E	383	GLU	CD-OE1	5.20	1.31	1.25
1	E	1009[A]	GLU	CD-OE1	5.19	1.31	1.25
1	E	1009[B]	GLU	CD-OE1	5.19	1.31	1.25
1	G	970	GLU	CD-OE1	5.19	1.31	1.25
1	E	299	GLU	CD-OE2	5.17	1.31	1.25
1	E	187	GLU	CD-OE2	5.16	1.31	1.25
1	A	219	GLU	CD-OE1	5.13	1.31	1.25
1	C	189	GLU	CD-OE2	5.13	1.31	1.25
1	C	142	GLU	CD-OE2	5.13	1.31	1.25
1	A	892	GLU	CD-OE2	5.13	1.31	1.25
1	G	299	GLU	CD-OE2	5.13	1.31	1.25
2	D	161	GLU	CD-OE2	5.13	1.31	1.25
1	A	552	GLU	CD-OE2	5.11	1.31	1.25
1	G	468	GLU	CD-OE1	5.11	1.31	1.25
1	A	72	GLU	CD-OE2	5.10	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	624	GLU	CD-OE1	5.10	1.31	1.25
1	A	468	GLU	CD-OE1	5.08	1.31	1.25
1	G	467	GLU	CD-OE1	5.06	1.31	1.25
1	G	40	GLU	CD-OE1	5.06	1.31	1.25
1	A	208	GLU	CD-OE1	5.06	1.31	1.25
1	E	926	GLU	CD-OE1	5.06	1.31	1.25
1	G	142	GLU	CD-OE2	5.06	1.31	1.25
1	A	580	TYR	CB-CG	-5.05	1.44	1.51
1	C	215	GLU	CD-OE1	5.05	1.31	1.25
1	E	628	GLU	CD-OE1	5.05	1.31	1.25
1	E	892	GLU	CD-OE2	5.05	1.31	1.25
1	C	841	GLU	CD-OE2	5.02	1.31	1.25
1	C	633	GLU	CD-OE1	5.02	1.31	1.25
1	G	1060	GLU	CD-OE2	5.00	1.31	1.25
1	E	916	GLU	CD-OE2	5.00	1.31	1.25

All (665) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	912[A]	ARG	NE-CZ-NH2	-15.00	112.80	120.30
1	A	912[B]	ARG	NE-CZ-NH2	-15.00	112.80	120.30
1	A	912[A]	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	A	912[B]	ARG	NE-CZ-NH1	14.54	127.57	120.30
1	C	667	ASP	CB-CG-OD1	-13.42	106.22	118.30
1	E	998	ARG	NE-CZ-NH1	13.38	126.99	120.30
1	E	1004	ARG	NE-CZ-NH1	12.87	126.73	120.30
1	A	735	ARG	NE-CZ-NH2	-12.73	113.94	120.30
1	G	631	ARG	NE-CZ-NH2	-12.32	114.14	120.30
1	E	675	ARG	NE-CZ-NH1	11.66	126.13	120.30
2	D	215	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	E	43	ARG	NE-CZ-NH2	-10.17	115.22	120.30
1	A	675	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	G	43	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	A	518	ASP	CB-CG-OD1	-10.01	109.29	118.30
1	G	579	ASP	CB-CG-OD1	-9.58	109.68	118.30
1	C	675	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	A	592	ASP	CB-CG-OD1	-9.52	109.73	118.30
1	C	769	ASP	CB-CG-OD1	-9.37	109.87	118.30
2	D	212	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	G	675	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	A	43	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	C	530	ASP	CB-CG-OD2	-8.99	110.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	999	PRO	N-CA-C	-8.93	88.89	112.10
1	E	130	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	E	43	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	E	912	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	A	226	ASP	CB-CG-OD1	-8.85	110.33	118.30
1	A	121	ASP	CB-CG-OD1	-8.85	110.34	118.30
1	G	133	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	E	611	ASP	CB-CG-OD1	-8.79	110.39	118.30
1	C	684	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	A	684	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	A	735	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	C	571	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	E	912	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	C	757	ASP	CB-CG-OD1	-8.63	110.54	118.30
1	C	514	ARG	NE-CZ-NH2	-8.62	115.99	120.30
2	B	211	ASP	CB-CG-OD2	-8.59	110.57	118.30
1	C	361	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	E	471	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	G	611	ASP	CB-CG-OD1	-8.41	110.73	118.30
1	A	646	THR	CA-CB-CG2	-8.41	100.62	112.40
1	E	1004	ARG	NE-CZ-NH2	-8.40	116.10	120.30
2	B	215	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	G	265	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	G	82	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	E	530	ASP	CB-CG-OD1	8.25	125.72	118.30
1	E	592	ASP	CB-CG-OD1	-8.23	110.89	118.30
1	A	609	ASP	CB-CG-OD2	-8.21	110.92	118.30
1	C	223	ASP	CB-CG-OD2	-8.19	110.93	118.30
2	D	334	ASP	CB-CG-OD1	-8.11	111.00	118.30
1	E	509	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	E	434	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	6	ASP	CB-CG-OD1	-8.04	111.07	118.30
1	C	128	ASP	CB-CG-OD1	7.98	125.48	118.30
1	C	197	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	G	62	ASP	CB-CA-C	7.93	126.26	110.40
2	B	368	ASP	CB-CG-OD1	-7.92	111.17	118.30
1	G	615	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	104	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	G	667	ASP	CB-CG-OD1	-7.87	111.22	118.30
1	E	514	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	G	460	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	E	609	ASP	CB-CG-OD2	-7.84	111.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	ASP	CB-CG-OD1	-7.83	111.25	118.30
1	A	753	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	372	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	A	226	ASP	CB-CG-OD2	7.78	125.31	118.30
1	E	579	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	C	43	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	C	670	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	C	57	ASP	CB-CG-OD1	-7.70	111.37	118.30
1	C	265	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	E	671	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	C	372	ASP	CB-CG-OD1	7.66	125.20	118.30
1	C	609	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	G	62	ASP	CB-CG-OD2	7.59	125.13	118.30
1	E	667	ASP	CB-CG-OD1	-7.57	111.49	118.30
1	E	539	ASP	CB-CG-OD1	-7.54	111.51	118.30
1	A	684	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	C	435	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	G	410	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	A	670	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	E	1003	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	E	579	ASP	CB-CG-OD1	7.50	125.05	118.30
2	H	139	ASP	CB-CG-OD1	7.48	125.03	118.30
1	A	712	LEU	N-CA-CB	-7.47	95.47	110.40
1	C	494	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	C	769	ASP	CB-CG-OD2	7.45	125.00	118.30
1	C	27	ASP	CB-CG-OD2	7.44	125.00	118.30
1	C	867	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	G	956	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	C	121	ASP	CB-CG-OD2	7.39	124.95	118.30
1	C	435	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	C	430	ASP	CB-CG-OD1	-7.35	111.68	118.30
1	C	530	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	730	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	E	757	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	A	791	ASP	CB-CG-OD2	-7.27	111.75	118.30
2	D	112	ASP	CB-CG-OD1	-7.27	111.76	118.30
2	D	211	ASP	CB-CG-OD2	-7.26	111.76	118.30
2	F	262	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	C	372	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	C	416	ASP	CB-CG-OD1	-7.21	111.81	118.30
1	G	579	ASP	CB-CG-OD2	7.21	124.79	118.30
2	F	211	ASP	CB-CG-OD2	-7.20	111.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	441	ASP	CB-CG-OD1	-7.18	111.84	118.30
1	E	27	ASP	CB-CG-OD2	7.17	124.75	118.30
1	G	338	ASP	CB-CG-OD1	-7.16	111.85	118.30
2	H	207	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	E	670	ASP	CB-CG-OD1	-7.14	111.88	118.30
1	C	6	ASP	CB-CG-OD2	7.13	124.72	118.30
1	E	416	ASP	CB-CG-OD1	-7.13	111.88	118.30
1	C	763	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	C	84	ASP	CB-CG-OD1	-7.11	111.91	118.30
1	C	333	ASP	CB-CG-OD1	7.09	124.68	118.30
1	C	912	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	E	333	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	E	4	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	579	ASP	CB-CG-OD2	7.03	124.62	118.30
1	C	625	ASP	CB-CG-OD2	7.01	124.61	118.30
1	C	84	ASP	CB-CG-OD2	7.01	124.61	118.30
2	F	227	ASP	CB-CG-OD2	-7.00	112.00	118.30
2	H	139	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	G	670	ASP	CB-CG-OD2	6.98	124.58	118.30
2	F	317	ASP	CB-CG-OD1	-6.97	112.02	118.30
1	E	558	ASP	CB-CG-OD2	-6.96	112.03	118.30
2	D	262	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	G	62	ASP	CB-CG-OD1	-6.93	112.06	118.30
1	G	43	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	G	434	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	C	487	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	C	518	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	C	684	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	521	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	E	517	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	G	57	ASP	CB-CG-OD1	-6.89	112.10	118.30
1	A	670	ASP	CB-CG-OD2	6.88	124.50	118.30
1	G	726	GLU	N-CA-CB	-6.88	98.21	110.60
1	C	1004	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	E	471	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	471	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	G	121	ASP	CB-CG-OD1	-6.87	112.12	118.30
2	H	211	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	C	733	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	C	558	ASP	CB-CG-OD2	-6.86	112.13	118.30
2	F	114	ASP	CB-CG-OD1	-6.84	112.14	118.30
1	G	670	ASP	CB-CG-OD1	-6.83	112.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	136	ASP	CB-CG-OD1	-6.83	112.16	118.30
1	E	133	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	434	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	207	ASP	CB-CG-OD2	-6.82	112.17	118.30
1	E	372	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	246	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	A	730	ASP	CB-CG-OD2	6.80	124.42	118.30
1	E	223	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	972	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	434	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	G	84	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	C	223	ASP	CB-CG-OD1	6.78	124.41	118.30
1	E	999	PRO	N-CA-CB	6.78	111.44	103.30
1	A	611	ASP	CB-CG-OD1	-6.78	112.20	118.30
1	A	579	ASP	CB-CG-OD1	-6.78	112.20	118.30
1	C	670	ASP	CB-CG-OD2	6.78	124.40	118.30
1	E	667	ASP	CB-CG-OD2	6.76	124.38	118.30
2	D	342	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	579	ASP	CB-CG-OD2	6.72	124.35	118.30
1	C	499	ASP	CB-CG-OD2	6.72	124.35	118.30
1	G	207	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	C	514	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	A	558	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	1003	ASP	CB-CG-OD1	-6.67	112.29	118.30
1	C	959	ASP	CB-CG-OD2	-6.67	112.30	118.30
2	H	234	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	A	161	ASP	CB-CG-OD1	-6.65	112.31	118.30
1	G	609	ASP	CB-CG-OD2	-6.65	112.31	118.30
2	D	344	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	E	530	ASP	CB-CG-OD2	-6.64	112.33	118.30
2	H	342	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	F	97	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	59	GLU	CG-CD-OE1	-6.62	105.06	118.30
2	B	368	ASP	CB-CG-OD2	6.61	124.25	118.30
2	D	334	ASP	CB-CG-OD2	6.61	124.25	118.30
1	E	539	ASP	CB-CG-OD2	6.61	124.25	118.30
2	B	249	ASP	CB-CG-OD1	-6.60	112.36	118.30
2	D	116	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	G	459	ASP	CB-CG-OD1	-6.60	112.36	118.30
1	A	904	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	A	580	TYR	CB-CG-CD2	-6.58	117.05	121.00
2	H	334	ASP	CB-CG-OD1	-6.58	112.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	249	ASP	CB-CG-OD1	-6.56	112.39	118.30
1	E	338	ASP	CB-CG-OD1	-6.56	112.39	118.30
1	C	416	ASP	CB-CG-OD2	6.56	124.20	118.30
1	E	410	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	G	973	ALA	N-CA-CB	6.55	119.27	110.10
1	C	1003	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	G	416	ASP	CB-CG-OD1	-6.54	112.41	118.30
1	C	579	ASP	CB-CG-OD1	-6.54	112.42	118.30
1	G	27	ASP	CB-CG-OD2	6.53	124.18	118.30
1	G	499	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	A	592	ASP	CB-CG-OD2	6.52	124.17	118.30
2	H	93	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	B	139	ASP	CB-CG-OD1	6.51	124.16	118.30
2	B	262	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	E	733	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	A	1030	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	F	136	ASP	CB-CG-OD1	-6.50	112.45	118.30
2	D	244	ASP	CB-CG-OD1	-6.48	112.47	118.30
1	G	530	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	G	972	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	G	490[A]	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	G	490[B]	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	677	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	G	558	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	G	904	ASP	CB-CG-OD1	-6.46	112.48	118.30
1	E	807	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	62	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	514	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	753	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	G	27	ASP	CB-CG-OD1	-6.46	112.49	118.30
2	F	317	ASP	CB-CG-OD2	6.45	124.11	118.30
1	A	430	ASP	CB-CG-OD1	-6.44	112.50	118.30
1	C	614	ASP	CB-CG-OD1	-6.44	112.50	118.30
1	G	518	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	A	530	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	E	82	ARG	NE-CZ-NH2	-6.43	117.08	120.30
2	B	344	ASP	CB-CG-OD1	-6.43	112.52	118.30
1	A	133	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	G	226	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	G	950	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	487	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	494	ARG	NE-CZ-NH1	6.40	123.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	518	ASP	CB-CG-OD2	6.40	124.06	118.30
1	C	129	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	G	207	ASP	CB-CG-OD1	6.38	124.04	118.30
1	G	625	ASP	CB-CG-OD2	6.37	124.03	118.30
2	H	97	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	C	441	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	G	6	ASP	CB-CG-OD1	-6.36	112.57	118.30
2	D	188	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	A	758	ASP	CB-CG-OD2	6.36	124.02	118.30
2	B	227	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	E	416	ASP	CB-CG-OD2	6.35	124.01	118.30
1	A	791	ASP	CB-CG-OD1	6.35	124.01	118.30
1	E	434	ASP	CB-CG-OD1	6.34	124.00	118.30
2	F	97	ASP	CB-CG-OD1	-6.34	112.60	118.30
2	F	139	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	G	1003	ASP	CB-CG-OD1	-6.32	112.61	118.30
1	C	487	ASP	CB-CG-OD1	6.32	123.99	118.30
1	E	84	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	E	372	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	C	434	ASP	CB-CG-OD2	-6.30	112.63	118.30
2	F	262	ASP	CB-CG-OD1	6.29	123.97	118.30
2	B	211	ASP	CB-CG-OD1	6.29	123.96	118.30
2	H	249	ASP	CB-CG-OD2	6.29	123.96	118.30
1	C	528	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	D	114	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	514	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	C	343	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	G	450	ASP	CB-CG-OD1	-6.27	112.66	118.30
1	G	434	ASP	CB-CG-OD1	6.27	123.94	118.30
1	G	197	ASP	CB-CG-OD2	-6.26	112.67	118.30
2	F	139	ASP	CB-CG-OD1	6.26	123.93	118.30
1	G	75	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	E	518	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	G	223	ASP	CB-CG-OD1	6.25	123.93	118.30
1	E	124	ASP	CB-CG-OD2	-6.25	112.68	118.30
2	D	344	ASP	CB-CG-OD2	6.25	123.92	118.30
2	D	18	ARG	NE-CZ-NH1	6.25	123.42	120.30
2	D	234	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	729	TYR	CB-CG-CD2	6.24	124.74	121.00
2	D	212	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	E	487	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	C	57	ASP	CB-CG-OD2	6.24	123.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	769	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	A	609	ASP	CB-CG-OD1	6.23	123.91	118.30
1	C	226	ASP	CB-CG-OD1	-6.22	112.70	118.30
1	E	38	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	43	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	C	197	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	580	TYR	N-CA-CB	-6.20	99.44	110.60
1	G	333	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	E	823	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	410	ASP	CB-CG-OD2	6.18	123.87	118.30
1	E	614	ASP	CB-CG-OD1	-6.18	112.73	118.30
1	E	410	ASP	CB-CG-OD1	6.18	123.86	118.30
2	B	114	ASP	CB-CG-OD2	6.17	123.85	118.30
2	D	262	ASP	CB-CG-OD1	6.16	123.84	118.30
1	G	807	ASP	CB-CG-OD1	-6.16	112.76	118.30
2	F	227	ASP	CB-CG-OD1	6.16	123.84	118.30
2	B	215	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	G	614	ASP	CB-CG-OD2	6.15	123.84	118.30
1	G	631	ARG	NH1-CZ-NH2	6.15	126.17	119.40
1	G	410	ASP	CB-CG-OD1	6.15	123.83	118.30
2	H	334	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	62	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	C	499	ASP	CB-CG-OD1	-6.13	112.78	118.30
2	F	188	ASP	CB-CG-OD2	-6.13	112.79	118.30
1	G	128	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	539	ASP	N-CA-CB	6.12	121.62	110.60
2	B	317	ASP	CB-CG-OD2	6.12	123.81	118.30
1	G	338	ASP	CB-CG-OD2	6.12	123.81	118.30
1	C	441	ASP	CB-CG-OD2	6.12	123.80	118.30
1	A	521	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	671	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	C	733	ASP	CB-CG-OD1	6.09	123.78	118.30
1	E	723	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	490	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	C	747	ASP	CB-CG-OD2	6.09	123.78	118.30
1	C	791	ASP	CB-CG-OD2	-6.09	112.82	118.30
2	H	362	ASP	CB-CG-OD1	-6.08	112.82	118.30
1	E	303	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	E	121	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	A	530	ASP	CB-CG-OD1	6.07	123.76	118.30
2	F	50	ARG	CB-CA-C	6.07	122.54	110.40
2	H	50	ARG	NE-CZ-NH1	6.07	123.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ASP	CB-CG-OD1	6.07	123.76	118.30
1	E	571	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	912	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	E	765	ASP	CB-CG-OD2	6.04	123.74	118.30
1	E	807	ASP	CB-CG-OD1	-6.04	112.86	118.30
2	B	317	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	G	733	ASP	CB-CG-OD1	-6.04	112.86	118.30
1	E	128	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	G	226	ASP	CB-CG-OD2	6.04	123.73	118.30
2	F	114	ASP	CB-CG-OD2	6.03	123.73	118.30
1	G	246	ASP	CB-CG-OD1	-6.03	112.87	118.30
1	G	867	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	G	667	ASP	CB-CG-OD2	6.03	123.73	118.30
1	G	674	ASP	CB-CG-OD1	-6.03	112.87	118.30
1	G	757	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	G	757	ASP	CB-CG-OD2	6.01	123.71	118.30
1	G	128	ASP	CB-CG-OD1	6.01	123.70	118.30
1	G	460	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	E	615	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	769	ASP	CB-CG-OD1	-6.00	112.90	118.30
1	E	956	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	E	223	ASP	CB-CG-OD1	5.98	123.69	118.30
1	G	258	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	G	521	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	G	765	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	C	133	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	A	410	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	E	558	ASP	CB-CG-OD1	5.98	123.68	118.30
1	G	791	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	161	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	84	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	A	758	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	C	757	ASP	CB-CG-OD2	5.94	123.65	118.30
1	G	223	ASP	CB-CG-OD2	-5.94	112.95	118.30
2	D	112	ASP	CB-CG-OD2	5.93	123.64	118.30
1	G	487	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	E	959	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	1041	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	C	539	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	C	609	ASP	CB-CG-OD1	5.92	123.62	118.30
1	A	416	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	G	539	ASP	CB-CG-OD1	-5.91	112.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	234	ASP	CB-CG-OD1	5.90	123.61	118.30
1	G	753	ASP	CB-CG-OD2	-5.90	112.99	118.30
2	F	188	ASP	CB-CG-OD1	5.90	123.61	118.30
2	H	249	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	C	592	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	C	807	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	E	84	ASP	CB-CG-OD2	5.88	123.59	118.30
2	F	211	ASP	CB-CG-OD1	5.87	123.59	118.30
1	A	642	TYR	CB-CG-CD2	-5.87	117.48	121.00
2	B	344	ASP	CB-CG-OD2	5.87	123.58	118.30
2	D	139	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	G	509	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	807	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	E	733	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	333	ASP	CB-CG-OD2	-5.85	113.03	118.30
2	H	188	ASP	CB-CG-OD1	5.85	123.56	118.30
2	B	244	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	124	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	E	730	ASP	CB-CG-OD2	5.83	123.55	118.30
2	D	148	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	E	161	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	A	426	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	C	450	ASP	CB-CG-OD1	-5.82	113.06	118.30
2	B	249	ASP	CB-CG-OD2	5.81	123.53	118.30
2	B	139	ASP	CB-CG-OD2	-5.81	113.07	118.30
2	H	136	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	625	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	E	521	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	E	226	ASP	CB-CG-OD2	5.80	123.52	118.30
1	G	197	ASP	CB-CG-OD1	5.80	123.52	118.30
1	E	333	ASP	CB-CG-OD1	5.79	123.51	118.30
1	E	226	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	E	705	ALA	CB-CA-C	5.78	118.78	110.10
1	G	82	ARG	CG-CD-NE	-5.78	99.66	111.80
2	D	215	ARG	CB-CA-C	5.77	121.93	110.40
1	C	747	ASP	CB-CG-OD1	-5.77	113.11	118.30
2	H	262	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	459	ASP	CB-CG-OD1	-5.76	113.11	118.30
2	F	67	ASP	CB-CG-OD1	-5.76	113.11	118.30
2	D	114	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	A	197	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	A	642	TYR	CB-CG-CD1	5.75	124.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1041	ASP	CB-CG-OD2	5.74	123.47	118.30
2	B	227	ASP	CB-CG-OD1	5.74	123.47	118.30
1	E	611	ASP	CB-CG-OD2	5.74	123.47	118.30
1	C	430	ASP	CB-CG-OD2	5.74	123.46	118.30
1	G	904	ASP	CB-CG-OD2	5.73	123.46	118.30
2	D	139	ASP	CB-CG-OD1	5.73	123.46	118.30
1	E	27	ASP	CB-CG-OD1	-5.73	113.14	118.30
1	E	258	ASP	CB-CG-OD1	5.73	123.46	118.30
2	B	67	ASP	CB-CG-OD1	-5.73	113.14	118.30
1	E	972	ASP	CB-CG-OD2	-5.72	113.15	118.30
2	B	342	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	G	104	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	B	244	ASP	CB-CG-OD1	-5.71	113.16	118.30
2	D	244	ASP	CB-CG-OD2	5.71	123.44	118.30
1	G	959	ASP	CB-CG-OD1	5.71	123.44	118.30
1	C	972	ASP	CB-CG-OD2	-5.71	113.17	118.30
2	D	136	ASP	CB-CG-OD1	-5.70	113.17	118.30
2	H	69	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	E	758	ASP	CB-CG-OD2	5.69	123.42	118.30
1	G	611	ASP	CB-CG-OD2	5.69	123.42	118.30
2	H	69	ASP	CB-CG-OD2	5.69	123.42	118.30
2	B	136	ASP	CB-CG-OD1	-5.68	113.19	118.30
2	F	286	MET	CG-SD-CE	-5.68	91.11	100.20
1	C	258	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	G	372	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	A	197	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	953	ASP	CB-CG-OD2	5.66	123.40	118.30
2	F	234	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	C	121	ASP	CB-CG-OD1	-5.66	113.20	118.30
1	A	578	PHE	CB-CA-C	5.66	121.71	110.40
1	G	675	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	F	234	ASP	CB-CG-OD1	5.65	123.39	118.30
2	F	10	GLU	CB-CA-C	-5.64	99.12	110.40
1	G	848	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	D	123	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	E	959	ASP	CB-CG-OD1	5.63	123.36	118.30
1	C	558	ASP	CB-CG-OD1	5.62	123.36	118.30
1	G	459	ASP	CB-CG-OD2	5.62	123.36	118.30
1	G	646	THR	CA-CB-CG2	-5.62	104.53	112.40
1	C	521	ASP	CB-CG-OD1	-5.62	113.25	118.30
2	B	97	ASP	CB-CG-OD2	5.61	123.35	118.30
1	C	807	ASP	CB-CG-OD2	5.61	123.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	671	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	459	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	333	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	C	246	ASP	CB-CG-OD2	5.60	123.34	118.30
1	E	747	ASP	CB-CG-OD1	-5.59	113.27	118.30
2	B	69	ASP	CB-CG-OD2	5.59	123.33	118.30
1	E	417	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	E	1025	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	G	625	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	A	333	ASP	CB-CG-OD1	5.59	123.33	118.30
1	E	747	ASP	CB-CG-OD2	5.58	123.33	118.30
1	E	487	ASP	CB-CG-OD1	5.58	123.32	118.30
2	H	188	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	C	75	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	C	62	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	246	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	904	ASP	CB-CG-OD2	5.56	123.31	118.30
1	C	867	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	E	207	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	C	161	ASP	CB-CG-OD1	-5.56	113.30	118.30
2	F	249	ASP	CB-CG-OD2	5.56	123.30	118.30
2	H	227	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	667	ASP	CB-CG-OD1	-5.55	113.31	118.30
1	E	614	ASP	CB-CG-OD2	5.54	123.29	118.30
1	G	133	ASP	CB-CG-OD1	5.54	123.29	118.30
2	F	368	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	27	ASP	CB-CG-OD2	5.54	123.28	118.30
1	G	558	ASP	CB-CG-OD1	5.54	123.28	118.30
1	E	57	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	G	1057	ASP	CB-CG-OD1	-5.53	113.33	118.30
2	D	227	ASP	CB-CG-OD1	5.53	123.27	118.30
1	E	615	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	614	ASP	CB-CG-OD2	5.52	123.26	118.30
2	H	234	ASP	CB-CG-OD1	5.51	123.26	118.30
2	B	362	ASP	CB-CG-OD2	5.51	123.26	118.30
1	G	758	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	133	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	416	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	258	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	509	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	F	120	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	361	ARG	NE-CZ-NH2	-5.50	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	733	ASP	CB-CG-OD2	5.50	123.25	118.30
1	G	185	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	763	ASP	CB-CG-OD1	-5.49	113.36	118.30
2	D	211	ASP	CB-CG-OD1	5.49	123.24	118.30
2	F	368	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	G	84	ASP	CB-CG-OD2	5.49	123.24	118.30
1	E	197	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	E	207	ASP	CB-CG-OD1	5.48	123.23	118.30
2	B	362	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	C	460	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	E	6	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	G	758	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	C	43	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	757[A]	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	757[B]	ASP	CB-CG-OD2	5.46	123.22	118.30
2	D	368	ASP	CB-CG-OD2	5.46	123.21	118.30
1	G	416	ASP	CB-CG-OD2	5.46	123.21	118.30
1	G	592	ASP	CB-CG-OD1	-5.46	113.39	118.30
1	A	959	ASP	CB-CG-OD2	-5.45	113.39	118.30
2	B	69	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	G	121	ASP	CB-CG-OD2	5.45	123.20	118.30
1	C	1003	ASP	CB-CG-OD2	5.45	123.20	118.30
1	E	517	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	E	845	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	E	592	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	1003	ASP	CB-CG-OD2	5.42	123.18	118.30
2	H	84	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	845	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	944	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	E	441	ASP	CB-CG-OD2	5.42	123.18	118.30
1	E	459	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	A	169	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	539	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	C	490	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	G	57	ASP	CB-CG-OD2	5.41	123.17	118.30
1	G	1041	ASP	CB-CG-OD2	5.41	123.17	118.30
1	G	285	GLN	N-CA-CB	5.41	120.33	110.60
1	G	642	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	G	1057	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	667	ASP	CB-CG-OD2	5.40	123.16	118.30
2	D	45	ASP	CB-CG-OD2	5.40	123.16	118.30
1	E	121	ASP	CB-CG-OD2	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	615	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	G	487	ASP	CB-CG-OD1	5.39	123.16	118.30
1	A	807	ASP	CB-CG-OD2	5.39	123.15	118.30
1	E	730	ASP	CB-CG-OD1	-5.39	113.45	118.30
2	F	244	ASP	CB-CG-OD2	5.39	123.15	118.30
2	B	48	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	G	161	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	6	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	758	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	1057	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	E	680	HIS	CA-CB-CG	-5.38	104.46	113.60
1	C	450	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	1021	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	G	810	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	1027	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	758	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	C	953	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	G	530	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	845	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	1025	ASP	CB-CG-OD2	5.34	123.11	118.30
1	G	753	ASP	CB-CG-OD1	5.34	123.11	118.30
1	G	1003	ASP	CB-CG-OD2	5.34	123.11	118.30
2	H	244	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	128	ASP	CB-CG-OD1	5.33	123.09	118.30
1	E	1003	ASP	CB-CG-OD2	5.33	123.10	118.30
2	F	372	GLU	CB-CG-CD	-5.33	99.82	114.20
2	H	123	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	G	609	ASP	CB-CG-OD1	5.32	123.09	118.30
2	F	136	ASP	CB-CG-OD2	5.31	123.08	118.30
1	G	848	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	C	410	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	E	338	ASP	CB-CG-OD2	5.31	123.08	118.30
2	H	344	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	220	VAL	CB-CA-C	-5.29	101.35	111.40
1	E	735	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	B	114	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	E	124	ASP	CB-CG-OD1	5.28	123.05	118.30
1	E	343	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	F	344	ASP	CB-CG-OD2	5.28	123.05	118.30
1	G	161	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	G	6	ASP	CB-CG-OD2	5.27	123.05	118.30
1	C	998	ARG	NE-CZ-NH1	5.27	122.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	82	ARG	NE-CZ-NH1	5.27	122.94	120.30
2	B	84	ASP	CB-CG-OD1	5.26	123.04	118.30
1	G	769	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	487	ASP	CB-CG-OD1	5.26	123.04	118.30
1	C	425	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	763	ASP	CB-CG-OD2	5.26	123.03	118.30
2	F	362	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	E	559	ARG	N-CA-CB	5.26	120.06	110.60
1	E	285	GLN	N-CA-CB	5.25	120.05	110.60
1	A	450	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	C	201	THR	CA-CB-CG2	-5.24	105.06	112.40
1	C	830	PHE	CB-CA-C	-5.24	99.91	110.40
2	D	45	ASP	CB-CG-OD1	-5.24	113.58	118.30
2	B	188	ASP	CB-CG-OD1	5.24	123.02	118.30
2	D	227	ASP	CB-CG-OD2	-5.24	113.58	118.30
2	F	244	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	G	747	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	614	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	C	1057	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	715	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	G	559	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	194	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	265	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	G	959	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	D	136	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	1041	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	G	614	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	C	459	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	G	972	ASP	CB-CG-OD1	5.19	122.97	118.30
1	E	1041	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	128	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	G	528	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	B	136	ASP	CB-CG-OD2	5.18	122.96	118.30
2	D	208	MET	CA-CB-CG	-5.18	104.50	113.30
1	E	1031	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	F	344	ASP	CB-CG-OD1	-5.17	113.65	118.30
1	C	434	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	28	TYR	CB-CG-CD1	5.16	124.09	121.00
2	H	11	ASP	CB-CG-OD1	-5.16	113.66	118.30
2	H	368	ASP	CB-CG-OD1	-5.16	113.66	118.30
2	F	69	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	C	306	ARG	NE-CZ-NH2	-5.15	117.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	362	ASP	CB-CG-OD2	5.15	122.94	118.30
2	H	211	ASP	CB-CG-OD1	5.15	122.93	118.30
1	C	1025	ASP	CB-CG-OD1	-5.15	113.67	118.30
2	H	342	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	441	ASP	CB-CG-OD2	5.14	122.93	118.30
1	E	499	ASP	CB-CG-OD1	-5.14	113.68	118.30
1	G	807	ASP	CB-CG-OD2	5.13	122.92	118.30
1	G	373	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	G	294	ARG	NE-CZ-NH2	-5.13	117.74	120.30
2	H	67	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	747	ASP	CB-CG-OD1	-5.12	113.69	118.30
2	F	11	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	1057	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	C	426	ARG	NE-CZ-NH1	5.12	122.86	120.30
2	D	342	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	128	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	667	ASP	CB-CG-OD2	5.11	122.90	118.30
1	G	246	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	959	ASP	CB-CG-OD1	5.11	122.89	118.30
1	G	1041	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	A	471	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	G	1031	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	769	ASP	CB-CG-OD2	5.09	122.88	118.30
1	E	735	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	E	514	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	1021	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	226	ASP	CB-CG-OD2	5.08	122.87	118.30
1	E	444	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	223	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	84	ASP	CB-CG-OD2	5.07	122.86	118.30
1	G	715	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	G	674	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	521	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	1041	ASP	CB-CG-OD1	-5.06	113.74	118.30
1	A	130	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	D	368	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	G	729	TYR	CB-CG-CD2	5.05	124.03	121.00
2	F	45	ASP	CB-CG-OD2	5.05	122.84	118.30
1	G	441	ASP	CB-CG-OD2	5.04	122.84	118.30
1	G	518	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	1025	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	E	459	ASP	CB-CG-OD2	5.03	122.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	791	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	G	810	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	A	765	ASP	CB-CG-OD1	-5.03	113.78	118.30
1	E	765	ASP	CB-CG-OD1	-5.03	113.78	118.30
1	E	1057	ASP	CB-CG-OD2	5.03	122.82	118.30
2	H	84	ASP	CB-CG-OD1	5.02	122.82	118.30
1	C	306	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	G	185	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	684	ARG	CD-NE-CZ	5.01	130.62	123.60
2	F	84	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	294	ARG	NE-CZ-NH1	5.00	122.80	120.30
2	F	120	ARG	NE-CZ-NH2	-5.00	117.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	50	ARG	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	1008	GLY	Mainchain

## 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	8288	0	8332	325	0
1	C	8268	0	8308	306	0
1	E	8284	0	8321	276	0
1	G	8279	0	8320	437	0
2	B	2895	0	2863	146	0
2	D	2895	0	2863	85	0
2	F	2895	0	2863	126	0
2	H	2895	0	2863	160	0
3	A	3	0	0	0	0
3	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
4	E	5	0	0	0	0
4	G	4	0	0	0	0
4	H	1	0	0	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
5	E	2	0	0	2	0
5	G	4	0	0	0	0
6	A	62	0	26	3	0
6	C	62	0	26	1	0
6	E	62	0	25	3	0
6	G	62	0	26	4	0
7	A	9	0	11	1	0
7	C	9	0	11	1	0
7	E	9	0	11	1	0
7	G	9	0	11	1	0
8	A	9	0	20	6	0
8	C	9	0	20	4	0
8	E	9	0	20	6	0
8	G	9	0	20	4	0
9	A	677	0	0	21	0
9	B	169	0	0	2	0
9	C	624	0	0	20	0
9	D	234	0	0	2	0
9	E	650	0	0	13	0
9	F	193	0	0	7	0
9	G	530	0	0	22	0
9	H	165	0	0	6	0
All	All	48307	0	44960	1851	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 21.

All (1851) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:967:GLN:HG2	1:C:1054:LEU:HD13	1.26	1.16
1:C:574:GLN:NE2	1:C:645:GLN:H	1.44	1.13
1:A:172:PHE:HB3	1:A:200:PRO:HG2	1.32	1.12
2:F:322:PRO:HB2	2:F:324:ASN:HD21	1.12	1.10
1:C:574:GLN:HE22	1:C:645:GLN:N	1.51	1.09
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.31	1.07
1:G:994:VAL:HG23	1:G:1001:ILE:HD11	1.32	1.05
1:C:953:ASP:HB3	1:C:1044:LEU:HD22	1.39	1.03
2:F:324:ASN:HD22	2:F:324:ASN:N	1.54	1.03
1:E:695:VAL:HG11	1:E:701:ALA:HB2	1.39	1.00
2:D:322:PRO:HB2	2:D:324:ASN:HD21	1.28	0.99
1:E:172:PHE:HB3	1:E:200:PRO:HG2	1.39	0.99
2:B:322:PRO:HB2	2:B:324:ASN:HD21	1.27	0.99
1:A:695:VAL:HG11	1:A:701:ALA:HB2	1.44	0.98
1:G:694:THR:HG23	1:G:749:PRO:HB2	1.46	0.98
2:H:324:ASN:HD22	2:H:324:ASN:H	1.08	0.98
2:H:322:PRO:HB2	2:H:324:ASN:HD21	1.29	0.96
1:C:784:GLN:H	1:C:784:GLN:HE21	1.11	0.96
1:E:712:LEU:HD11	1:E:752:LEU:HB3	1.48	0.96
1:C:687:LEU:HD13	1:C:812:GLN:HG2	1.47	0.95
1:C:954:LYS:HG2	1:C:980:VAL:HG21	1.48	0.95
1:A:1017:THR:HG21	1:A:1023:ILE:HA	1.45	0.95
2:D:324:ASN:HD22	2:D:324:ASN:N	1.58	0.95
1:E:574:GLN:HE21	1:E:720:LEU:HD21	1.31	0.95
1:C:784:GLN:H	1:C:784:GLN:NE2	1.65	0.94
1:E:130:ARG:HG3	1:E:148:ILE:HG13	1.49	0.94
2:F:324:ASN:ND2	2:F:324:ASN:H	1.66	0.94
1:G:1029:ILE:H	1:G:1029:ILE:HD12	1.32	0.93
1:E:676:GLU:HB2	1:E:694:THR:HG21	1.50	0.93
1:E:71:TRP:CH2	1:E:105:GLN:HG2	2.03	0.93
2:F:327:VAL:HG13	2:F:337:LEU:HD11	1.51	0.93
1:A:992:ASN:ND2	1:A:996:GLU:HB2	1.84	0.93
2:F:322:PRO:HB2	2:F:324:ASN:ND2	1.84	0.92
1:C:1001:ILE:HD12	1:C:1002:GLN:H	1.34	0.92
1:G:172:PHE:HB3	1:G:200:PRO:HG2	1.49	0.92
1:G:828:VAL:HG13	1:G:842:VAL:HG22	1.52	0.92
2:H:322:PRO:HB2	2:H:324:ASN:ND2	1.82	0.92
1:C:1017:THR:HG21	1:C:1023:ILE:HA	1.53	0.91
1:A:563:MET:HE3	1:A:635:PRO:HG3	1.53	0.91
2:D:324:ASN:ND2	2:D:324:ASN:H	1.61	0.91
1:A:574:GLN:NE2	1:A:645:GLN:H	1.68	0.90
2:D:133:ILE:HD12	2:D:143:ALA:HB2	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1086:NET:H22	8:A:1086:NET:H42	1.53	0.89
1:G:670:ASP:HB3	1:G:677:ARG:HH21	1.37	0.89
1:E:147:GLY:HA3	1:E:158:VAL:HG11	1.55	0.89
2:B:150:PHE:CD1	2:B:151:PRO:HD2	2.08	0.88
1:E:574:GLN:HE22	1:E:645:GLN:H	0.96	0.88
1:A:993:LYS:HB2	1:A:996:GLU:HG3	1.56	0.88
1:C:684:ARG:HH11	1:C:684:ARG:HG3	1.39	0.88
1:G:147:GLY:HA3	1:G:158:VAL:HG11	1.53	0.88
1:C:676:GLU:HB2	1:C:694:THR:HG21	1.56	0.87
2:H:327:VAL:HG13	2:H:337:LEU:HD11	1.55	0.87
1:A:784:GLN:NE2	1:A:784:GLN:H	1.73	0.87
1:G:695:VAL:HG11	1:G:701:ALA:CB	2.05	0.87
1:C:951:GLU:HA	1:C:954:LYS:HD2	1.55	0.87
1:A:574:GLN:HE22	1:A:645:GLN:H	1.22	0.86
2:D:322:PRO:HB2	2:D:324:ASN:ND2	1.90	0.86
2:H:324:ASN:HD22	2:H:324:ASN:N	1.67	0.86
2:B:322:PRO:HB2	2:B:324:ASN:ND2	1.88	0.86
1:G:1:MET:HG3	1:G:2:PRO:HD2	1.55	0.86
2:F:286:MET:HE3	2:F:289:GLY:HA2	1.55	0.86
2:F:150:PHE:CD1	2:F:151:PRO:HD2	2.10	0.85
1:G:685:LEU:HD11	1:G:819:GLU:CB	2.07	0.85
1:C:994:VAL:HG23	1:C:1001:ILE:HD11	1.59	0.85
1:G:574:GLN:NE2	1:G:645:GLN:HB2	1.91	0.84
2:F:201:ALA:HB2	2:F:239:SER:HB2	1.60	0.84
1:G:563:MET:HE3	1:G:635:PRO:HG3	1.59	0.84
1:G:772:MET:SD	1:G:880:THR:HG22	2.17	0.84
2:H:228:VAL:HA	2:H:231:MET:HE3	1.58	0.84
1:E:574:GLN:NE2	1:E:645:GLN:H	1.75	0.83
2:H:57:TYR:CD1	2:H:58:PRO:HD2	2.13	0.83
1:A:695:VAL:HG12	1:A:738:PHE:CZ	2.12	0.83
1:A:993:LYS:HB2	1:A:996:GLU:CG	2.08	0.83
1:G:858:GLY:HA2	1:G:1069:HIS:CE1	2.14	0.83
1:G:687:LEU:HD13	1:G:812:GLN:HG2	1.58	0.83
2:B:324:ASN:N	2:B:324:ASN:HD22	1.73	0.82
1:G:152:MET:HE1	1:G:189:GLU:HA	1.61	0.82
1:G:713:VAL:HG22	1:G:727:ILE:HG12	1.61	0.82
1:C:687:LEU:HD13	1:C:812:GLN:CG	2.10	0.82
1:E:784:GLN:H	1:E:784:GLN:NE2	1.76	0.82
1:A:4:ARG:NH2	1:A:7:ILE:HD11	1.94	0.82
1:C:571:ARG:HD2	1:C:574:GLN:HB2	1.62	0.81
1:A:723:ARG:NH1	1:A:724:ALA:H	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:1950:NET:H42	8:C:1950:NET:H22	1.61	0.81
1:A:784:GLN:HE21	1:A:784:GLN:H	1.26	0.81
1:C:922:ARG:HE	1:C:1061:LYS:HD3	1.44	0.81
1:G:981:LEU:HD12	1:G:988:PRO:HG3	1.61	0.81
1:C:1001:ILE:HD12	1:C:1002:GLN:N	1.95	0.81
1:C:574:GLN:HE21	1:C:720:LEU:HD21	1.43	0.81
1:E:967:GLN:HG2	1:E:1054:LEU:HD13	1.63	0.81
1:C:858:GLY:HA2	1:C:1069:HIS:CE1	2.16	0.80
2:F:324:ASN:H	2:F:324:ASN:HD22	0.85	0.80
1:G:110:GLU:HG2	1:G:111:PHE:CE1	2.15	0.80
1:E:784:GLN:H	1:E:784:GLN:HE21	1.29	0.80
1:G:147:GLY:HA3	1:G:158:VAL:CG1	2.10	0.80
1:A:694:THR:HG23	1:A:749:PRO:HB2	1.64	0.80
1:E:574:GLN:NE2	1:E:720:LEU:HD21	1.96	0.80
1:A:1017:THR:HG21	1:A:1023:ILE:CA	2.13	0.79
1:A:906:LEU:HD12	1:A:907:LEU:H	1.47	0.79
1:G:154:GLU:O	1:G:158:VAL:HG23	1.83	0.79
1:G:168:ILE:HD13	1:G:191:ILE:HG21	1.64	0.79
1:G:967:GLN:HG2	1:G:1054:LEU:HD13	1.63	0.79
1:C:403:GLU:CD	1:C:646:THR:HG21	2.04	0.78
2:F:201:ALA:HB2	2:F:239:SER:CB	2.14	0.78
1:C:716:PRO:HD2	1:C:725:MET:HG2	1.66	0.78
1:E:1000:HIS:HD2	1:E:1003:ASP:H	1.32	0.78
1:G:861:LEU:HD21	9:G:4404:HOH:O	1.83	0.78
1:G:403:GLU:CD	1:G:646:THR:HG21	2.04	0.78
2:D:324:ASN:HD22	2:D:324:ASN:H	0.81	0.78
1:G:126:ALA:HB3	1:G:302:PRO:HG3	1.66	0.77
2:H:324:ASN:H	2:H:324:ASN:ND2	1.81	0.77
1:C:693:ALA:CB	1:C:708:ILE:HD11	2.13	0.77
1:E:1020:ARG:HB2	9:E:3584:HOH:O	1.85	0.77
1:C:172:PHE:HB3	1:C:200:PRO:HG2	1.67	0.77
8:G:3950:NET:H22	8:G:3950:NET:H42	1.65	0.77
1:E:1:MET:HG3	1:E:2:PRO:HD2	1.66	0.77
1:A:710:TYR:HB3	1:A:711:PRO:HA	1.66	0.76
1:C:716:PRO:HG2	1:C:723:ARG:O	1.85	0.76
1:E:991:VAL:CG2	1:E:1001:ILE:HG23	2.15	0.76
2:F:262:ASP:HB2	9:F:2830:HOH:O	1.84	0.76
1:A:72:GLU:O	1:A:75:ARG:HB3	1.85	0.76
2:F:85:LEU:HD12	2:F:86:PRO:HD2	1.68	0.76
1:C:57:ASP:HB2	1:C:60:MET:HG2	1.68	0.76
1:A:574:GLN:NE2	1:A:645:GLN:HB2	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:GLU:OE1	2:B:330:LYS:HE3	1.86	0.76
1:E:1029:ILE:H	1:E:1029:ILE:HD12	1.51	0.75
1:A:695:VAL:HG12	1:A:738:PHE:HZ	1.49	0.75
2:B:341:HIS:ND1	2:B:342:ARG:N	2.35	0.75
2:H:201:ALA:HB2	2:H:239:SER:CB	2.17	0.75
2:D:57:TYR:CD1	2:D:58:PRO:HD2	2.21	0.75
1:E:991:VAL:HG21	1:E:1001:ILE:HG23	1.68	0.75
2:F:228:VAL:O	2:F:231:MET:HG3	1.86	0.75
1:A:676:GLU:HB2	1:A:694:THR:HG21	1.67	0.75
1:A:403:GLU:OE1	1:A:646:THR:HG21	1.86	0.75
1:C:146:SER:HB2	1:C:205:LEU:HD11	1.67	0.75
8:A:1086:NET:H62	8:A:1086:NET:H82	1.68	0.75
1:C:998:ARG:HG2	1:C:998:ARG:HH11	1.51	0.75
1:A:695:VAL:HG11	1:A:701:ALA:CB	2.16	0.74
2:B:248:CYS:O	2:B:252:ILE:HG13	1.87	0.74
1:C:1027:ARG:HH21	1:C:1031:ARG:HH11	1.35	0.74
2:D:277:LEU:HD21	2:D:283:THR:HG23	1.69	0.74
1:G:1001:ILE:HD12	1:G:1002:GLN:HB2	1.69	0.74
1:E:695:VAL:HG11	1:E:701:ALA:CB	2.15	0.74
1:C:313:LYS:HE2	1:C:608:THR:O	1.88	0.74
1:E:563:MET:HE3	1:E:635:PRO:HG3	1.68	0.73
2:H:255:ILE:HG22	2:H:259:LEU:CD1	2.19	0.73
1:A:344:THR:HB	1:A:345:PRO:HD2	1.70	0.73
1:E:286:PHE:CD1	1:E:295:LEU:HD11	2.23	0.73
2:B:324:ASN:HD22	2:B:325:LEU:N	1.86	0.73
1:C:772:MET:SD	1:C:880:THR:HG22	2.28	0.73
8:E:2950:NET:H22	8:E:2950:NET:H42	1.71	0.73
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.71	0.73
1:E:126:ALA:HB3	1:E:302:PRO:HG3	1.71	0.73
1:A:85:ALA:HB1	1:A:116:ILE:HG12	1.70	0.73
1:E:147:GLY:HA3	1:E:158:VAL:CG1	2.17	0.73
1:A:694:THR:HG23	1:A:749:PRO:CB	2.19	0.73
1:G:403:GLU:OE2	1:G:646:THR:HG21	1.89	0.73
1:A:267:ALA:O	1:A:271:VAL:HG23	1.89	0.72
1:A:679:GLN:HA	1:A:689:GLN:HE22	1.54	0.72
1:A:954:LYS:HG2	1:A:980:VAL:HG21	1.69	0.72
2:F:228:VAL:HA	2:F:231:MET:HE3	1.71	0.72
1:G:574:GLN:HE21	1:G:645:GLN:HB2	1.54	0.72
2:F:318:GLU:O	2:F:321:LEU:HB2	1.89	0.72
1:A:873:SER:OG	1:A:876:GLU:HG3	1.88	0.72
2:B:324:ASN:HD22	2:B:325:LEU:H	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:713:VAL:HG22	1:G:727:ILE:CG1	2.19	0.72
1:C:951:GLU:O	1:C:954:LYS:HB2	1.89	0.72
1:E:105:GLN:HG3	9:E:3514:HOH:O	1.89	0.72
1:C:579:ASP:O	1:C:583:VAL:HG23	1.90	0.72
2:H:27:VAL:HG22	2:H:131:CYS:HB2	1.70	0.72
1:G:3:LYS:HB3	1:G:330:TYR:CZ	2.25	0.72
2:F:2:ILE:HD12	2:F:3:LYS:N	2.05	0.71
1:G:130:ARG:O	1:G:134:VAL:HG23	1.90	0.71
2:B:235:GLY:HA3	2:B:374:ILE:HD11	1.71	0.71
2:B:246:ALA:HB3	2:B:247:PRO:HD3	1.73	0.71
2:H:186:LYS:O	2:H:189:GLU:HB2	1.90	0.71
1:E:679:GLN:HA	1:E:689:GLN:HE22	1.54	0.71
1:G:700:MET:SD	1:G:703:GLU:HG2	2.31	0.71
1:G:479:VAL:CG2	1:G:483:GLY:HA3	2.19	0.71
2:H:201:ALA:HB2	2:H:239:SER:HB2	1.71	0.71
2:D:215:ARG:HH11	2:D:215:ARG:HG3	1.54	0.71
1:E:482:THR:HB	9:E:3533:HOH:O	1.89	0.71
1:G:574:GLN:NE2	1:G:645:GLN:H	1.89	0.71
1:G:574:GLN:HG3	1:G:720:LEU:HD11	1.73	0.71
2:B:330:LYS:HE2	2:B:335:GLY:O	1.91	0.70
2:B:324:ASN:N	2:B:324:ASN:ND2	2.38	0.70
1:A:1017:THR:CG2	1:A:1023:ILE:HG13	2.21	0.70
1:C:678:PHE:CZ	1:C:842:VAL:HG23	2.25	0.70
2:B:27:VAL:O	2:B:78:GLN:HG2	1.91	0.70
2:F:2:ILE:HD11	9:F:2530:HOH:O	1.91	0.70
1:G:75:ARG:HH11	1:G:75:ARG:HG2	1.55	0.70
1:E:1000:HIS:CD2	1:E:1000:HIS:H	2.09	0.70
2:F:228:VAL:HA	2:F:231:MET:CE	2.22	0.70
2:F:327:VAL:HG13	2:F:337:LEU:CD1	2.20	0.70
2:H:215:ARG:HH11	2:H:215:ARG:HG3	1.55	0.70
1:C:712:LEU:HD11	1:C:752:LEU:HB3	1.74	0.70
1:C:727:ILE:HG13	1:C:909:PRO:HG3	1.74	0.70
1:E:954:LYS:HG2	1:E:980:VAL:HG21	1.74	0.70
1:G:922:ARG:HE	1:G:1061:LYS:HD3	1.56	0.70
2:D:64:GLY:HA3	2:D:94:ASN:OD1	1.92	0.70
1:G:828:VAL:HG13	1:G:842:VAL:CG2	2.22	0.70
1:E:3:LYS:HB3	1:E:330:TYR:CE1	2.27	0.69
1:G:726:GLU:HG3	1:G:737:TYR:CG	2.26	0.69
2:B:153:LEU:HA	2:B:156:MET:HE3	1.74	0.69
1:G:152:MET:CE	1:G:189:GLU:HA	2.21	0.69
2:H:8:VAL:HG22	2:H:14:GLN:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:574:GLN:HE22	1:E:645:GLN:N	1.81	0.69
1:E:951:GLU:O	1:E:954:LYS:HB2	1.92	0.69
1:G:951:GLU:HA	1:G:954:LYS:HD2	1.73	0.69
2:H:255:ILE:HG22	2:H:259:LEU:HD12	1.74	0.69
1:C:691:ALA:O	1:C:708:ILE:HG23	1.92	0.69
1:G:1017:THR:HG21	1:G:1023:ILE:HA	1.74	0.69
1:C:1027:ARG:HH21	1:C:1031:ARG:NH1	1.89	0.69
2:B:142:LEU:O	2:B:146:LYS:HG3	1.92	0.69
1:E:417:ASP:HB3	1:E:420:ALA:HB2	1.75	0.69
2:H:55:LEU:HD13	2:H:60:ILE:HD12	1.75	0.69
1:E:1017:THR:HG22	1:E:1018:SER:H	1.58	0.69
1:E:694:THR:CG2	1:E:749:PRO:HB2	2.23	0.69
2:F:334:ASP:OD1	2:F:336:THR:HG23	1.93	0.69
1:G:1029:ILE:CD1	1:G:1029:ILE:H	2.06	0.69
2:H:324:ASN:O	2:H:342:ARG:HD2	1.92	0.69
1:A:57:ASP:O	1:A:60:MET:HB2	1.94	0.68
1:E:579:ASP:O	1:E:583:VAL:HG23	1.93	0.68
1:C:473:GLU:HG2	1:C:505:LEU:CD1	2.23	0.68
2:H:171:THR:O	2:H:185:LYS:HB2	1.92	0.68
2:H:218:ILE:N	2:H:218:ILE:HD13	2.08	0.68
2:F:345:LYS:HB3	2:F:346:PRO:HD2	1.74	0.68
1:G:481:ILE:HG21	1:G:508:VAL:HG11	1.75	0.68
1:E:1017:THR:HG21	1:E:1023:ILE:HA	1.75	0.68
1:G:172:PHE:CB	1:G:200:PRO:HG2	2.23	0.68
2:H:345:LYS:HB3	2:H:346:PRO:HD2	1.75	0.68
1:C:471:ARG:HD2	9:C:4389:HOH:O	1.92	0.68
2:D:6:LEU:HD22	2:D:138:PRO:HB2	1.76	0.68
1:G:1001:ILE:HD12	1:G:1002:GLN:N	2.08	0.68
1:G:695:VAL:CG1	1:G:701:ALA:HB2	2.17	0.68
1:E:976:GLY:O	1:E:980:VAL:HG23	1.94	0.68
1:E:992:ASN:HB3	1:E:996:GLU:HB3	1.75	0.68
1:G:579:ASP:O	1:G:583:VAL:HG23	1.93	0.68
1:A:1000:HIS:CD2	1:A:1003:ASP:H	2.12	0.67
1:A:772[B]:MET:HE1	1:A:880:THR:HB	1.76	0.67
1:C:693:ALA:HB3	1:C:708:ILE:HD11	1.76	0.67
1:G:267:ALA:O	1:G:271:VAL:HG23	1.94	0.67
1:C:473:GLU:HG2	1:C:505:LEU:HD11	1.75	0.67
2:D:133:ILE:CD1	2:D:143:ALA:HB2	2.23	0.67
1:E:80:LYS:HB2	9:E:3512:HOH:O	1.94	0.67
1:G:119:THR:HG23	9:G:4481:HOH:O	1.94	0.67
1:G:770:GLY:HA2	1:G:823:ARG:NH1	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:GLU:HG2	1:E:111:PHE:CD2	2.28	0.67
1:G:704:LYS:O	1:G:707:GLU:HB2	1.94	0.67
1:G:93:GLN:HB2	1:G:174:MET:HG2	1.76	0.67
1:A:772[B]:MET:HE2	1:A:880:THR:HG22	1.74	0.67
1:G:695:VAL:HG21	1:G:701:ALA:HA	1.75	0.67
2:F:145:GLU:HG3	9:F:2667:HOH:O	1.94	0.67
1:G:1063:ILE:HD13	1:G:1068:MET:CG	2.25	0.67
1:A:46:LEU:O	1:A:46:LEU:HG	1.94	0.67
2:B:71:GLU:O	2:B:203:ARG:HG3	1.94	0.67
1:C:816:LEU:HD11	1:C:839:LEU:HD21	1.74	0.67
2:D:237:PHE:CE1	2:D:268:ILE:HD12	2.30	0.67
1:G:43:ARG:NH2	1:G:81:GLU:OE1	2.28	0.67
1:C:828:VAL:HG22	1:C:842:VAL:HG13	1.76	0.67
1:E:1017:THR:HG22	1:E:1018:SER:N	2.10	0.67
1:G:1041:ASP:HA	7:G:3920:ORN:O	1.94	0.67
1:G:640:VAL:O	1:G:647:PRO:HB2	1.94	0.67
1:A:695:VAL:CG1	1:A:701:ALA:HB2	2.22	0.67
1:G:955:GLU:HB2	9:G:4511:HOH:O	1.93	0.67
2:B:300:VAL:HG22	2:B:328:THR:O	1.95	0.66
1:C:694:THR:HG23	1:C:749:PRO:HB2	1.77	0.66
1:E:172:PHE:CB	1:E:200:PRO:HG2	2.22	0.66
1:E:43:ARG:NH2	1:E:81:GLU:OE1	2.28	0.66
1:G:1000:HIS:O	1:G:1003:ASP:HB2	1.94	0.66
1:A:1004:ARG:HH22	1:G:983:GLU:HG2	1.58	0.66
1:A:906:LEU:HD12	1:A:907:LEU:N	2.09	0.66
1:E:93:GLN:HB2	1:E:174:MET:HG2	1.76	0.66
1:G:525:VAL:HG22	1:G:548:GLU:H	1.58	0.66
2:H:83:ARG:O	2:H:83:ARG:HD2	1.95	0.66
1:A:1000:HIS:HD2	1:A:1003:ASP:H	1.42	0.66
1:C:50:ASN:ND2	1:C:53:THR:HG23	2.11	0.66
1:E:684:ARG:HH11	1:E:684:ARG:HG3	1.60	0.66
2:H:197:TYR:HB3	2:H:199:PHE:CZ	2.31	0.66
1:G:850:VAL:HB	1:G:851:PRO:HD3	1.76	0.66
1:A:172:PHE:CB	1:A:200:PRO:HG2	2.19	0.66
2:B:306:MET:HB2	2:B:362:ASP:HB3	1.77	0.66
1:G:300:MET:O	1:G:300:MET:HG3	1.95	0.66
1:E:403:GLU:CD	1:E:646:THR:HG21	2.15	0.66
1:G:812:GLN:O	1:G:816:LEU:HG	1.95	0.66
2:B:285:LYS:HG3	2:B:314:PHE:CE1	2.31	0.66
1:C:740:THR:O	1:C:744:VAL:HG13	1.96	0.66
2:F:197:TYR:HB3	2:F:199:PHE:CZ	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:NH2	1:A:81:GLU:OE1	2.28	0.66
1:C:3:LYS:NZ	9:C:4567:HOH:O	2.29	0.66
1:G:676:GLU:HB2	1:G:694:THR:HG21	1.76	0.66
1:A:51:PRO:O	1:A:855:LYS:NZ	2.29	0.66
1:A:863:LYS:HE2	9:A:1712:HOH:O	1.95	0.66
1:E:716:PRO:HD2	1:E:725:MET:HG2	1.78	0.66
1:G:1001:ILE:O	1:G:1005:ILE:HG13	1.96	0.66
1:G:71:TRP:CZ3	1:G:105:GLN:HG2	2.31	0.66
1:G:694:THR:HG23	1:G:749:PRO:CB	2.24	0.66
2:F:324:ASN:ND2	2:F:324:ASN:N	2.31	0.65
1:G:872:LYS:HG2	1:G:877:GLN:HG3	1.77	0.65
1:G:1063:ILE:HD13	1:G:1068:MET:HG3	1.78	0.65
1:G:906:LEU:O	1:G:912:ARG:NH2	2.29	0.65
1:A:35:LYS:O	1:A:39:GLU:HG3	1.96	0.65
2:B:57:TYR:CD1	2:B:58:PRO:HD2	2.32	0.65
1:E:313:LYS:NZ	1:E:603:PRO:O	2.29	0.65
1:A:101:GLU:OE1	1:A:104:ARG:NE	2.30	0.65
2:B:269:CYS:O	2:B:272:HIS:HB3	1.96	0.65
1:C:906:LEU:O	1:C:912:ARG:NH2	2.29	0.65
2:D:327:VAL:HG13	2:D:337:LEU:HD11	1.79	0.65
2:F:193:HIS:N	2:F:234:ASP:OD2	2.29	0.65
1:G:1001:ILE:HD12	1:G:1002:GLN:H	1.60	0.65
2:B:350:PHE:HD2	2:B:354:PRO:HD3	1.61	0.65
2:D:150:PHE:CD1	2:D:151:PRO:HD2	2.30	0.65
1:G:810:ARG:HG3	1:G:810:ARG:HH11	1.60	0.65
2:F:261:THR:OG1	2:F:263:ILE:HG13	1.97	0.65
1:A:583:VAL:HG12	1:A:587:LEU:HD22	1.79	0.65
2:B:264:PRO:HB3	2:B:373:LEU:HB3	1.79	0.65
1:E:574:GLN:NE2	1:E:645:GLN:HB2	2.12	0.65
1:G:367:PHE:CE1	1:G:912:ARG:HG2	2.31	0.65
1:C:742:VAL:HA	1:C:745:SER:HB2	1.79	0.65
1:A:1017:THR:HG21	1:A:1023:ILE:HG13	1.79	0.65
1:C:784:GLN:N	1:C:784:GLN:HE21	1.91	0.65
1:G:853:VAL:HG12	1:G:861:LEU:HD11	1.79	0.65
1:A:731:GLU:O	1:A:734:LEU:HB3	1.97	0.65
1:C:998:ARG:NH1	1:C:998:ARG:HG2	2.08	0.65
1:E:569:PRO:O	1:E:571:ARG:NH1	2.30	0.64
1:G:168:ILE:HG23	1:G:204:LEU:HD22	1.78	0.64
1:G:667:ASP:OD1	1:G:677:ARG:NH2	2.30	0.64
1:A:410:ASP:OD2	1:A:504:LYS:NZ	2.30	0.64
1:E:289:ASN:HB3	1:E:292:ASN:OD1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:500:ALA:O	1:E:504:LYS:HG3	1.97	0.64
1:G:679:GLN:HG3	1:G:689:GLN:NE2	2.13	0.64
1:G:702:VAL:HG21	1:G:735:ARG:NH1	2.13	0.64
2:H:23:THR:HG23	2:H:134:ALA:O	1.97	0.64
1:A:563:MET:CE	1:A:635:PRO:HG3	2.28	0.64
2:B:38:GLY:O	2:B:42:ILE:HD12	1.98	0.64
1:G:905:PRO:HB2	1:G:1040:TYR:OH	1.97	0.64
2:H:228:VAL:O	2:H:231:MET:HG3	1.97	0.64
1:A:906:LEU:O	1:A:912[A]:ARG:NH2	2.26	0.64
1:C:336:MET:HB3	1:C:342:GLY:HA2	1.79	0.64
1:G:129:ARG:HB3	1:G:205:LEU:HD22	1.78	0.64
1:A:698:ILE:O	1:A:702:VAL:HG23	1.97	0.64
1:C:822:VAL:O	1:C:823:ARG:HD3	1.97	0.64
1:C:964:LEU:O	1:C:969:PHE:HB2	1.97	0.64
1:E:1004:ARG:NH1	1:E:1009[A]:GLU:OE2	2.30	0.64
1:E:910:GLU:O	1:E:912:ARG:NH1	2.31	0.64
2:H:71:GLU:O	2:H:203:ARG:HG3	1.98	0.64
1:C:953:ASP:HB3	1:C:1044:LEU:CD2	2.20	0.64
1:E:1004:ARG:HD3	1:E:1009[B]:GLU:OE2	1.98	0.64
1:C:944:ARG:NH1	1:C:972:ASP:OD1	2.30	0.63
1:E:722:GLY:N	6:E:2910:ANP:O1B	2.29	0.63
1:E:403:GLU:HG3	1:E:569:PRO:HD2	1.80	0.63
1:E:403:GLU:OE2	1:E:646:THR:HG21	1.99	0.63
1:G:89:THR:O	1:G:304:VAL:HG22	1.98	0.63
1:C:698:ILE:O	1:C:702:VAL:HG23	1.99	0.63
1:C:922:ARG:HH21	1:C:1061:LYS:HB3	1.63	0.63
1:E:110:GLU:HG2	1:E:111:PHE:CE2	2.34	0.63
1:G:1001:ILE:O	1:G:1005:ILE:N	2.29	0.63
1:G:1066:GLN:HB2	9:G:4018:HOH:O	1.99	0.63
1:G:110:GLU:HG2	1:G:111:PHE:CD1	2.34	0.63
2:H:195:VAL:HG23	2:H:233:PRO:HB3	1.81	0.63
1:E:71:TRP:CZ3	1:E:105:GLN:HG2	2.33	0.63
2:H:269:CYS:O	2:H:272:HIS:HB3	1.98	0.63
1:A:27:ASP:OD1	1:A:53:THR:HB	1.98	0.63
1:E:130:ARG:O	1:E:134:VAL:HG23	1.99	0.63
1:E:166:CYS:C	1:E:167:ILE:HD12	2.19	0.63
1:E:184:ASN:OD1	1:E:186:GLU:HB3	1.99	0.63
2:F:199:PHE:O	2:F:241:GLY:HA3	1.98	0.63
1:C:678:PHE:CE1	1:C:842:VAL:HG23	2.32	0.63
2:H:327:VAL:HG13	2:H:337:LEU:CD1	2.26	0.63
1:A:417:ASP:OD2	1:A:423:LYS:NZ	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:224:SER:O	2:F:228:VAL:HG23	1.98	0.63
1:A:175:GLY:N	6:A:1083:ANP:O1G	2.26	0.62
2:H:104:ARG:HG2	2:H:105:HIS:CD2	2.34	0.62
1:A:368:ALA:N	9:A:1521:HOH:O	2.31	0.62
1:C:569:PRO:O	1:C:571:ARG:NH1	2.31	0.62
1:C:64:THR:O	1:C:1065:VAL:HG23	1.98	0.62
2:F:254:ALA:O	2:F:257:LYS:HB2	1.98	0.62
1:G:403:GLU:HG3	1:G:569:PRO:HD2	1.82	0.62
2:B:273:GLN:O	2:B:277:LEU:HG	1.99	0.62
1:C:278:GLU:HG2	9:C:4561:HOH:O	1.99	0.62
1:A:39:GLU:OE2	9:A:1380:HOH:O	2.16	0.62
1:C:722:GLY:N	6:C:1910:ANP:O1B	2.30	0.62
1:C:951:GLU:HA	1:C:954:LYS:CD	2.26	0.62
1:A:259:LYS:HD3	2:B:175:TRP:CE3	2.35	0.62
1:E:258:ASP:O	1:E:262:GLN:HG2	1.99	0.62
1:A:313:LYS:HE2	1:A:608:THR:O	1.99	0.62
1:A:375:THR:OG1	1:A:376:THR:N	2.32	0.62
1:G:994:VAL:HG22	1:G:1000:HIS:ND1	2.15	0.62
1:E:168:ILE:HD13	1:E:191:ILE:CG2	2.30	0.62
1:E:300:MET:O	1:E:300:MET:HG3	1.99	0.62
1:C:659:VAL:HG13	1:C:660:PRO:HD2	1.82	0.62
1:C:9:SER:OG	1:C:83:PRO:HA	2.00	0.62
1:E:152:MET:O	1:E:156:LEU:HG	2.00	0.62
1:G:563:MET:CE	1:G:635:PRO:HG3	2.30	0.62
1:E:1019:GLY:O	1:E:1023:ILE:HD12	2.00	0.61
1:G:712:LEU:HG	1:G:753:ASP:O	2.00	0.61
1:A:583:VAL:HG12	1:A:587:LEU:CD2	2.30	0.61
2:B:299:ASP:OD2	2:B:302:LYS:HD2	2.00	0.61
1:G:147:GLY:CA	1:G:158:VAL:HG11	2.28	0.61
1:A:868:VAL:HA	1:A:872:LYS:O	2.00	0.61
2:B:345:LYS:HB3	2:B:346:PRO:CD	2.31	0.61
1:C:1017:THR:HG21	1:C:1023:ILE:CA	2.28	0.61
1:G:675:ARG:HG3	1:G:717:SER:OG	2.01	0.61
1:C:759:ALA:O	1:C:784:GLN:HB2	2.01	0.61
1:G:767:ILE:HG23	1:G:824:GLY:O	2.01	0.61
2:H:324:ASN:HA	2:H:343:THR:OG1	2.00	0.61
1:E:147:GLY:CA	1:E:158:VAL:HG11	2.29	0.61
1:E:946:LEU:C	1:E:947:LEU:HD12	2.21	0.61
1:G:153:GLU:O	1:G:153:GLU:HG3	1.99	0.61
1:A:1017:THR:HG22	1:A:1018:SER:N	2.15	0.61
1:C:574:GLN:NE2	1:C:720:LEU:HD21	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:ARG:O	2:D:120:ARG:HG3	2.01	0.61
1:E:3:LYS:HB3	1:E:330:TYR:CZ	2.35	0.61
2:F:174:SER:HB2	2:F:211:ASP:OD2	1.99	0.61
1:A:62:ASP:OD1	1:A:62:ASP:N	2.31	0.61
2:F:272:HIS:HA	2:F:349:SER:HB2	1.81	0.61
1:G:318:PRO:HG3	1:G:610:TYR:OH	2.00	0.61
1:C:953:ASP:CB	1:C:1044:LEU:HD22	2.23	0.61
1:C:873:SER:O	1:C:877:GLN:HG3	2.00	0.61
1:C:941:LYS:NZ	1:C:1056:ALA:O	2.34	0.61
2:F:218:ILE:HD13	2:F:218:ILE:N	2.16	0.61
2:F:185:LYS:HG2	2:F:189:GLU:OE1	2.00	0.61
1:G:685:LEU:HD11	1:G:819:GLU:HB2	1.81	0.61
1:G:679:GLN:HA	1:G:689:GLN:HE22	1.66	0.61
1:C:892:GLU:OE2	7:C:1920:ORN:NE	2.30	0.61
2:D:168:TYR:CE2	2:D:218:ILE:HG13	2.35	0.61
2:D:48:TYR:HA	2:D:51:GLN:HE21	1.65	0.61
1:E:375:THR:OG1	1:E:376:THR:N	2.30	0.61
2:F:259:LEU:HD13	2:F:342:ARG:NH1	2.16	0.61
1:G:181:ILE:HD11	1:G:376:THR:HG23	1.81	0.61
1:A:482:THR:HB	9:A:1595:HOH:O	2.00	0.60
2:F:286:MET:CE	2:F:289:GLY:HA2	2.27	0.60
1:G:190:GLU:O	1:G:194:ARG:NH1	2.33	0.60
1:G:710:TYR:HB3	1:G:711:PRO:HA	1.83	0.60
1:A:50:ASN:ND2	1:A:53:THR:HG23	2.16	0.60
1:C:686:LYS:HA	9:C:4403:HOH:O	2.01	0.60
2:H:227:ASP:O	2:H:230:LYS:HB2	2.01	0.60
1:C:956:ARG:NH2	9:C:4548:HOH:O	2.33	0.60
2:F:194:VAL:N	2:F:215:ARG:O	2.30	0.60
1:E:944:ARG:NH1	1:E:972:ASP:OD1	2.29	0.60
2:H:249:ASP:OD1	2:H:250:TYR:N	2.30	0.60
2:F:214:CYS:SG	2:F:371:ILE:HD11	2.41	0.60
1:G:340:THR:O	1:G:343:ARG:NE	2.35	0.60
1:G:471:ARG:HD2	9:G:4379:HOH:O	2.01	0.60
2:B:255:ILE:HA	2:B:258:PHE:HD2	1.67	0.60
1:C:403:GLU:OE1	1:C:646:THR:HG21	2.00	0.60
1:E:1000:HIS:CD2	1:E:1003:ASP:H	2.16	0.60
1:A:42:TYR:N	9:A:1112:HOH:O	2.35	0.60
2:D:324:ASN:N	2:D:324:ASN:ND2	2.32	0.60
1:E:150:HIS:CD2	1:E:203:GLU:HB2	2.37	0.60
2:H:253:THR:HG22	2:H:254:ALA:N	2.16	0.60
2:B:326:ARG:O	2:B:326:ARG:HG3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:504:LYS:NZ	9:G:4453:HOH:O	2.32	0.60
1:G:695:VAL:HG12	1:G:738:PHE:CZ	2.37	0.60
2:B:174:SER:HB2	2:B:211:ASP:OD2	2.02	0.60
2:D:199:PHE:O	2:D:241:GLY:HA3	2.01	0.60
1:C:990:LEU:HD13	1:E:990:LEU:HD22	1.83	0.60
1:G:1:MET:CG	1:G:2:PRO:HD2	2.30	0.60
2:H:152:GLY:O	2:H:156:MET:HE3	2.02	0.60
2:B:215:ARG:HG3	2:B:215:ARG:HH11	1.67	0.59
2:B:228:VAL:HG12	2:B:229:LEU:N	2.16	0.59
1:C:694:THR:HG23	1:C:749:PRO:CB	2.32	0.59
1:C:883:VAL:O	1:C:884:ILE:HD13	2.02	0.59
1:E:168:ILE:CD1	1:E:191:ILE:HG21	2.32	0.59
1:G:479:VAL:HG23	1:G:483:GLY:HA3	1.84	0.59
1:A:799:TYR:CD2	1:A:800:THR:HG22	2.37	0.59
1:C:946:LEU:C	1:C:947:LEU:HD12	2.22	0.59
1:G:685:LEU:HD11	1:G:819:GLU:HG2	1.83	0.59
1:C:400:ARG:HD3	9:C:4133:HOH:O	2.02	0.59
1:E:695:VAL:CG1	1:E:701:ALA:HB2	2.24	0.59
1:A:722:GLY:C	1:A:725:MET:HG3	2.23	0.59
2:B:324:ASN:ND2	2:B:325:LEU:N	2.50	0.59
1:C:807:ASP:OD1	1:C:810:ARG:NH1	2.34	0.59
1:G:631:ARG:NH2	9:G:4493:HOH:O	2.33	0.59
1:C:1048:PHE:O	1:C:1052:MET:HG3	2.03	0.59
1:E:15:ALA:HB3	5:E:2980:CL:CL	2.40	0.59
1:E:403:GLU:OE1	1:E:646:THR:HG21	2.02	0.59
2:F:133:ILE:HG22	2:F:138:PRO:HB3	1.83	0.59
1:G:1001:ILE:CG1	1:G:1002:GLN:H	2.15	0.59
1:G:1017:THR:HG22	1:G:1018:SER:N	2.18	0.59
1:G:40:GLU:OE2	1:G:325:LYS:HE2	2.01	0.59
1:G:333:ASP:N	1:G:333:ASP:OD1	2.31	0.59
1:C:698:ILE:N	1:C:698:ILE:HD12	2.18	0.59
1:E:757:ASP:O	1:E:833:LYS:NZ	2.30	0.59
2:F:116:ARG:O	2:F:120:ARG:HG3	2.03	0.59
1:G:118:ALA:HA	9:G:4481:HOH:O	2.03	0.59
1:E:906:LEU:O	1:E:912:ARG:NH2	2.36	0.59
1:G:1001:ILE:CD1	1:G:1002:GLN:H	2.16	0.59
8:A:1086:NET:H82	8:A:1086:NET:C6	2.27	0.59
1:C:671:ARG:NH2	1:C:819:GLU:O	2.36	0.59
1:E:700:MET:O	1:E:704:LYS:HB2	2.03	0.59
1:A:967:GLN:HG2	1:A:1054:LEU:HD13	1.85	0.59
1:E:472:LEU:O	1:E:476:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:LYS:HE2	9:G:4301:HOH:O	2.02	0.59
1:G:685:LEU:HD11	1:G:819:GLU:CG	2.33	0.59
1:G:574:GLN:CG	1:G:720:LEU:HD11	2.33	0.59
1:A:699:GLU:OE2	1:A:735:ARG:NH2	2.34	0.59
2:B:345:LYS:HB3	2:B:346:PRO:HD2	1.85	0.59
2:D:370:PHE:O	2:D:374:ILE:HG13	2.03	0.59
1:A:1000:HIS:HD2	1:A:1003:ASP:HB2	1.66	0.58
1:A:993:LYS:CB	1:A:996:GLU:HG3	2.32	0.58
2:B:144:LEU:O	2:B:144:LEU:HD12	2.03	0.58
1:C:18:ILE:HG23	1:C:23:ALA:HA	1.85	0.58
1:C:6:ASP:OD1	1:C:6:ASP:N	2.33	0.58
1:C:820:LEU:O	1:C:821:GLN:HB2	2.00	0.58
1:E:172:PHE:HB2	1:E:200:PRO:HD2	1.83	0.58
2:F:272:HIS:HA	2:F:349:SER:CB	2.32	0.58
1:G:148:ILE:HG22	1:G:150:HIS:CE1	2.38	0.58
1:G:313:LYS:NZ	1:G:603:PRO:O	2.35	0.58
1:A:166:CYS:C	1:A:167:ILE:HD12	2.23	0.58
1:A:166:CYS:HB2	1:A:207:ASP:O	2.02	0.58
1:E:683:GLU:OE1	1:E:683:GLU:HA	2.03	0.58
1:E:222:ARG:NH2	1:E:226:ASP:OD1	2.35	0.58
1:E:991:VAL:HG21	1:E:1001:ILE:CG2	2.33	0.58
1:G:240:MET:HE3	6:G:3900:ANP:C4	2.34	0.58
1:G:731:GLU:CD	1:G:732:ALA:H	2.06	0.58
1:G:403:GLU:OE1	1:G:646:THR:HG21	2.03	0.58
1:G:715:ARG:HA	1:G:725:MET:HG2	1.85	0.58
1:A:101:GLU:O	1:A:101:GLU:HG3	2.03	0.58
2:B:267:GLY:O	2:B:349:SER:HB2	2.03	0.58
2:B:48:TYR:O	2:B:51:GLN:HB2	2.04	0.58
1:C:337:ASN:OD1	9:C:4485:HOH:O	2.17	0.58
2:D:261:THR:OG1	2:D:263:ILE:HG13	2.04	0.58
2:H:277:LEU:HD23	2:H:281:ALA:O	2.03	0.58
2:H:7:LEU:HB3	2:H:15:PHE:HB2	1.85	0.58
1:A:784:GLN:HE21	1:A:784:GLN:N	2.00	0.58
1:E:17:PRO:HG3	1:E:917:VAL:CG1	2.33	0.58
1:G:1007:ASN:HB2	1:G:1009:GLU:HG3	1.86	0.58
2:H:193:HIS:O	2:H:234:ASP:HB2	2.04	0.58
1:A:953:ASP:HB3	1:A:1044:LEU:HD22	1.86	0.58
2:B:324:ASN:H	2:B:324:ASN:ND2	1.99	0.58
1:E:694:THR:HG23	1:E:749:PRO:HB2	1.84	0.58
2:F:345:LYS:HB3	2:F:346:PRO:CD	2.32	0.58
1:G:573:GLY:O	1:G:720:LEU:HD13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:ARG:HH11	2:B:215:ARG:CG	2.17	0.58
1:E:574:GLN:HE21	1:E:720:LEU:CD2	2.13	0.58
2:H:78:GLN:NE2	9:H:3324:HOH:O	2.36	0.58
2:D:158:LEU:HD23	2:D:161:GLU:HG3	1.86	0.57
1:G:174:MET:HE3	1:G:303:ARG:CZ	2.34	0.57
1:A:22:GLN:CD	8:A:1086:NET:H41	2.25	0.57
2:B:218:ILE:HD13	2:B:218:ILE:N	2.18	0.57
2:B:228:VAL:O	2:B:231:MET:HG3	2.03	0.57
8:C:1950:NET:H42	8:C:1950:NET:C2	2.27	0.57
1:A:3:LYS:HB3	1:A:330:TYR:CZ	2.39	0.57
1:C:783:GLU:N	1:C:783:GLU:OE1	2.34	0.57
2:D:208:MET:O	2:D:212:ARG:HG3	2.05	0.57
2:D:368:ASP:HB2	9:D:1592:HOH:O	2.05	0.57
1:G:166:CYS:C	1:G:167:ILE:HD12	2.23	0.57
2:B:190:LEU:HB2	2:B:215:ARG:HB3	1.86	0.57
1:C:110:GLU:HG2	1:C:110:GLU:O	2.03	0.57
1:C:675:ARG:HD2	1:C:716:PRO:O	2.04	0.57
1:G:151:THR:O	1:G:155:ALA:N	2.29	0.57
1:A:25:GLU:N	1:A:25:GLU:OE1	2.33	0.57
1:A:814:GLN:NE2	9:A:1315:HOH:O	2.36	0.57
1:C:1019:GLY:O	1:C:1023:ILE:HD12	2.04	0.57
1:G:784:GLN:HE22	1:G:1043:THR:HB	1.69	0.57
1:A:574:GLN:HE21	1:A:720:LEU:HD21	1.70	0.57
1:G:1029:ILE:N	1:G:1029:ILE:HD12	2.11	0.57
1:G:475:LYS:O	1:G:479:VAL:HG13	2.04	0.57
1:A:704:LYS:O	1:A:707:GLU:HB2	2.05	0.57
2:D:174:SER:O	2:D:182:PRO:HD3	2.03	0.57
1:E:1004:ARG:NH1	1:E:1009[B]:GLU:OE2	2.31	0.57
2:F:139:ASP:OD2	2:F:142:LEU:HB2	2.04	0.57
1:G:10:ILE:HD11	1:G:42:TYR:CD1	2.40	0.57
1:G:82:ARG:N	1:G:83:PRO:HD3	2.18	0.57
2:H:201:ALA:HA	2:H:240:ASN:OD1	2.03	0.57
1:A:946:LEU:C	1:A:947:LEU:HD12	2.24	0.57
1:E:471:ARG:HD2	9:E:3384:HOH:O	2.03	0.57
1:A:76:LYS:HD2	1:A:1059:THR:O	2.04	0.57
1:A:959:ASP:O	1:A:963:LYS:HG3	2.05	0.57
2:B:195:VAL:HG23	2:B:233:PRO:HB3	1.87	0.57
2:F:133:ILE:HD12	2:F:143:ALA:HB2	1.85	0.57
1:G:822:VAL:C	1:G:823:ARG:HG2	2.25	0.57
1:G:628:GLU:OE1	9:G:4185:HOH:O	2.17	0.56
1:G:820:LEU:O	1:G:821:GLN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:156:MET:HG2	2:H:158:LEU:HG	1.87	0.56
2:B:225:ALA:O	2:B:228:VAL:HB	2.05	0.56
1:E:236:ASN:OD1	1:E:244:THR:HG22	2.04	0.56
1:G:1004:ARG:O	1:G:1009:GLU:HB2	2.04	0.56
1:G:683:GLU:OE1	1:G:683:GLU:HA	2.05	0.56
1:A:164:PHE:HB3	1:A:165:PRO:HA	1.87	0.56
1:C:560:GLU:OE2	1:C:636:LYS:HE3	2.05	0.56
1:C:868:VAL:HG23	1:C:877:GLN:NE2	2.21	0.56
1:E:164:PHE:HB3	1:E:165:PRO:HA	1.88	0.56
1:E:670:ASP:HB3	1:E:677:ARG:HH21	1.69	0.56
2:F:306:MET:HB3	2:F:362:ASP:HB3	1.88	0.56
1:E:675:ARG:NH2	1:E:841:GLU:OE1	2.39	0.56
2:F:64:GLY:HA3	2:F:94:ASN:OD1	2.05	0.56
2:H:345:LYS:HB3	2:H:346:PRO:CD	2.35	0.56
1:A:975:HIS:HD1	1:G:975:HIS:HD1	0.70	0.56
2:F:191:PRO:HD2	2:F:213:GLY:O	2.05	0.56
2:H:364:ALA:N	2:H:365:PRO:HD2	2.20	0.56
1:C:717:SER:HB3	1:C:748:ALA:HB3	1.88	0.56
1:E:941:LYS:NZ	1:E:1056:ALA:O	2.30	0.56
1:E:684:ARG:HD3	1:E:819:GLU:OE2	2.04	0.56
1:G:157:ALA:O	1:G:160:ALA:HB3	2.06	0.56
1:G:194:ARG:HB2	1:G:194:ARG:NH1	2.20	0.56
1:G:579:ASP:OD1	1:G:607:SER:HB3	2.06	0.56
1:A:26:PHE:O	1:A:30:GLY:N	2.30	0.56
1:E:1029:ILE:HD12	1:E:1029:ILE:N	2.20	0.56
1:E:727:ILE:HG13	1:E:909:PRO:HG3	1.86	0.56
1:A:475:LYS:HE2	1:A:488:PHE:CE2	2.40	0.56
1:A:559:ARG:NH2	9:A:1677:HOH:O	2.28	0.56
2:D:355:GLU:N	2:D:355:GLU:OE1	2.33	0.56
1:G:872:LYS:HG2	1:G:877:GLN:CG	2.36	0.56
1:A:583:VAL:O	1:A:587:LEU:HD22	2.05	0.56
1:A:51:PRO:HG3	1:A:918:MET:HB2	1.86	0.56
1:C:975:HIS:HE2	1:E:992:ASN:ND2	2.04	0.56
1:E:365:GLU:HG2	1:E:366:LYS:N	2.19	0.56
2:F:48:TYR:HA	2:F:51:GLN:HE21	1.70	0.56
1:G:1017:THR:HG22	1:G:1023:ILE:HG13	1.86	0.56
1:G:151:THR:H	1:G:154:GLU:HB2	1.71	0.56
2:H:254:ALA:O	2:H:257:LYS:HB2	2.05	0.56
2:H:272:HIS:HA	2:H:349:SER:HB2	1.87	0.56
2:F:59:HIS:ND1	2:F:84:ASP:OD2	2.34	0.56
1:G:167:ILE:HD12	1:G:167:ILE:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:336:MET:HB3	1:G:342:GLY:HA2	1.88	0.56
2:H:255:ILE:O	2:H:259:LEU:HD12	2.06	0.56
1:A:1061:LYS:HG3	9:A:1389:HOH:O	2.06	0.56
1:E:138:LYS:NZ	1:E:274:GLU:OE2	2.39	0.56
1:G:859:VAL:O	1:G:861:LEU:HG	2.05	0.56
1:A:761:GLU:HB3	1:A:781:HIS:ND1	2.21	0.55
2:D:306:MET:HB2	2:D:362:ASP:HB3	1.87	0.55
2:F:171:THR:O	2:F:185:LYS:HB2	2.05	0.55
2:F:227:ASP:O	2:F:231:MET:HE2	2.06	0.55
1:G:1017:THR:CG2	1:G:1023:ILE:HG13	2.36	0.55
1:G:930:LYS:NZ	1:G:1058:ALA:O	2.37	0.55
1:G:223:ASP:CG	1:G:227:ASN:HB2	2.26	0.55
1:G:671:ARG:HG2	1:G:677:ARG:CZ	2.36	0.55
1:G:667:ASP:CG	1:G:677:ARG:HH22	2.10	0.55
1:G:949:VAL:O	1:G:954:LYS:HE3	2.06	0.55
2:H:26:ALA:O	2:H:131:CYS:HA	2.06	0.55
1:A:1060:GLU:HB3	9:A:1350:HOH:O	2.05	0.55
1:A:196:LEU:HG	1:A:204:LEU:HD11	1.88	0.55
1:A:534:ALA:O	2:B:123:ARG:HD3	2.06	0.55
2:D:222:GLN:H	2:D:222:GLN:HE21	1.55	0.55
1:E:579:ASP:OD2	1:E:605:THR:HB	2.05	0.55
1:G:259:LYS:HE2	2:H:69:ASP:OD1	2.06	0.55
1:A:26:PHE:HA	1:A:29:SER:HB2	1.87	0.55
1:E:172:PHE:HB3	1:E:200:PRO:CG	2.26	0.55
2:F:324:ASN:HA	2:F:343:THR:OG1	2.06	0.55
1:G:1:MET:HG3	1:G:2:PRO:CD	2.31	0.55
1:A:1001:ILE:HD13	1:A:1029:ILE:HG13	1.88	0.55
1:A:922:ARG:HH21	1:A:1061:LYS:HB3	1.71	0.55
2:B:244:ASP:OD1	2:B:245:PRO:HD2	2.06	0.55
1:C:313:LYS:NZ	1:C:603:PRO:O	2.40	0.55
1:E:998:ARG:CG	1:E:998:ARG:HH11	2.19	0.55
1:G:1001:ILE:CD1	1:G:1002:GLN:HB2	2.37	0.55
2:H:275:LEU:HD23	2:H:349:SER:OG	2.07	0.55
2:D:285:LYS:HG3	2:D:314:PHE:CE2	2.42	0.55
1:G:784:GLN:H	1:G:784:GLN:HE21	1.55	0.55
1:A:654:LEU:O	1:A:659:VAL:HG23	2.07	0.55
1:A:588:ALA:HB2	1:A:863:LYS:HG2	1.87	0.55
1:C:225:ASN:ND2	1:C:331:THR:HG21	2.22	0.55
1:C:343:ARG:NH2	1:C:539:ASP:OD2	2.40	0.55
1:C:990:LEU:HD23	1:E:979:ILE:HG12	1.87	0.55
1:G:1017:THR:HG22	1:G:1018:SER:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:698:ILE:O	1:G:702:VAL:N	2.30	0.55
1:G:93:GLN:HB2	1:G:174:MET:CG	2.36	0.55
2:H:255:ILE:HG22	2:H:259:LEU:HD11	1.88	0.55
2:H:277:LEU:HD21	2:H:283:THR:HG23	1.89	0.55
2:H:6:LEU:HD11	2:H:8:VAL:HG23	1.89	0.55
1:A:806:GLN:HA	1:A:809:MET:HE2	1.89	0.55
1:C:698:ILE:H	1:C:698:ILE:HD12	1.72	0.55
1:G:802:SER:O	1:G:805:ILE:HG22	2.07	0.55
2:H:193:HIS:HA	2:H:215:ARG:HG2	1.89	0.55
2:H:236:ILE:HB	2:H:265:VAL:HG22	1.88	0.55
1:A:1000:HIS:CD2	1:A:1003:ASP:HB2	2.42	0.55
1:C:690:PRO:HG3	1:C:756:LEU:HD11	1.89	0.55
1:E:169:ARG:O	1:E:205:LEU:N	2.38	0.55
1:E:712:LEU:C	1:E:712:LEU:HD23	2.28	0.55
1:G:152:MET:HE1	1:G:192:CYS:HB2	1.88	0.55
1:C:751:LEU:O	1:C:752:LEU:HD12	2.07	0.54
1:C:922:ARG:NH2	1:C:1061:LYS:HB3	2.21	0.54
2:D:226:GLU:O	2:D:230:LYS:HG3	2.07	0.54
1:E:930:LYS:HE3	9:E:3016:HOH:O	2.07	0.54
1:C:574:GLN:NE2	1:C:645:GLN:HB2	2.22	0.54
2:D:8:VAL:HG22	2:D:14:GLN:HG2	1.89	0.54
1:A:4:ARG:CZ	1:A:7:ILE:HD11	2.37	0.54
1:C:678:PHE:O	1:C:682:VAL:HG23	2.06	0.54
1:E:75:ARG:HG2	1:E:75:ARG:HH11	1.72	0.54
2:F:6:LEU:HD22	2:F:138:PRO:HB2	1.89	0.54
1:G:782:ILE:N	1:G:782:ILE:HD12	2.22	0.54
1:A:339:ILE:CD1	1:A:530:ASP:HA	2.37	0.54
2:D:33:ASN:OD1	2:D:35:SER:HB2	2.07	0.54
1:G:674:ASP:O	1:G:677:ARG:HB2	2.07	0.54
2:H:276:ALA:O	2:H:281:ALA:HB3	2.08	0.54
1:C:1051:ALA:O	1:C:1054:LEU:HB2	2.07	0.54
1:E:1004:ARG:HD3	1:E:1009[A]:GLU:OE2	2.06	0.54
1:E:168:ILE:HD11	1:E:182:ALA:HB2	1.90	0.54
2:B:350:PHE:CG	2:B:366:LEU:HD22	2.42	0.54
1:C:1027:ARG:NE	1:C:1031:ARG:HD3	2.22	0.54
1:C:43:ARG:NH2	1:C:81:GLU:OE1	2.29	0.54
1:C:956:ARG:NH2	1:C:1048:PHE:CD2	2.75	0.54
1:E:344:THR:HB	1:E:345:PRO:HD2	1.90	0.54
1:A:82:ARG:N	1:A:83:PRO:HD3	2.23	0.54
1:E:950:ARG:HD3	9:E:3431:HOH:O	2.06	0.54
1:G:676:GLU:O	1:G:680:HIS:ND1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ASP:N	1:G:6:ASP:OD1	2.36	0.54
1:G:70:HIS:CE1	1:G:72:GLU:HB2	2.42	0.54
1:C:761:GLU:HG2	1:C:781:HIS:CE1	2.42	0.54
1:C:890:VAL:HG23	1:C:927:ALA:HB1	1.89	0.54
1:E:264:MET:O	1:E:267:ALA:HB3	2.08	0.54
1:E:583:VAL:HG12	1:E:587:LEU:CD2	2.38	0.54
1:E:715:ARG:NH1	1:E:753:ASP:OD2	2.40	0.54
1:G:922:ARG:NE	1:G:1061:LYS:HD3	2.21	0.54
1:C:159:ALA:HB2	1:C:188:PHE:CZ	2.42	0.54
1:G:509:ARG:HB2	1:G:509:ARG:HH11	1.72	0.54
1:G:588:ALA:HB2	1:G:863:LYS:HG2	1.90	0.54
1:A:1036:TYR:C	1:A:1037:LYS:HG2	2.28	0.54
1:A:693:ALA:HB3	1:A:708:ILE:HD11	1.90	0.54
2:B:324:ASN:HA	2:B:343:THR:OG1	2.07	0.54
1:A:345:PRO:HG3	2:B:332:LEU:HB3	1.89	0.54
1:E:159:ALA:HB2	1:E:188:PHE:CZ	2.43	0.54
1:G:784:GLN:NE2	1:G:784:GLN:H	2.06	0.54
1:G:839:LEU:HD12	1:G:840:ILE:N	2.23	0.54
1:A:577:GLU:H	1:A:577:GLU:CD	2.11	0.53
1:C:868:VAL:HG23	1:C:877:GLN:HE22	1.73	0.53
1:E:675:ARG:HG3	1:E:717:SER:OG	2.08	0.53
2:F:201:ALA:CB	2:F:239:SER:HB2	2.36	0.53
1:G:741:ALA:O	1:G:745:SER:HB2	2.08	0.53
1:A:956:ARG:HB2	1:A:1044:LEU:HD23	1.90	0.53
1:A:527:LYS:HB2	1:A:544:TYR:CZ	2.42	0.53
1:A:74:VAL:O	1:A:78:ILE:HG13	2.08	0.53
2:B:133:ILE:HD12	2:B:143:ALA:HB2	1.89	0.53
2:B:324:ASN:O	2:B:342:ARG:HD2	2.08	0.53
1:E:26:PHE:HB2	5:E:2980:CL:CL	2.46	0.53
1:E:583:VAL:O	1:E:587:LEU:HD22	2.07	0.53
1:E:967:GLN:O	1:E:967:GLN:HG3	2.07	0.53
1:C:35:LYS:O	1:C:39:GLU:HG3	2.09	0.53
1:C:892:GLU:HG3	1:C:893:VAL:N	2.23	0.53
2:F:186:LYS:O	2:F:189:GLU:N	2.30	0.53
1:A:554:ASN:N	1:A:555:PRO:HD3	2.23	0.53
2:B:135:GLY:O	2:B:138:PRO:HD3	2.08	0.53
2:B:225:ALA:HA	2:B:258:PHE:CZ	2.44	0.53
2:B:228:VAL:HG11	2:B:258:PHE:CE1	2.44	0.53
2:B:322:PRO:CB	2:B:324:ASN:HD21	2.08	0.53
1:C:146:SER:CB	1:C:205:LEU:HD11	2.38	0.53
2:F:249:ASP:OD1	2:F:250:TYR:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:LEU:N	1:A:947:LEU:HD12	2.22	0.53
1:G:671:ARG:HG2	1:G:677:ARG:NH1	2.24	0.53
1:A:321:LYS:NZ	1:A:338:ASP:OD2	2.29	0.53
1:A:873:SER:O	1:A:877:GLN:HG3	2.08	0.53
2:B:255:ILE:HA	2:B:258:PHE:CD2	2.44	0.53
1:C:590:ARG:O	1:C:593:GLY:N	2.32	0.53
2:D:215:ARG:CG	2:D:215:ARG:HH11	2.21	0.53
1:E:318:PRO:HG3	1:E:610:TYR:OH	2.08	0.53
1:E:950:ARG:O	1:E:954:LYS:HD2	2.09	0.53
1:G:211:ILE:HG13	6:G:3900:ANP:H2	1.91	0.53
1:G:698:ILE:O	1:G:702:VAL:HG23	2.09	0.53
2:H:208:MET:SD	2:H:355:GLU:HA	2.49	0.53
2:H:232:ASN:N	2:H:233:PRO:HD3	2.22	0.53
1:A:344:THR:HB	1:A:345:PRO:CD	2.37	0.53
2:B:300:VAL:HG23	2:B:301:GLU:N	2.23	0.53
1:G:290:PRO:O	2:H:92:PHE:HB3	2.08	0.53
1:G:695:VAL:HG11	1:G:701:ALA:CA	2.39	0.53
1:A:70:HIS:ND1	1:A:72:GLU:HB2	2.23	0.53
1:C:403:GLU:OE2	1:C:646:THR:HG21	2.08	0.53
1:A:152:MET:O	1:A:156:LEU:HG	2.08	0.53
1:C:368:ALA:HB3	9:C:4425:HOH:O	2.09	0.53
2:D:327:VAL:HG13	2:D:337:LEU:CD1	2.39	0.53
1:E:299:GLU:HB2	9:E:3103:HOH:O	2.09	0.53
2:F:300:VAL:HG22	2:F:328:THR:O	2.08	0.53
1:G:1063:ILE:HD13	1:G:1068:MET:HG2	1.91	0.53
1:G:126:ALA:CB	1:G:302:PRO:HG3	2.36	0.53
1:A:1017:THR:HG22	1:A:1023:ILE:HG13	1.90	0.53
1:C:684:ARG:CG	1:C:684:ARG:HH11	2.17	0.53
1:E:36:ALA:HB2	1:E:321:LYS:CG	2.39	0.53
2:B:168:TYR:O	2:B:218:ILE:N	2.32	0.52
2:B:208:MET:O	2:B:211:ASP:HB2	2.08	0.52
1:C:583:VAL:HG12	1:C:587:LEU:HD22	1.91	0.52
1:A:54:ILE:O	1:A:57:ASP:N	2.41	0.52
1:A:892:GLU:OE1	7:A:1085:ORN:NE	2.40	0.52
2:B:139:ASP:OD2	2:B:142:LEU:HB2	2.09	0.52
1:G:1004:ARG:NH2	9:G:3990:HOH:O	2.43	0.52
1:G:873:SER:OG	1:G:876:GLU:HG3	2.09	0.52
2:H:277:LEU:O	2:H:280:GLY:N	2.39	0.52
1:A:17:PRO:HB2	1:A:894:VAL:HG21	1.91	0.52
1:A:757[B]:ASP:OD1	1:A:833:LYS:NZ	2.42	0.52
1:C:482:THR:HB	9:C:4517:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:762:VAL:HG12	1:E:763:ASP:N	2.24	0.52
1:E:947:LEU:N	1:E:947:LEU:HD12	2.25	0.52
2:F:46:PRO:HA	2:F:76:HIS:CG	2.44	0.52
1:G:426:ARG:HD3	1:G:426:ARG:C	2.29	0.52
1:G:561:LYS:O	1:G:636:LYS:N	2.40	0.52
2:H:29:GLU:OE2	2:H:285:LYS:NZ	2.38	0.52
2:H:300:VAL:HG22	2:H:328:THR:O	2.08	0.52
1:A:475:LYS:HE2	1:A:488:PHE:CZ	2.45	0.52
1:C:421:LEU:HB3	1:G:421:LEU:HB3	1.92	0.52
1:C:563:MET:HE3	1:C:635:PRO:HG3	1.90	0.52
1:E:713:VAL:N	1:E:753:ASP:O	2.32	0.52
2:F:244:ASP:OD1	2:F:245:PRO:HD2	2.10	0.52
1:G:158:VAL:O	1:G:161:ASP:HB3	2.09	0.52
2:B:116:ARG:O	2:B:120:ARG:HG3	2.09	0.52
1:C:354:TYR:CD1	1:C:387:ILE:HG23	2.44	0.52
1:G:180:GLY:HA2	1:G:376:THR:OG1	2.09	0.52
1:A:723:ARG:NH1	1:A:910:GLU:OE1	2.43	0.52
1:A:772[B]:MET:CE	1:A:880:THR:HG22	2.39	0.52
1:E:183:TYR:HB2	1:E:187:GLU:OE1	2.09	0.52
1:E:991:VAL:HG22	1:E:1001:ILE:HG23	1.88	0.52
2:F:34:THR:HA	2:F:56:THR:OG1	2.09	0.52
1:G:519:GLN:NE2	9:G:4492:HOH:O	2.43	0.52
1:G:703:GLU:HG3	1:G:704:LYS:N	2.22	0.52
1:G:722:GLY:HA2	1:G:725:MET:SD	2.49	0.52
2:H:313:GLY:HA3	9:H:3476:HOH:O	2.09	0.52
1:A:469:LEU:O	1:A:473:GLU:HG3	2.09	0.52
1:E:426:ARG:C	1:E:426:ARG:HD3	2.29	0.52
1:G:384:VAL:HG22	1:G:385:MET:N	2.24	0.52
1:G:703:GLU:HA	1:G:706:LYS:HD2	1.92	0.52
1:A:990:LEU:HD23	1:G:979:ILE:HG12	1.90	0.52
2:B:286:MET:HE1	2:B:312:HIS:ND1	2.24	0.52
1:C:46:LEU:HD13	1:C:55:MET:HE3	1.92	0.52
1:C:570:ASN:C	1:C:571:ARG:HG3	2.29	0.52
1:C:698:ILE:H	1:C:698:ILE:CD1	2.23	0.52
2:D:237:PHE:CZ	2:D:268:ILE:HD12	2.45	0.52
1:E:516:LEU:O	1:E:519:GLN:HB3	2.09	0.52
1:G:679:GLN:HG3	1:G:689:GLN:HE22	1.73	0.52
1:G:685:LEU:CD1	1:G:819:GLU:HG2	2.39	0.52
1:A:143:THR:HA	1:A:296:ILE:HG23	1.91	0.52
2:B:133:ILE:HG22	2:B:138:PRO:HB3	1.91	0.52
1:C:479:VAL:HB	1:C:483:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:951:GLU:CA	1:C:954:LYS:HD2	2.34	0.52
1:E:40:GLU:OE1	1:E:40:GLU:HA	2.10	0.52
1:G:425:ARG:NH1	9:G:4363:HOH:O	2.40	0.52
1:C:692:ASN:HB3	1:C:753:ASP:HA	1.91	0.52
1:C:70:HIS:ND1	1:C:72:GLU:HB2	2.24	0.52
2:D:26:ALA:O	2:D:131:CYS:HA	2.10	0.52
1:G:417:ASP:HB3	1:G:420:ALA:HB2	1.92	0.52
1:A:1061:LYS:HA	9:A:1389:HOH:O	2.09	0.51
1:A:672:ALA:HB3	1:A:844:PRO:HG3	1.91	0.51
1:E:671:ARG:NH2	1:E:819:GLU:O	2.43	0.51
1:G:166:CYS:SG	1:G:182:ALA:HB3	2.50	0.51
1:G:590:ARG:O	1:G:593:GLY:N	2.42	0.51
1:G:67:GLU:HB3	1:G:68:PRO:HD2	1.92	0.51
1:G:760:VAL:HG11	1:G:801:LEU:HD11	1.92	0.51
2:B:244:ASP:HB3	2:B:247:PRO:CD	2.40	0.51
2:D:345:LYS:HB3	2:D:346:PRO:HD2	1.91	0.51
1:E:126:ALA:CB	1:E:302:PRO:HG3	2.40	0.51
1:E:722:GLY:HA2	1:E:725:MET:HE3	1.91	0.51
2:F:259:LEU:O	2:F:345:LYS:HD2	2.09	0.51
2:F:275:LEU:HD23	2:F:349:SER:HB3	1.92	0.51
2:H:172:GLN:HG2	2:H:173:GLY:N	2.25	0.51
2:H:225:ALA:HA	2:H:258:PHE:CZ	2.46	0.51
2:H:46:PRO:HG2	2:H:200:GLY:O	2.11	0.51
1:A:700:MET:SD	1:A:703:GLU:HG2	2.51	0.51
1:A:57:ASP:OD1	1:A:855:LYS:HE3	2.10	0.51
1:C:289:ASN:HB3	1:C:292:ASN:OD1	2.11	0.51
1:E:684:ARG:NH1	1:E:684:ARG:HG3	2.24	0.51
2:F:236:ILE:HG22	2:F:237:PHE:N	2.24	0.51
1:G:191:ILE:HG22	1:G:192:CYS:N	2.25	0.51
1:G:805:ILE:HD12	1:G:832:VAL:HG11	1.92	0.51
1:A:331:THR:O	1:A:334:GLU:HB2	2.11	0.51
1:C:709:GLY:O	1:C:754:HIS:HD2	1.94	0.51
1:G:168:ILE:HD13	1:G:191:ILE:CG2	2.38	0.51
1:G:859:VAL:O	1:G:861:LEU:N	2.43	0.51
1:A:956:ARG:HB2	1:A:1044:LEU:CD2	2.40	0.51
1:A:11:LEU:HD12	1:A:45:ILE:O	2.10	0.51
1:A:343:ARG:NH2	1:A:539:ASP:OD1	2.38	0.51
1:C:146:SER:HB2	1:C:205:LEU:CD1	2.37	0.51
1:C:742:VAL:HG22	1:C:750:VAL:HG21	1.92	0.51
1:C:805:ILE:CD1	1:C:837:VAL:HG22	2.40	0.51
1:G:670:ASP:HB3	1:G:677:ARG:NH2	2.16	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:PRO:HG3	1:A:914:THR:HG23	1.93	0.51
1:C:722:GLY:HA2	1:C:725:MET:SD	2.50	0.51
1:G:57:ASP:HB2	1:G:60:MET:HG2	1.92	0.51
1:G:712:LEU:HB3	1:G:728:VAL:HG23	1.92	0.51
2:H:27:VAL:O	2:H:78:GLN:HG2	2.10	0.51
1:A:17:PRO:HG3	1:A:917:VAL:CG1	2.40	0.51
1:C:103:GLU:HG3	1:C:104:ARG:N	2.25	0.51
2:H:318:GLU:OE1	2:H:330:LYS:HE3	2.11	0.51
2:D:249:ASP:OD1	2:D:250:TYR:N	2.44	0.51
1:E:1029:ILE:CD1	1:E:1029:ILE:H	2.21	0.51
1:E:1065:VAL:O	1:E:1068:MET:HB2	2.10	0.51
6:E:2910:ANP:O3'	9:E:3414:HOH:O	2.19	0.51
2:H:114:ASP:O	2:H:117:LYS:HB3	2.10	0.51
1:A:731:GLU:O	1:A:735:ARG:HG3	2.11	0.51
1:C:947:LEU:HG	1:C:1014:ILE:CG2	2.41	0.51
2:D:78:GLN:HA	2:D:78:GLN:NE2	2.25	0.51
1:E:315:THR:O	1:E:531:THR:HG22	2.11	0.51
1:G:412:LYS:HE2	1:G:434:ASP:OD2	2.11	0.51
1:A:990:LEU:HG	1:G:979:ILE:CD1	2.41	0.51
2:B:302:LYS:HB2	2:B:304:VAL:HG13	1.92	0.50
1:C:1028:VAL:HG12	9:C:4605:HOH:O	2.11	0.50
1:C:269:MET:O	1:C:273:ARG:HG3	2.11	0.50
1:E:721:GLY:N	6:E:2910:ANP:O1G	2.30	0.50
1:E:36:ALA:HB2	1:E:321:LYS:HG2	1.93	0.50
2:H:215:ARG:NH1	2:H:215:ARG:HG3	2.23	0.50
1:A:289:ASN:OD1	1:A:290:PRO:HD2	2.12	0.50
1:A:333:ASP:N	1:A:333:ASP:OD1	2.42	0.50
1:C:554:ASN:N	1:C:555:PRO:HD3	2.26	0.50
1:E:858:GLY:HA2	1:E:1069:HIS:CE1	2.46	0.50
1:E:168:ILE:HD13	1:E:191:ILE:HG21	1.89	0.50
2:F:159:ALA:O	2:F:163:THR:HG22	2.11	0.50
2:F:269:CYS:O	2:F:272:HIS:HB3	2.11	0.50
1:G:194:ARG:HB2	1:G:194:ARG:HH11	1.76	0.50
1:G:259:LYS:HD3	2:H:175:TRP:CE3	2.47	0.50
1:G:271:VAL:HG12	1:G:300:MET:HE3	1.91	0.50
1:G:417:ASP:OD2	1:G:423:LYS:NZ	2.42	0.50
1:G:435:ARG:O	1:G:439:ILE:HG13	2.10	0.50
1:A:910:GLU:O	1:A:912[A]:ARG:HD3	2.11	0.50
1:E:25:GLU:N	1:E:25:GLU:OE1	2.28	0.50
1:G:810:ARG:HG3	1:G:810:ARG:NH1	2.26	0.50
1:G:899:LYS:O	1:G:901:PRO:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ILE:HD11	1:A:530:ASP:HA	1.92	0.50
1:A:574:GLN:HE22	1:A:645:GLN:HB2	1.73	0.50
1:A:70:HIS:O	1:A:74:VAL:HG23	2.11	0.50
2:B:150:PHE:CG	2:B:151:PRO:HD2	2.46	0.50
1:C:146:SER:HA	1:C:206:ILE:O	2.11	0.50
2:D:135:GLY:O	2:D:138:PRO:HD3	2.11	0.50
2:D:326:ARG:O	2:D:340:ILE:HA	2.12	0.50
1:G:950:ARG:HD3	9:G:4425:HOH:O	2.11	0.50
1:A:574:GLN:HE22	1:A:645:GLN:N	1.99	0.50
2:B:144:LEU:C	2:B:144:LEU:HD12	2.30	0.50
2:B:205:ILE:HG21	2:B:237:PHE:CE2	2.46	0.50
1:E:956:ARG:HB2	1:E:1044:LEU:HD21	1.94	0.50
2:F:310:GLN:NE2	2:F:352:GLY:HA3	2.27	0.50
2:F:6:LEU:HD23	2:F:6:LEU:O	2.11	0.50
1:G:998:ARG:HA	1:G:999:PRO:C	2.30	0.50
1:A:1003:ASP:OD1	1:A:1006:LYS:NZ	2.40	0.50
2:F:268:ILE:O	2:F:268:ILE:HG22	2.11	0.50
2:H:176:THR:O	2:H:180:GLY:N	2.41	0.50
2:H:39:TYR:CZ	2:H:61:GLY:HA2	2.46	0.50
1:A:1000:HIS:CD2	1:A:1000:HIS:H	2.30	0.50
1:A:1004:ARG:O	1:A:1009:GLU:HB2	2.11	0.50
1:A:1028:VAL:O	1:A:1032:SER:OG	2.29	0.50
1:G:994:VAL:HG22	1:G:1000:HIS:CE1	2.46	0.50
2:H:273:GLN:HE21	2:H:351:GLN:HE22	1.60	0.50
2:H:9:LEU:N	2:H:9:LEU:HD23	2.25	0.50
1:A:900:PHE:N	1:A:901:PRO:HD3	2.26	0.50
1:C:403:GLU:HG3	1:C:569:PRO:HD2	1.94	0.50
1:C:460:ARG:O	1:C:464:VAL:HG22	2.12	0.50
1:G:168:ILE:HD11	1:G:188:PHE:CD1	2.47	0.50
1:G:431:ALA:HB2	1:G:435:ARG:CZ	2.41	0.50
1:G:982:GLY:HA2	1:G:986:ILE:O	2.12	0.50
1:A:181:ILE:HD11	1:A:376:THR:HG23	1.94	0.50
1:A:403:GLU:CD	1:A:646:THR:HG21	2.32	0.50
1:A:675:ARG:NH2	1:A:841:GLU:OE1	2.45	0.50
2:B:249:ASP:OD1	2:B:250:TYR:N	2.45	0.50
1:G:349:GLU:O	2:H:294:ASN:HB2	2.12	0.50
1:C:294:ARG:NH1	9:C:4348:HOH:O	2.43	0.49
1:E:708:ILE:HG22	1:E:709:GLY:N	2.27	0.49
1:G:589:LEU:O	1:G:594:TYR:HB2	2.12	0.49
1:G:947:LEU:N	1:G:947:LEU:HD12	2.27	0.49
2:F:232:ASN:N	2:F:233:PRO:HD3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1001:ILE:HD12	1:G:1002:GLN:CB	2.41	0.49
1:G:1064:SER:OG	1:G:1067:GLU:HG3	2.13	0.49
1:A:85:ALA:HA	1:A:114:THR:O	2.13	0.49
1:A:1:MET:HB3	1:A:2:PRO:HD2	1.94	0.49
1:A:993:LYS:N	1:A:996:GLU:HG3	2.27	0.49
2:B:364:ALA:N	2:B:365:PRO:HD2	2.28	0.49
1:G:481:ILE:HG21	1:G:508:VAL:CG1	2.42	0.49
1:G:773:VAL:HG23	1:G:818:PHE:CZ	2.46	0.49
1:G:825:LEU:HG	1:G:865:ALA:CB	2.41	0.49
1:A:467:GLU:O	1:A:471:ARG:HG2	2.13	0.49
2:B:327:VAL:HG13	2:B:337:LEU:CD1	2.42	0.49
1:E:216:TYR:HB2	1:E:264:MET:HE1	1.95	0.49
1:G:46:LEU:O	1:G:46:LEU:HG	2.12	0.49
1:G:516:LEU:HD12	1:G:519:GLN:NE2	2.27	0.49
2:H:272:HIS:HA	2:H:349:SER:CB	2.42	0.49
1:A:158:VAL:O	1:A:161:ASP:HB3	2.12	0.49
1:C:1017:THR:HG22	1:C:1018:SER:N	2.27	0.49
1:C:688:LYS:HE2	1:C:838:TYR:CE2	2.47	0.49
1:E:327:ALA:HB2	9:E:3520:HOH:O	2.12	0.49
1:E:313:LYS:HE2	1:E:608:THR:O	2.13	0.49
2:F:66:ASN:HB3	2:F:93:ARG:O	2.13	0.49
2:H:160:LYS:HG3	2:H:161:GLU:HG2	1.94	0.49
1:A:586:SER:O	1:A:590:ARG:HB2	2.13	0.49
1:C:922:ARG:HH21	1:C:1061:LYS:CB	2.25	0.49
1:C:692:ASN:HA	1:C:708:ILE:HD13	1.95	0.49
1:C:768:CYS:HA	1:C:772:MET:O	2.12	0.49
1:E:563:MET:CE	1:E:635:PRO:HG3	2.38	0.49
2:F:206:LEU:HB3	2:F:216:LEU:CD1	2.43	0.49
1:G:152:MET:HB2	9:G:4034:HOH:O	2.13	0.49
1:G:716:PRO:HD2	1:G:725:MET:CG	2.42	0.49
1:A:1027:ARG:HH21	1:A:1031:ARG:HH11	1.59	0.49
2:B:246:ALA:HB3	2:B:247:PRO:CD	2.41	0.49
1:G:237:PHE:HB3	1:G:248:ILE:HB	1.93	0.49
1:G:712:LEU:HD11	1:G:752:LEU:HB3	1.94	0.49
2:H:225:ALA:O	2:H:228:VAL:HB	2.12	0.49
1:A:219:GLU:OE2	1:A:307:SER:HB2	2.12	0.49
2:B:356:ALA:HB3	9:B:1123:HOH:O	2.12	0.49
1:E:906:LEU:CD2	1:E:1023:ILE:HG23	2.43	0.49
1:E:130:ARG:CG	1:E:148:ILE:HG13	2.33	0.49
1:E:712:LEU:HD23	1:E:713:VAL:N	2.27	0.49
1:G:860:PRO:HB2	1:G:863:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:MET:HA	6:A:1083:ANP:O1B	2.13	0.49
2:B:33:ASN:HB3	2:B:55:LEU:HD23	1.94	0.49
1:C:44:VAL:N	1:C:62:ASP:OD2	2.30	0.49
1:E:10:ILE:HD13	1:E:37:LEU:HD13	1.93	0.49
1:E:692:ASN:HB3	1:E:753:ASP:OD1	2.13	0.49
1:E:784:GLN:HE21	1:E:784:GLN:N	2.02	0.49
2:F:259:LEU:O	2:F:345:LYS:HE3	2.12	0.49
1:G:698:ILE:HG13	1:G:698:ILE:H	1.47	0.49
1:G:929:ALA:HB2	1:G:1053:ALA:HB1	1.93	0.49
1:A:710:TYR:CB	1:A:711:PRO:HA	2.33	0.49
1:C:1001:ILE:HD12	1:C:1002:GLN:HB2	1.94	0.49
1:E:695:VAL:HG11	1:E:701:ALA:CA	2.42	0.49
2:F:66:ASN:OD1	2:F:68:ALA:HB3	2.13	0.49
1:G:365:GLU:HG2	1:G:366:LYS:N	2.27	0.49
1:G:716:PRO:HD2	1:G:725:MET:HG3	1.95	0.49
1:A:366:LYS:O	1:A:912[B]:ARG:NH1	2.46	0.48
1:A:820:LEU:O	1:A:821:GLN:HB2	2.13	0.48
1:A:890:VAL:HG12	1:A:931:ALA:CB	2.43	0.48
1:C:1027:ARG:NH2	1:C:1031:ARG:HH11	2.08	0.48
1:C:525:VAL:HG22	1:C:548:GLU:H	1.77	0.48
1:C:574:GLN:NE2	1:C:645:GLN:N	2.30	0.48
2:F:199:PHE:HB3	2:F:270:LEU:HD23	1.95	0.48
1:G:941:LYS:NZ	1:G:1056:ALA:O	2.38	0.48
2:H:46:PRO:HA	2:H:76:HIS:CG	2.48	0.48
1:A:1023:ILE:HG22	1:A:1024:GLU:N	2.27	0.48
1:G:853:VAL:CG1	1:G:861:LEU:HD11	2.43	0.48
1:G:767:ILE:HD13	1:G:865:ALA:HB2	1.94	0.48
2:H:201:ALA:CB	2:H:239:SER:HB2	2.41	0.48
1:A:574:GLN:HE21	1:A:645:GLN:HB2	1.74	0.48
2:B:334:ASP:CG	2:B:336:THR:HG23	2.33	0.48
1:C:574:GLN:CG	1:C:720:LEU:HD11	2.42	0.48
1:E:214:LYS:O	1:E:287:ALA:HA	2.13	0.48
1:E:796:LEU:HD23	1:E:796:LEU:C	2.33	0.48
2:F:194:VAL:O	2:F:216:LEU:HA	2.13	0.48
1:A:1051:ALA:O	1:A:1054:LEU:HB2	2.13	0.48
1:C:331:THR:OG1	1:C:334:GLU:HG3	2.12	0.48
1:C:456:THR:O	1:C:457:ASN:HB2	2.12	0.48
1:C:805:ILE:HD11	1:C:837:VAL:CG2	2.43	0.48
2:D:201:ALA:HB2	2:D:239:SER:CB	2.43	0.48
1:E:70:HIS:ND1	1:E:72:GLU:HB2	2.29	0.48
1:G:1028:VAL:O	1:G:1032:SER:OG	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:ARG:HD3	1:G:277:VAL:O	2.13	0.48
1:G:722:GLY:N	6:G:3910:ANP:O1B	2.39	0.48
1:G:780:GLU:HB2	1:G:801:LEU:HD12	1.94	0.48
2:B:367:PHE:O	2:B:370:PHE:HB3	2.14	0.48
1:C:1000:HIS:HD2	1:C:1003:ASP:H	1.61	0.48
1:C:704:LYS:O	1:C:707:GLU:HB2	2.14	0.48
1:C:805:ILE:HD11	1:C:837:VAL:HG22	1.94	0.48
1:G:723:ARG:NH1	1:G:910:GLU:OE1	2.46	0.48
2:H:51:GLN:O	2:H:78:GLN:N	2.39	0.48
1:C:639:ILE:HD13	1:C:869:MET:CE	2.43	0.48
1:E:712:LEU:HG	1:E:753:ASP:O	2.14	0.48
1:G:796:LEU:HD23	1:G:796:LEU:C	2.34	0.48
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.95	0.48
1:C:1027:ARG:HE	1:C:1031:ARG:HD3	1.78	0.48
1:C:671:ARG:HG2	1:C:677:ARG:NH1	2.28	0.48
2:F:142:LEU:O	2:F:146:LYS:HG3	2.14	0.48
2:F:197:TYR:HB3	2:F:199:PHE:CE2	2.48	0.48
1:G:148:ILE:CG2	1:G:150:HIS:CE1	2.97	0.48
1:A:671:ARG:NH2	1:A:819:GLU:O	2.47	0.48
2:B:244:ASP:HB3	2:B:247:PRO:CG	2.44	0.48
1:C:1000:HIS:CD2	1:C:1003:ASP:H	2.32	0.48
2:D:121:LEU:HD11	2:D:125:LYS:HD2	1.96	0.48
2:D:228:VAL:O	2:D:231:MET:HG3	2.14	0.48
2:D:251:ALA:O	2:D:255:ILE:HG13	2.13	0.48
2:F:370:PHE:O	2:F:373:LEU:N	2.46	0.48
1:G:358:LYS:HG2	1:G:359:ILE:N	2.28	0.48
1:G:554:ASN:N	1:G:555:PRO:HD3	2.29	0.48
1:G:693:ALA:HB3	1:G:708:ILE:HD11	1.96	0.48
1:G:839:LEU:HD12	1:G:840:ILE:H	1.79	0.48
2:H:34:THR:HA	2:H:56:THR:OG1	2.13	0.48
1:A:970:GLU:HG3	9:A:1524:HOH:O	2.12	0.48
1:G:23:ALA:HB3	1:G:25:GLU:OE2	2.14	0.48
2:H:46:PRO:HB2	2:H:200:GLY:O	2.14	0.48
8:A:1086:NET:C2	8:A:1086:NET:H42	2.29	0.48
1:A:213:TRP:HH2	1:A:294:ARG:HD3	1.78	0.48
2:B:249:ASP:N	2:B:249:ASP:OD1	2.46	0.48
1:C:224:LYS:HE2	1:C:329:GLY:O	2.14	0.48
1:C:796:LEU:C	1:C:796:LEU:HD23	2.35	0.48
2:D:244:ASP:OD1	2:D:245:PRO:HD2	2.14	0.48
2:F:354:PRO:HA	2:F:363:ALA:HB3	1.96	0.48
1:G:271:VAL:HG12	1:G:300:MET:CE	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:ILE:CD1	1:G:376:THR:HG23	2.44	0.48
1:G:679:GLN:CA	1:G:689:GLN:HE22	2.26	0.48
1:G:716:PRO:HB3	1:G:741:ALA:O	2.14	0.48
1:G:972:ASP:HB3	1:G:991:VAL:HG11	1.95	0.48
2:B:261:THR:OG1	2:B:263:ILE:HG13	2.14	0.47
2:B:58:PRO:HA	2:B:83:ARG:HB3	1.95	0.47
1:C:449:VAL:HG12	1:C:460:ARG:HG2	1.97	0.47
1:C:692:ASN:HB3	1:C:753:ASP:OD1	2.14	0.47
1:E:187:GLU:O	1:E:191:ILE:HD12	2.13	0.47
1:G:720:LEU:HD12	1:G:720:LEU:C	2.35	0.47
2:H:205:ILE:HG12	2:H:355:GLU:HG3	1.95	0.47
2:H:318:GLU:O	2:H:321:LEU:HB2	2.13	0.47
2:B:270:LEU:HD12	2:B:273:GLN:OE1	2.14	0.47
1:C:514:ARG:HD3	9:C:4176:HOH:O	2.14	0.47
1:C:517:ARG:HB3	1:C:522:LEU:O	2.14	0.47
1:C:820:LEU:HD23	1:C:820:LEU:HA	1.46	0.47
2:D:175:TRP:HA	2:D:180:GLY:O	2.13	0.47
2:F:46:PRO:HA	2:F:76:HIS:CD2	2.49	0.47
1:G:101:GLU:OE1	1:G:104:ARG:NH2	2.45	0.47
1:G:1063:ILE:CD1	1:G:1068:MET:HG3	2.43	0.47
1:G:419:GLU:O	1:G:423:LYS:HG3	2.14	0.47
1:G:565:LEU:HD23	1:G:565:LEU:N	2.25	0.47
1:G:912:ARG:NE	9:G:4346:HOH:O	2.30	0.47
1:G:937:SER:OG	1:G:938:THR:N	2.48	0.47
1:G:993:LYS:NZ	9:G:4423:HOH:O	2.47	0.47
1:C:312:SER:HA	1:C:317:PHE:O	2.14	0.47
1:C:412:LYS:HG2	1:C:438:TYR:CZ	2.50	0.47
1:C:516:LEU:HA	1:C:516:LEU:HD12	1.72	0.47
2:F:55:LEU:HA	2:F:55:LEU:HD23	1.59	0.47
1:G:904:ASP:CG	1:G:1027:ARG:HG3	2.35	0.47
2:H:342:ARG:NE	2:H:344:ASP:OD1	2.47	0.47
2:H:54:THR:HA	2:H:81:VAL:HB	1.95	0.47
2:B:205:ILE:HG21	2:B:237:PHE:CZ	2.48	0.47
1:E:417:ASP:OD1	1:E:418:PRO:HD2	2.14	0.47
1:G:27:ASP:OD1	1:G:53:THR:HB	2.13	0.47
1:G:804:GLU:O	1:G:808:VAL:HG23	2.14	0.47
2:H:153:LEU:CD2	2:H:158:LEU:HD11	2.44	0.47
1:C:967:GLN:HG2	1:C:1054:LEU:CD1	2.19	0.47
1:E:57:ASP:OD1	1:E:855:LYS:HE3	2.15	0.47
1:G:623:LEU:HD12	1:G:654:LEU:CD2	2.44	0.47
2:H:5:ALA:HB3	2:H:110:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:306:MET:HB2	2:H:362:ASP:HB3	1.95	0.47
2:B:299:ASP:HB3	2:B:304:VAL:HG22	1.95	0.47
1:C:106:GLY:HA2	9:C:4569:HOH:O	2.13	0.47
1:C:145:ARG:NH1	1:C:161:ASP:OD2	2.48	0.47
2:F:350:PHE:HB2	2:F:366:LEU:HD22	1.97	0.47
2:H:205:ILE:HG12	2:H:355:GLU:CG	2.45	0.47
1:A:221:VAL:HA	1:A:281:GLY:HA2	1.97	0.47
1:A:9:SER:OG	1:A:83:PRO:HA	2.14	0.47
1:E:164:PHE:HA	1:E:165:PRO:C	2.35	0.47
1:E:70:HIS:CE1	1:E:72:GLU:HB2	2.50	0.47
1:E:715:ARG:HA	1:E:725:MET:HG2	1.96	0.47
2:F:163:THR:OG1	2:F:164:THR:N	2.48	0.47
1:A:1004:ARG:HH22	1:G:983:GLU:CG	2.27	0.47
2:B:46:PRO:HA	2:B:76:HIS:CG	2.49	0.47
1:C:1019:GLY:C	1:C:1023:ILE:HD12	2.35	0.47
1:C:1036:TYR:C	1:C:1037:LYS:HG2	2.35	0.47
1:C:383:GLU:OE2	9:C:4593:HOH:O	2.20	0.47
1:C:574:GLN:HE22	1:C:645:GLN:H	0.67	0.47
2:D:212:ARG:HH11	2:D:212:ARG:CG	2.27	0.47
1:E:998:ARG:HH11	1:E:998:ARG:HG2	1.80	0.47
8:G:3950:NET:H23	8:G:3950:NET:H83	1.97	0.47
1:A:291:LYS:HD2	9:A:1552:HOH:O	2.15	0.47
1:A:588:ALA:O	1:A:591:GLU:HB2	2.15	0.47
1:A:772[B]:MET:HE1	1:A:880:THR:CB	2.43	0.47
1:C:904:ASP:HA	1:C:905:PRO:HD3	1.72	0.47
2:D:157:ASP:CG	2:D:160:LYS:HG2	2.35	0.47
1:E:587:LEU:HD12	1:E:587:LEU:HA	1.77	0.47
2:F:104:ARG:HG2	2:F:105:HIS:CD2	2.50	0.47
1:G:146:SER:HA	1:G:206:ILE:O	2.15	0.47
1:G:623:LEU:O	1:G:627:LEU:HG	2.14	0.47
1:G:685:LEU:HD11	1:G:819:GLU:HB3	1.92	0.47
1:A:198:LEU:HA	1:A:198:LEU:HD12	1.72	0.47
1:A:525:VAL:HG22	1:A:548:GLU:H	1.78	0.47
2:B:325:LEU:HA	2:B:325:LEU:HD23	1.68	0.47
1:C:1020:ARG:HA	1:C:1020:ARG:HD2	1.69	0.47
1:C:700:MET:CE	1:C:703:GLU:HG2	2.45	0.47
1:E:314:ALA:HB1	1:E:356:VAL:HG21	1.97	0.47
2:F:298:LYS:HE2	2:F:303:ASN:OD1	2.15	0.47
1:G:215:GLU:HG3	1:G:240:MET:SD	2.55	0.47
1:G:353:ASP:OD1	1:G:353:ASP:N	2.48	0.47
1:A:172:PHE:CE2	1:A:201:THR:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:THR:O	1:A:531:THR:HG22	2.15	0.47
2:B:201:ALA:HB2	2:B:239:SER:CB	2.45	0.47
1:E:1001:ILE:H	1:E:1001:ILE:HG13	1.46	0.47
1:E:955:GLU:HB2	9:E:3611:HOH:O	2.14	0.47
1:G:1002:GLN:O	1:G:1006:LYS:HB3	2.15	0.47
1:G:859:VAL:HG12	1:G:861:LEU:HD23	1.97	0.47
2:H:264:PRO:HB3	2:H:373:LEU:HB3	1.95	0.47
1:A:788:HIS:HD2	1:A:909:PRO:O	1.98	0.46
1:C:3:LYS:HB3	1:C:330:TYR:CZ	2.50	0.46
1:C:568:GLY:O	1:C:602:ASN:HB2	2.14	0.46
1:E:534:ALA:O	2:F:123:ARG:HD3	2.14	0.46
1:E:944:ARG:HA	1:E:970:GLU:O	2.14	0.46
1:G:503:ALA:HB2	1:G:513:ILE:HG13	1.97	0.46
1:G:560:GLU:OE2	1:G:636:LYS:HE3	2.15	0.46
1:G:973:ALA:O	1:G:990:LEU:HD12	2.14	0.46
1:G:972:ASP:HB3	1:G:991:VAL:CG1	2.46	0.46
2:H:325:LEU:HD23	2:H:342:ARG:HD2	1.97	0.46
1:A:579:ASP:O	1:A:583:VAL:HG23	2.15	0.46
1:C:145:ARG:HH12	1:C:161:ASP:CG	2.18	0.46
1:A:146:SER:HB2	1:A:206:ILE:O	2.15	0.46
1:A:932:GLN:O	1:A:937:SER:HB3	2.15	0.46
2:B:253:THR:O	2:B:256:GLN:HB2	2.14	0.46
1:C:731:GLU:H	1:C:731:GLU:HG3	1.38	0.46
2:H:195:VAL:CG2	2:H:233:PRO:HB3	2.44	0.46
1:A:990:LEU:HG	1:G:979:ILE:HD11	1.96	0.46
1:C:723:ARG:HD2	1:C:723:ARG:HA	1.72	0.46
2:D:87:LEU:HD12	2:D:87:LEU:HA	1.60	0.46
1:G:124:ASP:OD2	1:G:131:ARG:NH1	2.46	0.46
2:H:285:LYS:HG3	2:H:314:PHE:CE2	2.50	0.46
2:H:48:TYR:HA	2:H:51:GLN:HE21	1.79	0.46
1:A:493:LYS:HA	1:A:493:LYS:HD2	1.50	0.46
2:B:286:MET:CE	2:B:312:HIS:ND1	2.78	0.46
1:C:577:GLU:O	1:C:580:TYR:HB3	2.15	0.46
2:D:298:LYS:O	2:D:329:HIS:HA	2.15	0.46
2:D:286:MET:CE	2:D:312:HIS:ND1	2.78	0.46
1:G:146:SER:HB3	1:G:207:ASP:OD1	2.16	0.46
1:G:802:SER:O	1:G:806:GLN:HG3	2.15	0.46
2:H:253:THR:O	2:H:256:GLN:HB2	2.15	0.46
2:H:72:SER:OG	2:H:74:GLN:O	2.33	0.46
1:A:220:VAL:O	1:A:281:GLY:HA2	2.16	0.46
1:A:434:ASP:HB2	9:A:1457:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:ILE:O	1:E:69:ILE:HG22	2.16	0.46
1:A:1020:ARG:HA	1:A:1020:ARG:HD2	1.64	0.46
1:A:684:ARG:CG	1:A:684:ARG:HH11	2.29	0.46
1:C:57:ASP:HB3	1:C:59:GLU:OE1	2.15	0.46
1:C:801:LEU:HD23	1:C:801:LEU:HA	1.80	0.46
2:D:157:ASP:OD1	2:D:160:LYS:HG2	2.15	0.46
2:D:45:ASP:HB3	2:D:48:TYR:HD2	1.81	0.46
1:E:27:ASP:OD1	1:E:55:MET:HB3	2.15	0.46
1:E:583:VAL:HG12	1:E:587:LEU:HD22	1.97	0.46
2:F:305:VAL:HG12	2:F:306:MET:N	2.31	0.46
1:G:100:LEU:HA	1:G:103:GLU:HB3	1.98	0.46
1:G:172:PHE:CD2	1:G:201:THR:HG23	2.51	0.46
1:G:720:LEU:HD12	1:G:720:LEU:O	2.16	0.46
2:H:44:THR:O	2:H:46:PRO:HD3	2.15	0.46
1:A:325:LYS:O	1:A:330:TYR:HB2	2.15	0.46
1:C:482:THR:HG22	1:C:483:GLY:N	2.29	0.46
1:E:489:LEU:HD22	1:E:516:LEU:HD23	1.97	0.46
1:E:805:ILE:CD1	1:E:837:VAL:HG23	2.46	0.46
1:E:9:SER:HA	1:E:43:ARG:O	2.16	0.46
2:F:310:GLN:HE22	2:F:352:GLY:HA3	1.79	0.46
2:F:364:ALA:N	2:F:365:PRO:HD2	2.31	0.46
1:G:770:GLY:CA	1:G:823:ARG:NH1	2.79	0.46
1:G:972:ASP:OD1	1:G:989:ARG:HB3	2.15	0.46
2:H:57:TYR:CE1	2:H:58:PRO:HD2	2.49	0.46
1:A:236:ASN:OD1	1:A:244:THR:HG22	2.14	0.46
1:A:426:ARG:C	1:A:426:ARG:HD3	2.36	0.46
1:A:5:THR:HG23	1:A:6:ASP:N	2.30	0.46
1:A:951:GLU:HA	1:A:954:LYS:CD	2.46	0.46
2:B:117:LYS:NZ	9:B:1007:HOH:O	2.48	0.46
1:C:602:ASN:ND2	1:C:605:THR:CG2	2.79	0.46
2:D:215:ARG:CG	2:D:215:ARG:NH1	2.78	0.46
2:D:229:LEU:HA	2:D:229:LEU:HD23	1.77	0.46
2:D:273:GLN:O	2:D:277:LEU:HG	2.15	0.46
1:G:574:GLN:HE22	1:G:645:GLN:HB2	1.78	0.46
2:H:120:ARG:O	2:H:124:GLU:HB2	2.16	0.46
2:H:190:LEU:HD21	2:H:210:VAL:HG13	1.97	0.46
2:H:350:PHE:HB2	2:H:366:LEU:CD2	2.46	0.46
1:A:471:ARG:HG3	9:A:1484:HOH:O	2.15	0.46
1:A:82:ARG:N	1:A:83:PRO:CD	2.79	0.46
2:B:162:VAL:HG21	2:B:200:GLY:HA3	1.98	0.46
1:C:267:ALA:O	1:C:271:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:764:VAL:HA	1:C:777:GLY:O	2.16	0.46
1:E:693:ALA:HB3	1:E:708:ILE:HD11	1.98	0.46
2:F:330:LYS:NZ	9:F:2838:HOH:O	2.48	0.46
2:F:57:TYR:CD1	2:F:58:PRO:HD2	2.51	0.46
1:G:172:PHE:CD2	1:G:201:THR:CG2	2.99	0.46
1:A:1017:THR:CG2	1:A:1018:SER:N	2.78	0.45
1:A:299:GLU:HB2	9:A:1200:HOH:O	2.16	0.45
1:A:299:GLU:OE2	1:A:301:ASN:ND2	2.48	0.45
1:A:490:ARG:HA	1:A:522:LEU:HD21	1.98	0.45
1:A:949:VAL:O	1:A:954:LYS:HE3	2.16	0.45
1:C:1007:ASN:HB3	9:C:4604:HOH:O	2.16	0.45
1:C:550:GLU:HB2	2:D:117:LYS:HG3	1.97	0.45
2:D:212:ARG:NH1	2:D:212:ARG:CG	2.79	0.45
2:D:194:VAL:O	2:D:216:LEU:HA	2.16	0.45
2:D:371:ILE:O	2:D:374:ILE:HB	2.16	0.45
1:E:1017:THR:CG2	1:E:1018:SER:N	2.79	0.45
1:E:222:ARG:HD3	1:E:278:GLU:HA	1.97	0.45
1:E:820:LEU:O	1:E:821:GLN:HB2	2.16	0.45
1:G:1027:ARG:HE	1:G:1031:ARG:HD3	1.80	0.45
1:G:524:PRO:HD3	1:G:547:TYR:OH	2.17	0.45
1:C:349:GLU:O	2:D:294:ASN:HB2	2.16	0.45
1:C:82:ARG:N	1:C:83:PRO:CD	2.79	0.45
1:G:1000:HIS:CD2	1:G:1003:ASP:H	2.33	0.45
1:G:262:GLN:OE1	1:G:262:GLN:HA	2.15	0.45
8:G:3950:NET:H83	9:G:4270:HOH:O	2.16	0.45
1:G:75:ARG:HH11	1:G:75:ARG:CG	2.27	0.45
1:G:782:ILE:CD1	1:G:782:ILE:N	2.80	0.45
1:A:332:LEU:HB3	1:A:347:SER:HB3	1.98	0.45
1:A:708:ILE:CG2	1:A:754:HIS:HB2	2.46	0.45
2:B:133:ILE:CG2	2:B:138:PRO:HB3	2.46	0.45
2:B:224:SER:OG	2:B:227:ASP:OD2	2.34	0.45
2:B:235:GLY:HA3	2:B:374:ILE:CD1	2.43	0.45
1:E:100:LEU:HA	1:E:100:LEU:HD12	1.52	0.45
1:E:460:ARG:O	1:E:464:VAL:HG22	2.16	0.45
1:E:503:ALA:HB2	1:E:510:GLU:HA	1.97	0.45
1:E:716:PRO:HG2	1:E:723:ARG:O	2.15	0.45
1:E:999:PRO:HA	1:E:1003:ASP:OD2	2.16	0.45
1:G:64:THR:O	1:G:1065:VAL:HG23	2.16	0.45
1:G:339:ILE:HG22	1:G:540:THR:HG21	1.96	0.45
1:G:385:MET:HB2	1:G:603:PRO:HG3	1.98	0.45
2:H:286:MET:CE	2:H:312:HIS:ND1	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:HG3	1:A:148:ILE:HG13	1.98	0.45
1:E:154:GLU:O	1:E:158:VAL:HG23	2.16	0.45
1:E:125:LYS:HD3	1:E:275:ILE:HA	1.97	0.45
1:G:151:THR:N	1:G:154:GLU:HB2	2.31	0.45
1:G:874:LEU:HB3	1:G:879:VAL:O	2.17	0.45
1:A:167:ILE:N	1:A:167:ILE:HD12	2.32	0.45
1:A:456:THR:O	1:A:457:ASN:HB2	2.15	0.45
1:A:990:LEU:HD23	1:G:979:ILE:CD1	2.46	0.45
2:B:160:LYS:HG3	2:B:161:GLU:HG2	1.98	0.45
2:B:263:ILE:H	2:B:263:ILE:HG13	1.57	0.45
2:B:350:PHE:CG	2:B:366:LEU:CD2	3.00	0.45
1:C:1017:THR:HG22	1:C:1018:SER:H	1.81	0.45
1:C:431:ALA:HB2	1:C:435:ARG:CZ	2.47	0.45
1:C:579:ASP:OD1	1:C:605:THR:HB	2.17	0.45
1:C:82:ARG:HA	1:C:82:ARG:HD2	1.64	0.45
1:E:1067:GLU:O	1:E:1071:GLN:HG3	2.16	0.45
1:E:272:LEU:HD11	1:E:282:SER:HB2	1.99	0.45
1:E:1:MET:CG	1:E:2:PRO:HD2	2.42	0.45
1:G:363:ASN:ND2	1:G:365:GLU:OE2	2.49	0.45
1:G:677:ARG:O	1:G:680:HIS:HB2	2.17	0.45
2:H:324:ASN:N	2:H:324:ASN:ND2	2.42	0.45
2:H:306:MET:CE	2:H:329:HIS:CD2	3.00	0.45
2:H:63:VAL:HG12	2:H:91:ASN:HB2	1.99	0.45
1:A:979:ILE:HD13	1:G:990:LEU:HB3	1.97	0.45
2:B:193:HIS:CD2	2:B:215:ARG:CZ	3.00	0.45
1:E:1017:THR:CG2	1:E:1018:SER:H	2.29	0.45
1:E:711:PRO:HB3	1:E:729:TYR:CD1	2.52	0.45
1:G:318:PRO:O	1:G:322:VAL:HG23	2.16	0.45
1:G:35:LYS:HD2	9:G:4283:HOH:O	2.16	0.45
1:G:645:GLN:HG2	1:G:720:LEU:HG	1.98	0.45
1:G:711:PRO:HG2	1:G:755:PHE:HB3	1.98	0.45
1:G:891:LYS:HG2	1:G:892:GLU:N	2.29	0.45
1:A:71:TRP:CH2	1:A:105:GLN:HG2	2.51	0.45
1:C:213:TRP:N	1:C:213:TRP:CD1	2.84	0.45
1:C:843:ASN:O	1:C:845:ARG:N	2.45	0.45
2:D:299:ASP:OD2	2:D:302:LYS:HD2	2.16	0.45
1:E:695:VAL:HG12	1:E:738:PHE:CZ	2.51	0.45
2:F:299:ASP:O	2:F:303:ASN:N	2.48	0.45
2:F:367:PHE:O	2:F:370:PHE:HB3	2.17	0.45
1:G:167:ILE:CD1	1:G:167:ILE:N	2.80	0.45
2:H:210:VAL:HG22	2:H:214:CYS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:191:PRO:HD2	2:H:213:GLY:O	2.17	0.45
2:H:168:TYR:O	2:H:217:THR:HA	2.16	0.45
2:H:254:ALA:O	2:H:257:LYS:N	2.49	0.45
2:H:287:LYS:HD2	9:H:3198:HOH:O	2.17	0.45
1:A:899:LYS:C	1:A:901:PRO:HD3	2.37	0.45
2:B:168:TYR:O	2:B:217:THR:HA	2.17	0.45
2:B:364:ALA:N	2:B:365:PRO:CD	2.79	0.45
2:B:6:LEU:HD22	2:B:138:PRO:HB2	1.99	0.45
1:C:710:TYR:HB3	1:C:711:PRO:HA	1.98	0.45
2:D:364:ALA:N	2:D:365:PRO:CD	2.79	0.45
1:G:1063:ILE:HG12	1:G:1064:SER:N	2.32	0.45
1:G:174:MET:HE3	1:G:303:ARG:NH2	2.31	0.45
1:A:164:PHE:HA	1:A:165:PRO:C	2.35	0.45
1:A:723:ARG:O	1:A:724:ALA:HB3	2.17	0.45
1:C:224:LYS:NZ	9:C:3987:HOH:O	2.48	0.45
1:C:525:VAL:HG12	1:C:551:CYS:HB2	1.98	0.45
1:C:685:LEU:HD23	1:C:685:LEU:HA	1.84	0.45
1:E:989:ARG:NH2	1:E:1009[B]:GLU:OE1	2.42	0.45
1:E:574:GLN:HG2	1:E:720:LEU:HD11	1.98	0.45
1:E:695:VAL:HG21	1:E:701:ALA:HA	1.99	0.45
1:E:75:ARG:HG2	1:E:75:ARG:NH1	2.32	0.45
2:F:235:GLY:HA2	2:F:263:ILE:HG22	1.98	0.45
1:G:354:TYR:HB2	1:G:388:GLY:O	2.16	0.45
1:G:440:ALA:O	1:G:444:ARG:HG3	2.17	0.45
2:H:41:GLU:HG3	2:H:69:ASP:O	2.17	0.45
1:A:37:LEU:O	1:A:40:GLU:N	2.49	0.45
1:A:632:ILE:HG13	1:A:633:GLU:N	2.32	0.45
2:B:170:TRP:CD1	2:B:210:VAL:HG21	2.52	0.45
1:C:809:MET:O	1:C:813:VAL:HG23	2.17	0.45
1:C:998:ARG:HA	1:C:999:PRO:C	2.37	0.45
1:E:421:LEU:HD23	1:E:421:LEU:HA	1.71	0.45
1:E:833:LYS:O	1:E:834:ASN:HB2	2.16	0.45
2:F:197:TYR:OH	2:F:228:VAL:HG21	2.18	0.45
1:G:36:ALA:O	1:G:40:GLU:HG2	2.16	0.45
1:A:722:GLY:CA	1:A:725:MET:HG3	2.46	0.44
1:C:639:ILE:HD13	1:C:869:MET:HE3	1.98	0.44
8:E:2950:NET:H71	8:E:2950:NET:H23	1.63	0.44
1:E:3:LYS:CB	1:E:330:TYR:CE1	3.00	0.44
1:E:493:LYS:HD2	1:E:493:LYS:HA	1.69	0.44
1:G:1067:GLU:O	1:G:1070:ALA:HB3	2.18	0.44
1:G:289:ASN:HB3	1:G:292:ASN:OD1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:713:VAL:HG12	1:G:715:ARG:HG2	1.99	0.44
1:A:417:ASP:HA	1:A:418:PRO:HD3	1.80	0.44
2:B:22:ALA:N	2:B:107:ILE:O	2.46	0.44
2:B:49:SER:HA	2:B:76:HIS:O	2.18	0.44
1:C:656:ALA:HA	9:C:4594:HOH:O	2.17	0.44
1:C:695:VAL:HG11	1:C:701:ALA:CB	2.46	0.44
1:C:804:GLU:O	1:C:808:VAL:HG23	2.18	0.44
1:C:757:ASP:O	1:C:833:LYS:HE3	2.17	0.44
1:E:174:MET:CE	1:E:303:ARG:NH2	2.81	0.44
2:F:125:LYS:HB2	9:F:2666:HOH:O	2.17	0.44
2:F:310:GLN:NE2	2:F:352:GLY:CA	2.80	0.44
2:F:98:LEU:O	2:F:101:TYR:HB3	2.18	0.44
1:G:467:GLU:O	1:G:471:ARG:HG2	2.17	0.44
1:G:702:VAL:HG21	1:G:735:ARG:HH12	1.82	0.44
1:G:990:LEU:HA	1:G:990:LEU:HD12	1.77	0.44
1:A:163:GLY:O	1:A:166:CYS:HB3	2.17	0.44
1:A:159:ALA:HB2	1:A:188:PHE:CE1	2.51	0.44
1:A:570:ASN:C	1:A:571:ARG:HG3	2.37	0.44
1:A:956:ARG:HG3	9:A:1626:HOH:O	2.17	0.44
1:C:50:ASN:ND2	1:C:53:THR:CG2	2.80	0.44
1:C:698:ILE:O	1:C:701:ALA:N	2.49	0.44
2:D:64:GLY:N	2:D:89:ALA:HB1	2.32	0.44
1:E:168:ILE:HD13	1:E:191:ILE:HG22	2.00	0.44
1:E:991:VAL:CG2	1:E:992:ASN:N	2.80	0.44
2:F:236:ILE:CG2	2:F:237:PHE:N	2.80	0.44
1:G:139:ILE:HG13	1:G:141:LEU:HG	1.99	0.44
1:G:147:GLY:HA3	1:G:158:VAL:HG13	1.96	0.44
1:G:678:PHE:O	1:G:682:VAL:HG23	2.16	0.44
1:G:692:ASN:HB3	1:G:753:ASP:OD1	2.16	0.44
1:G:642:TYR:CE1	1:G:825:LEU:HD12	2.52	0.44
2:H:275:LEU:O	2:H:275:LEU:HG	2.15	0.44
2:H:337:LEU:HA	2:H:337:LEU:HD12	1.69	0.44
2:H:364:ALA:N	2:H:365:PRO:CD	2.80	0.44
1:A:1006:LYS:HB3	1:A:1006:LYS:HE3	1.57	0.44
2:B:48:TYR:HA	2:B:51:GLN:HE21	1.82	0.44
1:C:713:VAL:HG12	1:C:715:ARG:HG2	1.99	0.44
1:A:975:HIS:ND1	1:G:975:HIS:ND1	2.32	0.44
1:A:947:LEU:N	1:A:947:LEU:CD1	2.81	0.44
1:A:993:LYS:H	1:A:996:GLU:HG3	1.82	0.44
2:B:169:SER:HA	2:B:216:LEU:O	2.18	0.44
2:B:234:ASP:CG	2:B:378:ARG:HH11	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:ASP:O	2:F:138:PRO:HD3	2.18	0.44
2:F:142:LEU:HA	2:F:142:LEU:HD12	1.79	0.44
2:F:45:ASP:OD1	2:F:46:PRO:HD2	2.18	0.44
1:G:946:LEU:HB3	1:G:1013:ILE:HG12	1.99	0.44
1:G:75:ARG:NH1	1:G:75:ARG:HG2	2.26	0.44
1:G:75:ARG:CG	1:G:75:ARG:NH1	2.81	0.44
2:H:354:PRO:HB3	2:H:363:ALA:O	2.17	0.44
1:A:158:VAL:O	1:A:162:VAL:HG22	2.17	0.44
1:A:340:THR:O	1:A:343:ARG:NE	2.51	0.44
1:A:723:ARG:NH1	1:A:910:GLU:OE2	2.50	0.44
2:B:266:PHE:HB2	2:B:370:PHE:CD1	2.53	0.44
2:B:290:HIS:HB2	2:B:312:HIS:CD2	2.53	0.44
1:C:905:PRO:HB2	1:C:1040:TYR:OH	2.17	0.44
2:D:273:GLN:HE21	2:D:351:GLN:HE22	1.66	0.44
2:F:195:VAL:HG23	2:F:233:PRO:HB3	1.98	0.44
1:G:839:LEU:HA	1:G:839:LEU:HD13	1.61	0.44
2:H:266:PHE:CD1	2:H:348:PHE:CZ	3.06	0.44
8:A:1086:NET:C4	8:A:1086:NET:H22	2.38	0.44
1:A:172:PHE:HB3	1:A:200:PRO:CG	2.22	0.44
1:A:336:MET:HB3	1:A:342:GLY:HA2	1.99	0.44
1:C:158:VAL:HG11	1:C:206:ILE:HB	1.99	0.44
1:E:301:ASN:HA	1:E:302:PRO:HD3	1.80	0.44
2:H:274:LEU:HA	2:H:274:LEU:HD23	1.82	0.44
2:H:275:LEU:HD22	2:H:349:SER:HB3	2.00	0.44
2:H:363:ALA:C	2:H:365:PRO:HD2	2.37	0.44
1:A:45:ILE:HD13	1:A:81:GLU:HB3	2.00	0.44
1:A:717:SER:HB2	1:A:748:ALA:HB3	1.99	0.44
1:A:981:LEU:HD12	1:A:988:PRO:HG3	2.00	0.44
2:B:215:ARG:NH1	2:B:215:ARG:CG	2.80	0.44
1:E:423:LYS:O	1:E:426:ARG:HB3	2.18	0.44
1:E:436:ILE:CG2	1:E:437:TRP:CE3	3.01	0.44
1:E:890:VAL:O	1:E:918:MET:HA	2.17	0.44
2:F:232:ASN:N	2:F:233:PRO:CD	2.80	0.44
1:G:668:ALA:O	1:G:671:ARG:HB2	2.18	0.44
1:G:882:GLU:OE2	1:G:884:ILE:HD11	2.17	0.44
1:G:93:GLN:HG3	1:G:97:ASN:ND2	2.33	0.44
2:H:324:ASN:O	2:H:342:ARG:HA	2.18	0.44
1:A:487:ASP:HA	1:A:490:ARG:HH12	1.83	0.44
1:A:403:GLU:HG3	1:A:569:PRO:HD2	1.98	0.44
1:C:385:MET:HB2	1:C:603:PRO:HG3	2.00	0.44
2:D:237:PHE:HE1	2:D:268:ILE:HD12	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:237:PHE:CE1	2:F:268:ILE:HD12	2.52	0.44
1:G:994:VAL:CG2	1:G:1001:ILE:HD11	2.23	0.44
1:A:944:ARG:NH1	1:A:972:ASP:OD1	2.51	0.43
1:A:998:ARG:HA	1:A:999:PRO:C	2.38	0.43
1:C:1001:ILE:O	1:C:1005:ILE:HG13	2.18	0.43
1:E:166:CYS:HB2	1:E:207:ASP:O	2.18	0.43
2:F:259:LEU:CD1	2:F:342:ARG:NH1	2.80	0.43
1:G:375:THR:OG1	1:G:376:THR:N	2.49	0.43
2:H:83:ARG:O	2:H:112:ASP:HA	2.18	0.43
1:A:298:ILE:O	1:A:299:GLU:HB3	2.18	0.43
2:B:232:ASN:N	2:B:233:PRO:HD3	2.32	0.43
2:B:205:ILE:HD13	2:B:237:PHE:HZ	1.83	0.43
2:B:354:PRO:HB3	2:B:363:ALA:O	2.18	0.43
2:B:39:TYR:CZ	2:B:61:GLY:HA2	2.53	0.43
1:C:1044:LEU:HA	1:C:1044:LEU:HD12	1.82	0.43
1:C:981:LEU:HD12	1:C:988:PRO:HG3	2.00	0.43
1:E:1017:THR:HG21	1:E:1023:ILE:CA	2.44	0.43
1:E:198:LEU:HD12	1:E:198:LEU:HA	1.74	0.43
1:E:332:LEU:HB3	1:E:347:SER:HB3	1.99	0.43
2:F:208:MET:HE3	9:F:2590:HOH:O	2.18	0.43
2:F:332:LEU:HA	2:F:332:LEU:HD12	1.41	0.43
1:G:174:MET:O	1:G:177:SER:OG	2.30	0.43
1:G:726:GLU:HG3	1:G:737:TYR:CD2	2.53	0.43
2:H:199:PHE:O	2:H:241:GLY:HA3	2.18	0.43
1:A:48:ASN:O	1:A:66:ILE:HA	2.18	0.43
2:B:229:LEU:CD2	2:B:263:ILE:HD11	2.48	0.43
2:B:334:ASP:OD1	2:B:336:THR:HG23	2.19	0.43
1:C:45:ILE:HD13	1:C:83:PRO:HB3	1.99	0.43
2:D:194:VAL:HB	2:D:216:LEU:HD23	2.00	0.43
2:D:335:GLY:HA2	9:D:1770:HOH:O	2.18	0.43
1:G:655:GLU:HB2	9:G:4206:HOH:O	2.18	0.43
1:G:860:PRO:CB	1:G:863:LYS:HD2	2.47	0.43
2:H:326:ARG:NH2	2:H:341:HIS:CD2	2.86	0.43
2:H:33:ASN:OD1	2:H:35:SER:HB2	2.18	0.43
1:A:368:ALA:HB3	9:A:1521:HOH:O	2.18	0.43
1:A:313:LYS:NZ	1:A:603:PRO:O	2.44	0.43
1:A:731:GLU:HB3	9:A:1738:HOH:O	2.17	0.43
1:A:717:SER:CB	1:A:748:ALA:HB3	2.47	0.43
1:A:922:ARG:HE	1:A:1061:LYS:HD3	1.83	0.43
2:B:259:LEU:O	2:B:345:LYS:HE3	2.17	0.43
1:C:886:PRO:HD3	1:C:1072:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:693:ALA:HB2	1:C:708:ILE:HD11	1.94	0.43
1:E:101:GLU:OE1	1:E:104[A]:ARG:NH2	2.48	0.43
1:E:213:TRP:CZ3	1:E:296:ILE:HD12	2.53	0.43
1:E:830:PHE:CE1	1:E:839:LEU:HD13	2.53	0.43
1:E:991:VAL:HG22	1:E:992:ASN:N	2.33	0.43
1:G:237:PHE:CE2	1:G:458:ILE:HD13	2.53	0.43
1:G:524:PRO:HD3	1:G:547:TYR:CZ	2.53	0.43
1:G:9:SER:O	1:G:84:ASP:HB2	2.18	0.43
1:A:1004:ARG:NH2	1:G:983:GLU:HG2	2.30	0.43
2:H:6:LEU:HD11	2:H:8:VAL:CG2	2.48	0.43
1:A:574:GLN:HG2	1:A:720:LEU:HD21	1.99	0.43
1:C:922:ARG:NE	1:C:1061:LYS:HD3	2.23	0.43
1:C:712:LEU:HB3	1:C:728:VAL:HG23	2.01	0.43
1:E:358:LYS:HG2	1:E:359:ILE:N	2.33	0.43
1:G:159:ALA:HB2	1:G:188:PHE:CE1	2.54	0.43
2:H:325:LEU:HA	2:H:325:LEU:HD23	1.58	0.43
2:H:5:ALA:HA	2:H:133:ILE:O	2.18	0.43
1:A:126:ALA:HB3	1:A:302:PRO:HG3	2.01	0.43
1:A:412:LYS:NZ	9:A:1241:HOH:O	2.48	0.43
1:C:25:GLU:OE1	1:C:604:GLU:OE2	2.37	0.43
1:C:766:ALA:HB1	1:C:774:LEU:O	2.19	0.43
1:C:990:LEU:HD23	1:E:979:ILE:CD1	2.49	0.43
2:D:352:GLY:O	2:D:354:PRO:HD3	2.18	0.43
1:E:859:VAL:HA	1:E:860:PRO:HD3	1.85	0.43
2:F:195:VAL:HG11	2:F:228:VAL:HG13	2.00	0.43
2:F:44:THR:O	2:F:46:PRO:HD3	2.18	0.43
1:G:1000:HIS:NE2	1:G:1002:GLN:HB3	2.34	0.43
1:G:148:ILE:CG2	1:G:150:HIS:NE2	2.81	0.43
2:H:290:HIS:HB3	2:H:310:GLN:HB3	1.99	0.43
1:A:1017:THR:HG21	1:A:1023:ILE:CG1	2.48	0.43
1:A:880:THR:O	1:A:881[B]:LYS:HD2	2.19	0.43
2:B:264:PRO:HG3	2:B:373:LEU:O	2.18	0.43
1:C:197:ASP:OD2	1:C:1037:LYS:NZ	2.36	0.43
1:C:712:LEU:HG	1:C:753:ASP:O	2.19	0.43
1:C:975:HIS:HE2	1:E:992:ASN:HD21	1.67	0.43
2:D:120:ARG:HH11	2:D:120:ARG:HD2	1.69	0.43
1:G:820:LEU:HA	1:G:820:LEU:HD23	1.52	0.43
2:H:284:VAL:O	2:H:314:PHE:HB3	2.19	0.43
1:A:951:GLU:O	1:A:954:LYS:HB2	2.19	0.43
2:B:170:TRP:HD1	2:B:210:VAL:HG21	1.81	0.43
1:C:317:PHE:HA	1:C:318:PRO:HD3	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:ASN:ND2	1:C:605:THR:HG23	2.33	0.43
1:E:947:LEU:HG	1:E:1014:ILE:CG2	2.49	0.43
1:E:1018:SER:O	1:E:1022:ALA:HB3	2.19	0.43
2:F:164:THR:N	2:F:198:ASP:OD2	2.51	0.43
1:G:224:LYS:HE2	1:G:329:GLY:O	2.19	0.43
1:G:425:ARG:O	1:G:429:LYS:HB2	2.19	0.43
1:G:717:SER:CB	1:G:748:ALA:HB3	2.48	0.43
1:G:74:VAL:O	1:G:78:ILE:HG13	2.18	0.43
2:H:253:THR:CG2	2:H:254:ALA:N	2.82	0.43
1:A:170:PRO:HA	1:A:204:LEU:HA	2.01	0.43
1:C:28:TYR:O	1:C:32:GLN:HG3	2.19	0.43
1:C:475:LYS:HG2	1:C:488:PHE:CZ	2.54	0.43
1:E:646:THR:HB	1:E:647:PRO:HD3	2.01	0.43
1:E:739:GLN:O	1:E:743:SER:HB3	2.18	0.43
1:G:574:GLN:HE22	1:G:645:GLN:H	1.62	0.43
1:A:171:SER:O	1:A:172:PHE:HB2	2.18	0.43
1:A:38:ARG:HH11	1:A:61:ALA:CA	2.32	0.43
1:A:86:VAL:HG13	1:A:86:VAL:O	2.17	0.43
2:B:350:PHE:HB2	2:B:366:LEU:CD2	2.49	0.43
1:C:1071:GLN:HE21	1:C:1071:GLN:HB3	1.48	0.43
1:C:165:PRO:HA	1:C:182:ALA:O	2.19	0.43
1:C:198:LEU:HA	1:C:198:LEU:HD12	1.77	0.43
1:E:228:CYS:SG	1:E:269:MET:HG2	2.59	0.43
1:E:692:ASN:HB2	1:E:751:LEU:HD11	2.00	0.43
1:G:135:ALA:HB1	1:G:274:GLU:HG2	2.00	0.43
1:G:28:TYR:CZ	1:G:313:LYS:HE3	2.54	0.43
2:H:163:THR:OG1	2:H:198:ASP:O	2.30	0.43
2:H:232:ASN:HD22	2:H:232:ASN:HA	1.39	0.43
1:A:326:LEU:HD12	1:A:326:LEU:HA	1.85	0.42
1:A:528:ARG:HG2	1:A:543:MET:HG2	2.01	0.42
1:A:561:LYS:C	1:A:562:ILE:HG12	2.39	0.42
2:B:300:VAL:CG2	2:B:301:GLU:N	2.82	0.42
1:C:884:ILE:HD13	1:C:884:ILE:HA	1.73	0.42
1:C:885:PRO:HA	1:C:886:PRO:HD3	1.90	0.42
8:E:2950:NET:H52	8:E:2950:NET:H82	1.72	0.42
1:G:174:MET:CE	1:G:303:ARG:NH2	2.81	0.42
1:G:70:HIS:ND1	1:G:72:GLU:HB2	2.34	0.42
1:G:723:ARG:O	1:G:724:ALA:HB3	2.19	0.42
1:G:775:ILE:HA	1:G:775:ILE:HD13	1.82	0.42
1:A:145:ARG:HB2	1:A:208:GLU:CD	2.39	0.42
1:A:722:GLY:HA2	1:A:725:MET:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:LEU:HD23	1:A:981:LEU:HA	1.90	0.42
1:C:1013:ILE:O	1:C:1040:TYR:HA	2.19	0.42
1:C:574:GLN:HG2	1:C:720:LEU:HD11	2.02	0.42
1:E:145:ARG:HH12	1:E:161:ASP:CG	2.23	0.42
1:E:436:ILE:HG22	9:E:3065:HOH:O	2.19	0.42
1:E:702:VAL:HG22	1:E:734:LEU:HD23	2.01	0.42
1:E:901:PRO:O	1:E:903:VAL:N	2.52	0.42
1:G:164:PHE:HB3	1:G:183:TYR:O	2.19	0.42
1:G:623:LEU:HD12	1:G:654:LEU:HD23	2.01	0.42
2:H:265:VAL:O	2:H:347:ALA:HA	2.18	0.42
1:A:481:ILE:HD12	1:A:508:VAL:HG11	2.02	0.42
1:A:998:ARG:HG2	1:A:998:ARG:HH11	1.84	0.42
2:B:158:LEU:HA	2:B:158:LEU:HD23	1.86	0.42
1:C:421:LEU:HD23	1:C:421:LEU:HA	1.86	0.42
1:C:693:ALA:N	1:C:708:ILE:HD11	2.34	0.42
1:C:93:GLN:H	1:C:174:MET:HE3	1.84	0.42
2:D:269:CYS:O	2:D:272:HIS:HB3	2.19	0.42
2:D:367:PHE:O	2:D:370:PHE:HB3	2.19	0.42
1:E:803:GLN:O	1:E:806:GLN:HB2	2.19	0.42
2:F:255:ILE:HA	2:F:258:PHE:HD2	1.83	0.42
1:G:287:ALA:HB2	1:G:298:ILE:HD11	2.01	0.42
1:G:93:GLN:HG3	1:G:97:ASN:HD21	1.84	0.42
2:H:171:THR:HB	2:H:185:LYS:HB2	2.01	0.42
1:A:172:PHE:CD2	1:A:201:THR:CG2	3.02	0.42
1:A:696:THR:O	1:A:696:THR:HG23	2.19	0.42
2:B:285:LYS:HG3	2:B:314:PHE:CD1	2.54	0.42
2:B:302:LYS:C	2:B:304:VAL:HG13	2.39	0.42
1:C:186:GLU:HB2	9:C:4321:HOH:O	2.18	0.42
1:C:986:ILE:O	1:C:988:PRO:HD3	2.19	0.42
2:D:46:PRO:HA	2:D:76:HIS:CG	2.54	0.42
1:E:25:GLU:HG2	1:E:26:PHE:CD2	2.54	0.42
1:E:440:ALA:O	1:E:444:ARG:HG3	2.18	0.42
1:E:795:SER:HB2	1:E:890:VAL:HG22	2.02	0.42
1:E:900:PHE:HA	1:E:901:PRO:HD2	1.83	0.42
2:F:208:MET:SD	2:F:355:GLU:HA	2.59	0.42
1:G:198:LEU:HD12	1:G:198:LEU:HA	1.80	0.42
1:G:224:LYS:NZ	9:G:3992:HOH:O	2.34	0.42
1:G:658:GLY:O	1:G:660:PRO:HD3	2.19	0.42
1:A:40:GLU:OE1	1:A:40:GLU:HA	2.18	0.42
1:A:412:LYS:N	1:A:441:ASP:OD2	2.32	0.42
1:A:490:ARG:HB3	1:A:490:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1000:HIS:O	1:C:1003:ASP:HB2	2.19	0.42
1:C:79:GLU:HA	1:C:111:PHE:CE2	2.54	0.42
1:E:208:GLU:HG3	1:E:208:GLU:O	2.20	0.42
1:G:1031:ARG:HB3	1:G:1031:ARG:HE	1.23	0.42
1:G:675:ARG:HD2	1:G:716:PRO:O	2.20	0.42
2:H:255:ILE:C	2:H:259:LEU:HD12	2.38	0.42
2:H:46:PRO:HD3	2:H:72:SER:HB3	2.01	0.42
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.89	0.42
1:A:392:GLN:OE1	1:A:495:LYS:HD3	2.19	0.42
1:C:701:ALA:HB1	1:C:752:LEU:HD21	2.01	0.42
2:D:23:THR:HG23	2:D:134:ALA:O	2.19	0.42
1:E:907:LEU:HD11	7:E:2920:ORN:HD3	2.01	0.42
1:A:692:ASN:HB3	1:A:753:ASP:OD1	2.20	0.42
2:B:167:ALA:HA	2:B:218:ILE:O	2.19	0.42
2:B:176:THR:O	2:B:180:GLY:N	2.45	0.42
1:C:305:SER:H	1:C:308:SER:HB3	1.85	0.42
1:C:2:PRO:HB2	1:C:3:LYS:H	1.72	0.42
1:C:899:LYS:C	1:C:901:PRO:HD3	2.40	0.42
2:D:200:GLY:O	2:D:240:ASN:ND2	2.52	0.42
2:F:2:ILE:HD12	2:F:2:ILE:C	2.36	0.42
1:G:1001:ILE:CG1	1:G:1002:GLN:N	2.80	0.42
1:G:622:THR:OG1	1:G:625:ASP:OD2	2.29	0.42
1:G:768:CYS:HB2	1:G:817:ALA:HB1	2.02	0.42
1:A:135:ALA:HB1	1:A:274:GLU:CG	2.49	0.42
2:D:300:VAL:HG23	2:D:301:GLU:N	2.33	0.42
2:D:302:LYS:O	2:D:303:ASN:HB3	2.19	0.42
1:E:1017:THR:CG2	1:E:1023:ILE:HG13	2.49	0.42
1:E:1028:VAL:HG13	1:E:1029:ILE:HD12	2.01	0.42
1:G:526:TYR:CE1	1:G:545:SER:HB3	2.55	0.42
1:G:382:GLY:HA3	1:G:570:ASN:O	2.20	0.42
1:G:597:ILE:HG12	1:G:615:ARG:HB2	2.01	0.42
1:A:574:GLN:NE2	1:A:720:LEU:HD21	2.32	0.42
1:A:890:VAL:HG12	1:A:931:ALA:HB2	2.01	0.42
1:C:3:LYS:HB3	1:C:330:TYR:CE2	2.55	0.42
1:C:482:THR:HG22	9:C:4511:HOH:O	2.19	0.42
1:C:527:LYS:HB2	1:C:544:TYR:CZ	2.55	0.42
1:C:922:ARG:HH21	1:C:1061:LYS:CG	2.33	0.42
1:E:1028:VAL:O	1:E:1032:SER:OG	2.30	0.42
2:F:123:ARG:NH2	9:F:2627:HOH:O	2.53	0.42
2:F:237:PHE:CZ	2:F:268:ILE:HD12	2.53	0.42
1:G:755:PHE:CE1	6:G:3910:ANP:H2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:981:LEU:CD1	1:G:988:PRO:HG3	2.41	0.42
2:H:279:SER:HB2	2:H:325:LEU:HD11	2.00	0.42
2:H:298:LYS:O	2:H:329:HIS:HA	2.19	0.42
2:H:32:PHE:O	2:H:291:HIS:HB2	2.18	0.42
1:A:885:PRO:HG2	9:A:1623:HOH:O	2.19	0.42
2:B:332:LEU:HD12	2:B:332:LEU:HA	1.79	0.42
2:B:264:PRO:HG2	2:B:374:ILE:HG12	2.02	0.42
1:C:941:LYS:HE2	1:C:1054:LEU:HD23	2.01	0.42
1:C:774:LEU:HD12	1:C:775:ILE:N	2.35	0.42
1:C:784:GLN:N	1:C:784:GLN:NE2	2.49	0.42
1:C:859:VAL:HA	1:C:860:PRO:HD3	1.92	0.42
2:D:350:PHE:HB2	2:D:366:LEU:HD22	2.01	0.42
1:E:716:PRO:CD	1:E:725:MET:HG2	2.47	0.42
2:F:249:ASP:OD1	2:F:249:ASP:N	2.53	0.42
1:G:82:ARG:NH1	1:G:111:PHE:HE2	2.18	0.42
1:G:187:GLU:O	1:G:191:ILE:HD12	2.20	0.42
1:G:623:LEU:CD1	1:G:654:LEU:HD23	2.50	0.42
2:H:244:ASP:OD1	2:H:245:PRO:HD2	2.20	0.42
1:A:289:ASN:HB3	1:A:292:ASN:OD1	2.20	0.41
1:C:488:PHE:O	1:C:492:LEU:HG	2.20	0.41
1:C:890:VAL:HG23	1:C:927:ALA:CB	2.50	0.41
8:E:2950:NET:H43	8:E:2950:NET:H12	1.71	0.41
1:E:781:HIS:HE1	1:E:789:SER:HB2	1.85	0.41
2:F:321:LEU:HA	2:F:321:LEU:HD12	1.80	0.41
1:G:183:TYR:N	1:G:187:GLU:OE1	2.43	0.41
1:G:671:ARG:NH2	1:G:819:GLU:O	2.53	0.41
1:G:984:ALA:HB2	9:G:4514:HOH:O	2.20	0.41
2:H:138:PRO:HA	9:H:3552:HOH:O	2.20	0.41
1:A:238:ASP:HB2	1:A:247:SER:HB3	2.02	0.41
1:A:981:LEU:CD1	1:A:988:PRO:HG3	2.50	0.41
2:B:174:SER:O	2:B:182:PRO:HD3	2.20	0.41
2:B:307:ILE:O	2:B:362:ASP:HB2	2.19	0.41
1:C:85:ALA:HA	1:C:114:THR:O	2.20	0.41
1:C:585:ALA:HB2	1:C:642:TYR:CE2	2.55	0.41
1:C:367:PHE:CE1	1:C:912:ARG:HG2	2.56	0.41
1:E:1036:TYR:C	1:E:1037:LYS:HG2	2.41	0.41
1:E:94:THR:OG1	8:E:2950:NET:H71	2.20	0.41
1:G:1001:ILE:HD12	1:G:1002:GLN:CA	2.50	0.41
1:G:574:GLN:HG2	1:G:720:LEU:HD21	2.01	0.41
2:H:144:LEU:HD11	2:H:148:ARG:HE	1.86	0.41
2:H:205:ILE:HG21	2:H:237:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:HIS:CD2	1:A:1003:ASP:CB	3.03	0.41
1:A:745:SER:O	1:A:748:ALA:HB3	2.20	0.41
1:C:502:LEU:HA	1:C:502:LEU:HD23	1.77	0.41
1:G:332:LEU:O	1:G:346:ALA:HB3	2.21	0.41
1:G:453:PHE:HD1	1:G:458:ILE:O	2.03	0.41
1:G:816:LEU:HD11	1:G:839:LEU:HD21	2.02	0.41
1:G:883:VAL:O	1:G:884:ILE:HD13	2.20	0.41
1:A:363:ASN:OD1	1:A:381:VAL:HG21	2.21	0.41
2:B:277:LEU:HA	2:B:277:LEU:HD23	1.78	0.41
2:B:305:VAL:CG1	2:B:306:MET:N	2.83	0.41
2:B:285:LYS:CG	2:B:314:PHE:CE1	3.02	0.41
1:C:900:PHE:N	1:C:901:PRO:HD3	2.35	0.41
1:E:148:ILE:HD13	1:E:148:ILE:HA	1.93	0.41
1:E:172:PHE:CD2	1:E:201:THR:HG23	2.55	0.41
8:E:2950:NET:H63	8:E:2950:NET:H31	1.66	0.41
1:E:503:ALA:HB1	1:E:508:VAL:O	2.20	0.41
2:F:98:LEU:HG	2:F:102:LEU:HD11	2.01	0.41
2:F:310:GLN:HE22	2:F:352:GLY:CA	2.33	0.41
1:G:949:VAL:HB	1:G:1016:THR:OG1	2.20	0.41
1:G:675:ARG:NH2	1:G:841:GLU:OE1	2.54	0.41
2:H:158:LEU:HA	2:H:158:LEU:HD23	1.76	0.41
1:A:145:ARG:HB2	1:A:208:GLU:OE2	2.20	0.41
2:B:208:MET:HA	2:B:211:ASP:HB2	2.01	0.41
2:B:80:LEU:HA	2:B:80:LEU:HD12	1.85	0.41
1:G:1064:SER:OG	1:G:1066:GLN:HB2	2.21	0.41
1:G:3:LYS:CB	1:G:330:TYR:CE2	3.04	0.41
1:G:679:GLN:HG2	1:G:679:GLN:O	2.20	0.41
1:G:717:SER:HB3	1:G:748:ALA:HB3	2.03	0.41
1:G:642:TYR:OH	1:G:865:ALA:HB3	2.21	0.41
1:G:899:LYS:C	1:G:901:PRO:HD3	2.41	0.41
1:G:981:LEU:HD23	1:G:981:LEU:HA	1.78	0.41
2:H:354:PRO:HB2	2:H:367:PHE:CE2	2.56	0.41
1:A:1017:THR:HG22	1:A:1018:SER:H	1.83	0.41
1:A:347:SER:O	2:B:296:PRO:HB3	2.21	0.41
1:A:3:LYS:HB3	1:A:330:TYR:CE2	2.56	0.41
1:A:768:CYS:HB2	1:A:817:ALA:HB1	2.02	0.41
2:B:299:ASP:HA	2:B:329:HIS:CD2	2.55	0.41
2:B:350:PHE:CD1	2:B:366:LEU:HD21	2.55	0.41
1:C:1000:HIS:H	1:C:1000:HIS:CD2	2.39	0.41
1:C:809:MET:HG2	1:C:837:VAL:HG11	2.02	0.41
1:G:194:ARG:NH1	1:G:194:ARG:CB	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:ILE:HG22	1:G:66:ILE:O	2.20	0.41
2:H:2:ILE:HG13	2:H:2:ILE:O	2.20	0.41
2:H:60:ILE:O	2:H:86:PRO:HD2	2.21	0.41
1:A:904:ASP:HA	1:A:905:PRO:HD3	1.87	0.41
2:B:222:GLN:H	2:B:222:GLN:HE21	1.69	0.41
1:C:695:VAL:HG12	1:C:696:THR:N	2.34	0.41
1:C:99:ALA:HB1	1:C:115:MET:CE	2.51	0.41
1:E:1022:ALA:O	1:E:1025:ASP:HB2	2.21	0.41
1:E:174:MET:CE	1:E:303:ARG:CZ	2.99	0.41
1:E:998:ARG:NH1	1:E:998:ARG:CG	2.81	0.41
1:G:172:PHE:CE2	1:G:201:THR:HG21	2.55	0.41
1:G:698:ILE:O	1:G:701:ALA:HB3	2.20	0.41
1:G:578:PHE:HE1	1:G:846:ALA:O	2.03	0.41
2:H:169:SER:HA	2:H:216:LEU:O	2.20	0.41
1:A:424:ILE:O	1:A:428:LEU:HD13	2.21	0.41
1:C:698:ILE:C	1:C:702:VAL:HG23	2.41	0.41
1:C:828:VAL:HG13	1:C:842:VAL:HG22	2.03	0.41
1:E:171:SER:O	1:E:172:PHE:HB2	2.21	0.41
1:E:667:ASP:OD1	1:E:677:ARG:NH2	2.42	0.41
1:A:119:THR:H	1:A:119:THR:HG23	1.56	0.41
1:A:10:ILE:HG22	1:A:11:LEU:N	2.36	0.41
1:A:576:ILE:HG21	1:A:576:ILE:HD13	1.85	0.41
1:A:751:LEU:HG	1:A:752:LEU:N	2.36	0.41
1:A:822:VAL:C	1:A:823:ARG:HG2	2.41	0.41
2:B:122:LEU:O	2:B:126:GLY:N	2.53	0.41
2:B:286:MET:HE1	2:B:314:PHE:O	2.21	0.41
1:C:712:LEU:C	1:C:712:LEU:HD23	2.41	0.41
1:C:720:LEU:HD12	1:C:720:LEU:O	2.21	0.41
1:C:900:PHE:HA	1:C:901:PRO:HD2	1.68	0.41
1:E:516:LEU:HA	1:E:516:LEU:HD12	1.91	0.41
1:G:1000:HIS:O	1:G:1000:HIS:HD2	2.04	0.41
1:G:1073:LYS:HD3	1:G:1073:LYS:HA	1.78	0.41
8:G:3950:NET:H63	8:G:3950:NET:H31	1.57	0.41
1:G:770:GLY:CA	1:G:823:ARG:CZ	2.98	0.41
2:H:292:GLY:HA3	9:H:3478:HOH:O	2.21	0.41
1:A:470:VAL:O	1:A:473:GLU:HB2	2.21	0.41
1:A:523:HIS:HB3	1:A:524:PRO:HD2	2.02	0.41
1:A:646:THR:CB	1:A:647:PRO:HD3	2.51	0.41
2:B:71:GLU:C	2:B:203:ARG:HG3	2.41	0.41
1:C:648:LEU:HD12	1:C:648:LEU:HA	1.89	0.41
1:C:659:VAL:HA	1:C:660:PRO:HD3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:VAL:HA	1:E:65:TYR:O	2.21	0.41
2:F:154:ASN:HD22	2:F:155:GLY:N	2.19	0.41
2:F:217:THR:C	2:F:218:ILE:HD13	2.40	0.41
1:G:152:MET:O	1:G:156:LEU:HG	2.21	0.41
1:G:634:LYS:N	1:G:635:PRO:HD3	2.36	0.41
2:H:225:ALA:HB1	2:H:258:PHE:CE1	2.56	0.41
1:A:1000:HIS:NE2	1:A:1003:ASP:OD2	2.54	0.41
1:A:258:ASP:O	1:A:262:GLN:HG2	2.21	0.41
1:A:574:GLN:HG3	1:A:720:LEU:HD11	2.02	0.41
2:B:236:ILE:HG22	2:B:237:PHE:N	2.36	0.41
1:C:659:VAL:CG1	1:C:660:PRO:HD2	2.51	0.41
1:E:167:ILE:N	1:E:167:ILE:HD12	2.37	0.41
1:E:903:VAL:O	1:E:905:PRO:HD3	2.21	0.41
2:F:223:THR:HG22	2:F:228:VAL:HG23	2.02	0.41
2:F:255:ILE:HA	2:F:258:PHE:CD2	2.56	0.41
1:G:461:TRP:O	1:G:465:GLN:HG3	2.21	0.41
1:G:315:THR:O	1:G:531:THR:HG22	2.20	0.41
1:G:619:GLU:HB3	1:G:620:PRO:HD2	2.03	0.41
1:G:80:LYS:HG2	1:G:81:GLU:HG2	2.01	0.41
1:G:828:VAL:CG1	1:G:842:VAL:HG22	2.38	0.41
2:H:209:LEU:HD23	2:H:209:LEU:HA	1.91	0.41
2:H:341:HIS:ND1	2:H:347:ALA:O	2.54	0.41
1:A:906:LEU:HD21	1:A:1023:ILE:HG12	2.03	0.40
1:A:858:GLY:HA2	1:A:1069:HIS:CE1	2.56	0.40
1:A:1069:HIS:ND1	9:A:1644:HOH:O	2.37	0.40
8:C:1950:NET:H11	8:C:1950:NET:H83	1.76	0.40
1:C:286:PHE:CD1	1:C:295:LEU:HD11	2.55	0.40
1:C:683:GLU:O	1:C:686:LYS:N	2.53	0.40
1:E:1072:ILE:HG22	9:E:3630:HOH:O	2.20	0.40
1:E:174:MET:HE3	1:E:303:ARG:NH2	2.36	0.40
1:E:70:HIS:O	1:E:73:VAL:N	2.54	0.40
2:F:294:ASN:OD1	2:F:294:ASN:N	2.54	0.40
1:G:679:GLN:CB	1:G:689:GLN:HE22	2.34	0.40
1:G:679:GLN:CG	1:G:689:GLN:HE22	2.32	0.40
1:G:693:ALA:HB1	1:G:704:LYS:HG2	2.03	0.40
1:A:1020:ARG:O	1:A:1024:GLU:HG3	2.22	0.40
1:A:836:GLU:HB3	1:A:838:TYR:CE1	2.55	0.40
1:A:904:ASP:OD1	1:A:905:PRO:HD2	2.20	0.40
1:A:950:ARG:HG3	1:A:1016:THR:OG1	2.20	0.40
1:A:951:GLU:HA	1:A:954:LYS:HD2	2.04	0.40
1:A:990:LEU:HB3	1:G:979:ILE:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:ASP:OD1	2:B:345:LYS:N	2.54	0.40
8:C:1950:NET:H63	8:C:1950:NET:H31	1.90	0.40
1:E:1:MET:HG3	1:E:2:PRO:CD	2.44	0.40
1:G:761:GLU:HB3	1:G:781:HIS:ND1	2.36	0.40
2:H:127:ALA:HB2	9:H:3532:HOH:O	2.21	0.40
1:A:172:PHE:CD2	1:A:201:THR:HG23	2.56	0.40
1:A:82:ARG:HA	1:A:82:ARG:HD2	1.48	0.40
2:B:346:PRO:HB2	2:B:373:LEU:HD13	2.03	0.40
1:C:273:ARG:HD2	9:C:4089:HOH:O	2.22	0.40
1:C:354:TYR:CD1	1:C:387:ILE:CG2	3.04	0.40
2:D:201:ALA:HB2	2:D:239:SER:HB2	2.03	0.40
1:E:273:ARG:HH11	1:E:273:ARG:HD2	1.72	0.40
1:E:373:ARG:NH1	1:E:430:ASP:O	2.47	0.40
1:E:720:LEU:HD12	1:E:720:LEU:C	2.41	0.40
1:E:809:MET:O	1:E:813:VAL:HG23	2.21	0.40
1:G:1001:ILE:HG13	1:G:1002:GLN:H	1.86	0.40
1:G:148:ILE:HG23	1:G:203:GLU:HG3	2.02	0.40
1:G:236:ASN:OD1	1:G:244:THR:HG22	2.22	0.40
1:G:746:ASN:C	1:G:748:ALA:H	2.24	0.40
2:H:255:ILE:CG2	2:H:259:LEU:HD11	2.48	0.40
2:H:63:VAL:O	2:H:94:ASN:HB2	2.22	0.40
1:A:56:THR:O	1:A:855:LYS:HE2	2.22	0.40
1:C:385:MET:HG2	1:C:386:ALA:N	2.36	0.40
1:C:421:LEU:HD13	1:G:421:LEU:HD22	2.04	0.40
1:C:684:ARG:NH1	1:C:684:ARG:HG3	2.16	0.40
1:C:700:MET:HE1	1:C:703:GLU:HG2	2.02	0.40
1:C:843:ASN:HA	1:C:844:PRO:HD3	1.84	0.40
2:D:286:MET:HE2	2:D:312:HIS:ND1	2.36	0.40
2:D:324:ASN:HA	2:D:343:THR:OG1	2.21	0.40
1:E:339:ILE:HD11	1:E:531:THR:HG23	2.03	0.40
2:F:275:LEU:HD23	2:F:349:SER:CB	2.51	0.40
1:G:1:MET:CB	1:G:2:PRO:HD2	2.51	0.40
2:H:225:ALA:O	2:H:229:LEU:HD12	2.22	0.40
2:H:342:ARG:HA	2:H:342:ARG:HD2	1.76	0.40
1:A:211:ILE:HG13	6:A:1083:ANP:H2	2.04	0.40
1:A:4:ARG:CZ	1:A:7:ILE:CD1	3.00	0.40
1:C:1:MET:CB	1:C:2:PRO:HD2	2.52	0.40
1:C:641:GLN:NE2	1:C:664:THR:O	2.55	0.40
1:C:715:ARG:HA	1:C:716:PRO:HD2	2.00	0.40
2:D:286:MET:HE1	2:D:312:HIS:ND1	2.37	0.40
2:D:363:ALA:O	2:D:366:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:716:PRO:HB3	1:E:741:ALA:O	2.21	0.40
2:F:371:ILE:HD13	2:F:371:ILE:HA	1.88	0.40
1:G:825:LEU:HG	1:G:865:ALA:HB2	2.03	0.40
1:G:82:ARG:NH1	1:G:111:PHE:CE2	2.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1075/1073 (100%)	1008 (94%)	63 (6%)	4 (0%)	34	32
1	C	1071/1073 (100%)	1009 (94%)	54 (5%)	8 (1%)	22	18
1	E	1074/1073 (100%)	1020 (95%)	48 (4%)	6 (1%)	25	21
1	G	1073/1073 (100%)	993 (92%)	72 (7%)	8 (1%)	22	18
2	B	377/382 (99%)	350 (93%)	23 (6%)	4 (1%)	14	9
2	D	377/382 (99%)	363 (96%)	14 (4%)	0	100	100
2	F	377/382 (99%)	361 (96%)	14 (4%)	2 (0%)	29	26
2	H	377/382 (99%)	358 (95%)	19 (5%)	0	100	100
All	All	5801/5820 (100%)	5462 (94%)	307 (5%)	32 (1%)	25	21

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	975	HIS
2	F	136	ASP
1	G	975	HIS
2	B	346	PRO
1	C	707	GLU
1	C	975	HIS

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Mol	Chain	Res	Type
1	E	835	ASN
1	G	558	ASP
1	G	873	SER
1	G	1001	ILE
1	A	368	ALA
2	B	191	PRO
1	C	2	PRO
1	C	708	ILE
1	C	873	SER
1	E	708	ILE
2	F	243	GLY
1	G	707	GLU
1	A	2	PRO
1	A	24	CYS
2	B	229	LEU
1	C	821	GLN
1	E	2	PRO
1	E	707	GLU
1	E	975	HIS
1	G	71	TRP
1	G	860	PRO
1	C	341	GLY
1	C	698	ILE
1	G	2	PRO
1	E	902	GLY
2	B	228	VAL

### 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	882/878 (100%)	785 (89%)	97 (11%)	6	3
1	C	878/878 (100%)	783 (89%)	95 (11%)	6	3
1	E	881/878 (100%)	800 (91%)	81 (9%)	9	6
1	G	880/878 (100%)	761 (86%)	119 (14%)	4	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	308/310 (99%)	279 (91%)	29 (9%)	8	5
2	D	308/310 (99%)	290 (94%)	18 (6%)	20	17
2	F	308/310 (99%)	282 (92%)	26 (8%)	11	7
2	H	308/310 (99%)	276 (90%)	32 (10%)	7	4
All	All	4753/4752 (100%)	4256 (90%)	497 (10%)	7	4

All (497) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	25	GLU
1	A	38	ARG
1	A	46	LEU
1	A	49	SER
1	A	54	ILE
1	A	57	ASP
1	A	59	GLU
1	A	60	MET
1	A	62	ASP
1	A	76	LYS
1	A	103	GLU
1	A	105	GLN
1	A	109	GLU
1	A	119	THR
1	A	130	ARG
1	A	137	LYS
1	A	174	MET
1	A	185	ARG
1	A	197	ASP
1	A	236	ASN
1	A	279	THR
1	A	300	MET
1	A	306	ARG
1	A	326	LEU
1	A	403	GLU
1	A	412	LYS
1	A	416	ASP
1	A	482	THR
1	A	490	ARG
1	A	509	ARG
1	A	515	LYS

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Mol	Chain	Res	Type
1	A	518	ASP
1	A	542	TYR
1	A	548	GLU
1	A	558	ASP
1	A	559	ARG
1	A	562	ILE
1	A	571	ARG
1	A	587	LEU
1	A	592	ASP
1	A	604	GLU
1	A	613	SER
1	A	645	GLN
1	A	646	THR
1	A	671	ARG
1	A	675	ARG
1	A	684	ARG
1	A	688	LYS
1	A	694	THR
1	A	695	VAL
1	A	696	THR
1	A	698	ILE
1	A	699	GLU
1	A	700	MET
1	A	703	GLU
1	A	707	GLU
1	A	723	ARG
1	A	733	ASP
1	A	739	GLN
1	A	740	THR
1	A	745	SER
1	A	763	ASP
1	A	784	GLN
1	A	800	THR
1	A	805	ILE
1	A	821	GLN
1	A	833	LYS
1	A	839	LEU
1	A	849	THR
1	A	855	LYS
1	A	881[A]	LYS
1	A	881[B]	LYS
1	A	906	LEU

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Mol	Chain	Res	Type
1	A	912[A]	ARG
1	A	912[B]	ARG
1	A	923	THR
1	A	938	THR
1	A	948	SER
1	A	950	ARG
1	A	954	LYS
1	A	972	ASP
1	A	992	ASN
1	A	996	GLU
1	A	998	ARG
1	A	1000	HIS
1	A	1001	ILE
1	A	1004	ARG
1	A	1006	LYS
1	A	1009	GLU
1	A	1014	ILE
1	A	1020	ARG
1	A	1021	ARG
1	A	1023	ILE
1	A	1028	VAL
1	A	1032	SER
1	A	1037	LYS
2	B	2	ILE
2	B	3	LYS
2	B	6	LEU
2	B	47	SER
2	B	87	LEU
2	B	99	SER
2	B	104	ARG
2	B	106	ASN
2	B	113	ILE
2	B	123	ARG
2	B	154	ASN
2	B	169	SER
2	B	174	SER
2	B	183	GLN
2	B	192	PHE
2	B	215	ARG
2	B	222	GLN
2	B	238	LEU
2	B	239	SER

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Mol	Chain	Res	Type
2	B	263	ILE
2	B	324	ASN
2	B	326	ARG
2	B	331	SER
2	B	333	PHE
2	B	343	THR
2	B	348	PHE
2	B	357	SER
2	B	373	LEU
2	B	374	ILE
1	C	1	MET
1	C	2	PRO
1	C	4	ARG
1	C	5	THR
1	C	8	LYS
1	C	38	ARG
1	C	46	LEU
1	C	60	MET
1	C	103	GLU
1	C	109	GLU
1	C	137	LYS
1	C	174	MET
1	C	185	ARG
1	C	198	LEU
1	C	202	LYS
1	C	207	ASP
1	C	217	GLU
1	C	296	ILE
1	C	313	LYS
1	C	321	LYS
1	C	326	LEU
1	C	338	ASP
1	C	343	ARG
1	C	344	THR
1	C	363	ASN
1	C	384	VAL
1	C	403	GLU
1	C	414	SER
1	C	416	ASP
1	C	482	THR
1	C	518	ASP
1	C	542	TYR

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Mol	Chain	Res	Type
1	C	548	GLU
1	C	558	ASP
1	C	559	ARG
1	C	571	ARG
1	C	587	LEU
1	C	591	GLU
1	C	636	LYS
1	C	645	GLN
1	C	646	THR
1	C	652	ARG
1	C	665	SER
1	C	675	ARG
1	C	680	HIS
1	C	684	ARG
1	C	694	THR
1	C	696	THR
1	C	698	ILE
1	C	699	GLU
1	C	700	MET
1	C	703	GLU
1	C	707	GLU
1	C	715	ARG
1	C	717	SER
1	C	723	ARG
1	C	731	GLU
1	C	733	ASP
1	C	736	ARG
1	C	739	GLN
1	C	740	THR
1	C	745	SER
1	C	749	PRO
1	C	752	LEU
1	C	753	ASP
1	C	757	ASP
1	C	763	ASP
1	C	784	GLN
1	C	800	THR
1	C	805	ILE
1	C	812	GLN
1	C	815	LYS
1	C	821	GLN
1	C	834	ASN

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Mol	Chain	Res	Type
1	C	835	ASN
1	C	838	TYR
1	C	839	LEU
1	C	855	LYS
1	C	880	THR
1	C	891	LYS
1	C	912	ARG
1	C	937	SER
1	C	950	ARG
1	C	955	GLU
1	C	972	ASP
1	C	992	ASN
1	C	998	ARG
1	C	1000	HIS
1	C	1017	THR
1	C	1018	SER
1	C	1020	ARG
1	C	1021	ARG
1	C	1028	VAL
1	C	1031	ARG
1	C	1061	LYS
2	D	2	ILE
2	D	6	LEU
2	D	35	SER
2	D	49	SER
2	D	82	ILE
2	D	87	LEU
2	D	154	ASN
2	D	183	GLN
2	D	212	ARG
2	D	215	ARG
2	D	222	GLN
2	D	301	GLU
2	D	321	LEU
2	D	324	ASN
2	D	332	LEU
2	D	357	SER
2	D	366	LEU
2	D	379	LYS
1	E	1	MET
1	E	5	THR
1	E	46	LEU

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Mol	Chain	Res	Type
1	E	100	LEU
1	E	104[A]	ARG
1	E	104[B]	ARG
1	E	109	GLU
1	E	119	THR
1	E	137	LYS
1	E	158	VAL
1	E	185	ARG
1	E	197	ASP
1	E	202	LYS
1	E	236	ASN
1	E	275	ILE
1	E	278	GLU
1	E	294	ARG
1	E	296	ILE
1	E	300	MET
1	E	303	ARG
1	E	305	SER
1	E	358	LYS
1	E	412	LYS
1	E	414	SER
1	E	426	ARG
1	E	509	ARG
1	E	515	LYS
1	E	518	ASP
1	E	542	TYR
1	E	548	GLU
1	E	558	ASP
1	E	559	ARG
1	E	562	ILE
1	E	571	ARG
1	E	587	LEU
1	E	591	GLU
1	E	645	GLN
1	E	646	THR
1	E	649	LYS
1	E	652	ARG
1	E	675	ARG
1	E	680	HIS
1	E	688	LYS
1	E	696	THR
1	E	698	ILE

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Mol	Chain	Res	Type
1	E	699	GLU
1	E	700	MET
1	E	703	GLU
1	E	712	LEU
1	E	717	SER
1	E	720	LEU
1	E	731	GLU
1	E	733	ASP
1	E	739	GLN
1	E	745	SER
1	E	747	ASP
1	E	752	LEU
1	E	763	ASP
1	E	784	GLN
1	E	789	SER
1	E	805	ILE
1	E	839	LEU
1	E	849	THR
1	E	855	LYS
1	E	881	LYS
1	E	891	LYS
1	E	912	ARG
1	E	950	ARG
1	E	954	LYS
1	E	996	GLU
1	E	998	ARG
1	E	1000	HIS
1	E	1001	ILE
1	E	1006	LYS
1	E	1009[A]	GLU
1	E	1009[B]	GLU
1	E	1014	ILE
1	E	1018	SER
1	E	1021	ARG
1	E	1028	VAL
1	E	1032	SER
2	F	2	ILE
2	F	6	LEU
2	F	25	SER
2	F	73	SER
2	F	87	LEU
2	F	104	ARG

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Mol	Chain	Res	Type
2	F	154	ASN
2	F	163	THR
2	F	169	SER
2	F	178	THR
2	F	183	GLN
2	F	198	ASP
2	F	206	LEU
2	F	215	ARG
2	F	222	GLN
2	F	224	SER
2	F	231	MET
2	F	257	LYS
2	F	263	ILE
2	F	306	MET
2	F	321	LEU
2	F	324	ASN
2	F	332	LEU
2	F	357	SER
2	F	366	LEU
2	F	379	LYS
1	G	1	MET
1	G	5	THR
1	G	8	LYS
1	G	43	ARG
1	G	46	LEU
1	G	59	GLU
1	G	76	LYS
1	G	100	LEU
1	G	103	GLU
1	G	104	ARG
1	G	105	GLN
1	G	109	GLU
1	G	137	LYS
1	G	152	MET
1	G	153	GLU
1	G	174	MET
1	G	177	SER
1	G	185	ARG
1	G	197	ASP
1	G	202	LYS
1	G	207	ASP
1	G	236	ASN

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Mol	Chain	Res	Type
1	G	272	LEU
1	G	279	THR
1	G	285	GLN
1	G	300	MET
1	G	303	ARG
1	G	317	PHE
1	G	321	LYS
1	G	331	THR
1	G	343	ARG
1	G	344	THR
1	G	363	ASN
1	G	412	LYS
1	G	414	SER
1	G	416	ASP
1	G	426	ARG
1	G	471	ARG
1	G	481	ILE
1	G	482	THR
1	G	490[A]	ARG
1	G	490[B]	ARG
1	G	509	ARG
1	G	515	LYS
1	G	518	ASP
1	G	542	TYR
1	G	548	GLU
1	G	558	ASP
1	G	559	ARG
1	G	571	ARG
1	G	576	ILE
1	G	591	GLU
1	G	634	LYS
1	G	645	GLN
1	G	646	THR
1	G	648	LEU
1	G	652	ARG
1	G	655	GLU
1	G	671	ARG
1	G	675	ARG
1	G	684	ARG
1	G	686	LYS
1	G	689	GLN
1	G	696	THR

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Mol	Chain	Res	Type
1	G	698	ILE
1	G	699	GLU
1	G	700	MET
1	G	703	GLU
1	G	707	GLU
1	G	715	ARG
1	G	717	SER
1	G	723	ARG
1	G	726	GLU
1	G	731	GLU
1	G	733	ASP
1	G	736	ARG
1	G	739	GLN
1	G	740	THR
1	G	747	ASP
1	G	751	LEU
1	G	752	LEU
1	G	753	ASP
1	G	763	ASP
1	G	778	ILE
1	G	784	GLN
1	G	804	GLU
1	G	805	ILE
1	G	811	GLN
1	G	815	LYS
1	G	821	GLN
1	G	835	ASN
1	G	839	LEU
1	G	849	THR
1	G	855	LYS
1	G	880	THR
1	G	891	LYS
1	G	895	LEU
1	G	906	LEU
1	G	912	ARG
1	G	944	ARG
1	G	949	VAL
1	G	950	ARG
1	G	955	GLU
1	G	956	ARG
1	G	991	VAL
1	G	998	ARG

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Mol	Chain	Res	Type
1	G	999	PRO
1	G	1000	HIS
1	G	1001	ILE
1	G	1004	ARG
1	G	1014	ILE
1	G	1020	ARG
1	G	1021	ARG
1	G	1027	ARG
1	G	1028	VAL
1	G	1031	ARG
1	G	1032	SER
1	G	1061	LYS
1	G	1064	SER
2	H	2	ILE
2	H	4	SER
2	H	6	LEU
2	H	18	ARG
2	H	25	SER
2	H	35	SER
2	H	73	SER
2	H	87	LEU
2	H	104	ARG
2	H	110	ILE
2	H	144	LEU
2	H	154	ASN
2	H	169	SER
2	H	174	SER
2	H	175	TRP
2	H	185	LYS
2	H	186	LYS
2	H	215	ARG
2	H	222	GLN
2	H	223	THR
2	H	232	ASN
2	H	238	LEU
2	H	239	SER
2	H	253	THR
2	H	261	THR
2	H	263	ILE
2	H	275	LEU
2	H	301	GLU
2	H	321	LEU

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Mol	Chain	Res	Type
2	H	324	ASN
2	H	331	SER
2	H	332	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	266	ASN
1	A	285	GLN
1	A	457	ASN
1	A	574	GLN
1	A	679	GLN
1	A	689	GLN
1	A	754	HIS
1	A	784	GLN
1	A	803	GLN
1	A	812	GLN
1	A	814	GLN
1	A	834	ASN
1	A	942	HIS
1	A	987	ASN
1	A	992	ASN
1	A	1000	HIS
1	A	1007	ASN
1	A	1035	GLN
1	A	1055	ASN
1	A	1071	GLN
2	B	51	GLN
2	B	78	GLN
2	B	154	ASN
2	B	193	HIS
2	B	222	GLN
2	B	324	ASN
2	B	351	GLN
1	C	266	ASN
1	C	285	GLN
1	C	457	ASN
1	C	519	GLN
1	C	523	HIS
1	C	574	GLN
1	C	746	ASN

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Mol	Chain	Res	Type
1	C	754	HIS
1	C	784	GLN
1	C	821	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	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	150	HIS
1	E	266	ASN
1	E	285	GLN
1	E	457	ASN
1	E	574	GLN
1	E	689	GLN
1	E	784	GLN
1	E	803	GLN
1	E	834	ASN
1	E	843	ASN
1	E	942	HIS
1	E	992	ASN
1	E	1000	HIS
1	E	1035	GLN
1	E	1055	ASN
1	E	1071	GLN
2	F	51	GLN
2	F	76	HIS
2	F	78	GLN
2	F	105	HIS
2	F	154	ASN
2	F	222	GLN
2	F	324	ASN
2	F	351	GLN
1	G	105	GLN

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Mol	Chain	Res	Type
1	G	266	ASN
1	G	457	ASN
1	G	519	GLN
1	G	574	GLN
1	G	645	GLN
1	G	689	GLN
1	G	692	ASN
1	G	746	ASN
1	G	784	GLN
1	G	942	HIS
1	G	987	ASN
1	G	1000	HIS
1	G	1007	ASN
1	G	1035	GLN
1	G	1071	GLN
2	H	51	GLN
2	H	76	HIS
2	H	78	GLN
2	H	105	HIS
2	H	154	ASN
2	H	222	GLN
2	H	232	ASN
2	H	324	ASN
2	H	329	HIS
2	H	351	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 62 ligands modelled in this entry, 46 are monoatomic - leaving 16 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
6	ANP	E	2900	3	29,33,33	1.34	5 (17%)	31,52,52	1.73	5 (16%)
6	ANP	C	1900	3	29,33,33	1.35	6 (20%)	31,52,52	1.74	4 (12%)
6	ANP	A	1084	3	29,33,33	1.49	6 (20%)	31,52,52	1.75	6 (19%)
7	ORN	C	1920	-	4,8,8	0.50	0	3,9,9	0.20	0
8	NET	G	3950	-	8,8,8	0.69	0	10,10,10	0.56	0
8	NET	A	1086	-	8,8,8	0.77	0	10,10,10	0.49	0
7	ORN	A	1085	-	4,8,8	0.45	0	3,9,9	0.96	0
6	ANP	C	1910	3	29,33,33	1.42	5 (17%)	31,52,52	1.76	7 (22%)
7	ORN	G	3920	-	4,8,8	0.53	0	3,9,9	0.48	0
6	ANP	E	2910	3	29,33,33	1.39	5 (17%)	31,52,52	1.68	4 (12%)
6	ANP	G	3910	3	29,33,33	1.34	7 (24%)	31,52,52	1.81	7 (22%)
8	NET	E	2950	-	8,8,8	0.61	0	10,10,10	0.59	0
6	ANP	A	1083	3	29,33,33	1.58	6 (20%)	31,52,52	1.83	5 (16%)
8	NET	C	1950	-	8,8,8	0.67	0	10,10,10	0.69	0
6	ANP	G	3900	3	29,33,33	1.28	6 (20%)	31,52,52	1.86	5 (16%)
7	ORN	E	2920	-	4,8,8	0.70	0	3,9,9	0.25	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
6	ANP	E	2900	3	-	3/14/38/38	0/3/3/3
6	ANP	C	1900	3	-	2/14/38/38	0/3/3/3
6	ANP	A	1084	3	-	3/14/38/38	0/3/3/3
7	ORN	C	1920	-	-	4/4/8/8	-
8	NET	G	3950	-	-	6/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NET	A	1086	-	-	6/12/12/12	-
7	ORN	A	1085	-	-	3/4/8/8	-
6	ANP	C	1910	3	-	3/14/38/38	0/3/3/3
7	ORN	G	3920	-	-	4/4/8/8	-
6	ANP	E	2910	3	-	6/14/38/38	0/3/3/3
6	ANP	G	3910	3	-	4/14/38/38	0/3/3/3
8	NET	E	2950	-	-	12/12/12/12	-
6	ANP	A	1083	3	-	3/14/38/38	0/3/3/3
8	NET	C	1950	-	-	3/12/12/12	-
6	ANP	G	3900	3	-	2/14/38/38	0/3/3/3
7	ORN	E	2920	-	-	4/4/8/8	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1083	ANP	PG-O1G	5.08	1.54	1.46
6	C	1910	ANP	PB-O1B	4.11	1.52	1.46
6	E	2910	ANP	PB-O1B	4.08	1.52	1.46
6	A	1084	ANP	PB-O1B	4.05	1.52	1.46
6	A	1084	ANP	PG-O1G	3.58	1.51	1.46
6	E	2900	ANP	PG-O1G	3.44	1.51	1.46
6	A	1083	ANP	PB-O1B	3.35	1.51	1.46
6	E	2910	ANP	PG-O1G	3.12	1.51	1.46
6	A	1083	ANP	PG-O2G	-3.10	1.48	1.56
6	G	3900	ANP	PB-O1B	3.07	1.51	1.46
6	C	1900	ANP	PG-O1G	2.95	1.50	1.46
6	E	2900	ANP	PB-O1B	2.89	1.50	1.46
6	C	1910	ANP	PG-O1G	2.86	1.50	1.46
6	G	3910	ANP	PB-O1B	2.82	1.50	1.46
6	C	1900	ANP	PB-O1B	2.70	1.50	1.46
6	C	1910	ANP	PG-O2G	-2.51	1.50	1.56
6	G	3910	ANP	PB-O2B	-2.50	1.50	1.56
6	A	1084	ANP	PG-O2G	-2.43	1.50	1.56
6	G	3900	ANP	C2-N1	2.43	1.38	1.33
6	G	3900	ANP	O4'-C1'	-2.43	1.37	1.41
6	C	1900	ANP	PG-O2G	-2.43	1.50	1.56
6	G	3900	ANP	PG-O2G	-2.42	1.50	1.56
6	E	2910	ANP	PB-O2B	-2.42	1.50	1.56
6	C	1910	ANP	PB-O2B	-2.39	1.50	1.56
6	E	2900	ANP	PG-O2G	-2.39	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	3910	ANP	C6-N6	-2.37	1.25	1.34
6	G	3910	ANP	O4'-C1'	-2.35	1.37	1.41
6	A	1083	ANP	C2-N1	2.33	1.38	1.33
6	C	1900	ANP	O4'-C1'	-2.32	1.37	1.41
6	C	1910	ANP	C6-N6	-2.28	1.25	1.34
6	A	1084	ANP	C6-N6	-2.26	1.25	1.34
6	E	2900	ANP	PB-O2B	-2.26	1.50	1.56
6	G	3900	ANP	PG-O1G	2.23	1.49	1.46
6	G	3910	ANP	PG-O1G	2.22	1.49	1.46
6	E	2910	ANP	C6-N6	-2.22	1.25	1.34
6	E	2910	ANP	C2-N1	2.21	1.38	1.33
6	A	1084	ANP	PB-O2B	-2.20	1.50	1.56
6	A	1083	ANP	PB-O2B	-2.18	1.50	1.56
6	C	1900	ANP	C2-N1	2.14	1.37	1.33
6	E	2900	ANP	C2-N1	2.11	1.37	1.33
6	C	1900	ANP	C6-N6	-2.10	1.26	1.34
6	A	1084	ANP	C2-N1	2.05	1.37	1.33
6	G	3910	ANP	PG-O2G	-2.05	1.51	1.56
6	A	1083	ANP	C6-N6	-2.04	1.26	1.34
6	G	3900	ANP	C6-N6	-2.04	1.26	1.34
6	G	3910	ANP	C2-N1	2.02	1.37	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	3900	ANP	C5-C6-N6	5.59	128.84	120.35
6	A	1084	ANP	C5-C6-N6	5.12	128.13	120.35
6	C	1900	ANP	C5-C6-N6	4.61	127.35	120.35
6	G	3910	ANP	C2-N1-C6	4.53	126.51	118.75
6	G	3900	ANP	C2-N1-C6	4.53	126.50	118.75
6	A	1083	ANP	C5-C6-N6	4.51	127.20	120.35
6	A	1083	ANP	C2-N1-C6	4.50	126.44	118.75
6	A	1083	ANP	C5-C6-N1	-4.48	110.20	120.35
6	C	1910	ANP	C5-C6-N6	4.43	127.09	120.35
6	E	2910	ANP	C2-N1-C6	4.39	126.26	118.75
6	E	2900	ANP	C2-N1-C6	4.28	126.08	118.75
6	G	3900	ANP	C5-C6-N1	-4.27	110.66	120.35
6	C	1900	ANP	C2-N1-C6	4.27	126.05	118.75
6	G	3910	ANP	C5-C6-N1	-4.06	111.15	120.35
6	C	1910	ANP	C2-N1-C6	3.95	125.52	118.75
6	A	1084	ANP	C2-N1-C6	3.95	125.51	118.75
6	C	1910	ANP	C5-C6-N1	-3.94	111.42	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	2900	ANP	C5-C6-N1	-3.94	111.43	120.35
6	A	1084	ANP	C5-C6-N1	-3.83	111.67	120.35
6	E	2900	ANP	C5-C6-N6	3.81	126.15	120.35
6	E	2910	ANP	C5-C6-N6	3.81	126.14	120.35
6	E	2910	ANP	C5-C6-N1	-3.80	111.73	120.35
6	C	1900	ANP	C5-C6-N1	-3.78	111.78	120.35
6	G	3910	ANP	N3-C2-N1	-3.70	122.90	128.68
6	E	2910	ANP	N3-C2-N1	-3.54	123.14	128.68
6	C	1900	ANP	N3-C2-N1	-3.46	123.27	128.68
6	E	2900	ANP	N3-C2-N1	-3.44	123.29	128.68
6	A	1083	ANP	N3-C2-N1	-3.13	123.79	128.68
6	G	3910	ANP	C5-C6-N6	3.01	124.92	120.35
6	A	1084	ANP	O1B-PB-N3B	-2.99	107.37	111.77
6	A	1083	ANP	C3'-C2'-C1'	2.98	105.47	100.98
6	E	2900	ANP	C3'-C2'-C1'	2.92	105.37	100.98
6	G	3900	ANP	N3-C2-N1	-2.91	124.13	128.68
6	A	1084	ANP	N3-C2-N1	-2.82	124.28	128.68
6	C	1910	ANP	N3-C2-N1	-2.72	124.42	128.68
6	G	3910	ANP	N6-C6-N1	2.58	123.93	118.57
6	C	1910	ANP	C3'-C2'-C1'	2.45	104.67	100.98
6	A	1084	ANP	C3'-C2'-C1'	2.43	104.64	100.98
6	G	3900	ANP	O2G-PG-O1G	-2.36	107.51	113.45
6	C	1910	ANP	O3'-C3'-C2'	2.17	118.83	111.82
6	G	3910	ANP	C3'-C2'-C1'	2.15	104.22	100.98
6	G	3910	ANP	O2G-PG-O1G	-2.15	108.05	113.45
6	C	1910	ANP	O2G-PG-O1G	-2.14	108.08	113.45

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1920	ORN	N-CA-CB-CG
7	C	1920	ORN	C-CA-CB-CG
6	E	2910	ANP	PB-N3B-PG-O1G
6	E	2910	ANP	PG-N3B-PB-O1B
6	E	2910	ANP	PG-N3B-PB-O3A
6	E	2910	ANP	C5'-O5'-PA-O3A
6	E	2900	ANP	PB-N3B-PG-O1G
6	E	2900	ANP	PG-N3B-PB-O1B
6	E	2900	ANP	PG-N3B-PB-O3A
6	C	1910	ANP	PB-N3B-PG-O1G
6	C	1910	ANP	PG-N3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
6	C	1910	ANP	PG-N3B-PB-O3A
7	G	3920	ORN	C-CA-CB-CG
6	G	3900	ANP	PB-N3B-PG-O1G
6	G	3900	ANP	PG-N3B-PB-O1B
6	G	3910	ANP	PB-N3B-PG-O1G
6	G	3910	ANP	PG-N3B-PB-O1B
6	G	3910	ANP	C5'-O5'-PA-O3A
6	C	1900	ANP	PB-N3B-PG-O1G
6	C	1900	ANP	PG-N3B-PB-O1B
6	A	1084	ANP	PB-N3B-PG-O1G
6	A	1084	ANP	PG-N3B-PB-O1B
7	A	1085	ORN	C-CA-CB-CG
6	A	1083	ANP	PB-N3B-PG-O1G
6	A	1083	ANP	PG-N3B-PB-O1B
6	A	1083	ANP	PG-N3B-PB-O3A
7	E	2920	ORN	N-CA-CB-CG
7	E	2920	ORN	C-CA-CB-CG
8	G	3950	NET	C4-C3-N1-C1
8	A	1086	NET	C4-C3-N1-C1
8	E	2950	NET	C4-C3-N1-C1
8	A	1086	NET	C8-C7-N1-C5
8	A	1086	NET	C8-C7-N1-C3
8	A	1086	NET	C8-C7-N1-C1
8	E	2950	NET	C4-C3-N1-C5
8	E	2950	NET	C4-C3-N1-C7
8	A	1086	NET	C4-C3-N1-C7
7	G	3920	ORN	CA-CB-CG-CD
8	A	1086	NET	C4-C3-N1-C5
8	E	2950	NET	C8-C7-N1-C3
7	C	1920	ORN	CA-CB-CG-CD
8	G	3950	NET	C4-C3-N1-C5
8	G	3950	NET	C4-C3-N1-C7
8	C	1950	NET	C4-C3-N1-C7
8	C	1950	NET	C4-C3-N1-C5
8	E	2950	NET	C8-C7-N1-C1
8	E	2950	NET	C2-C1-N1-C5
7	E	2920	ORN	CA-CB-CG-CD
8	C	1950	NET	C4-C3-N1-C1
8	E	2950	NET	C8-C7-N1-C5
8	E	2950	NET	C2-C1-N1-C3
8	E	2950	NET	C2-C1-N1-C7
8	E	2950	NET	C6-C5-N1-C1

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Mol	Chain	Res	Type	Atoms
8	G	3950	NET	C6-C5-N1-C7
8	G	3950	NET	C6-C5-N1-C1
8	E	2950	NET	C6-C5-N1-C7
8	G	3950	NET	C6-C5-N1-C3
8	E	2950	NET	C6-C5-N1-C3
7	C	1920	ORN	NE-CD-CG-CB
6	E	2910	ANP	C5'-O5'-PA-O2A
6	G	3910	ANP	C5'-O5'-PA-O2A
6	A	1084	ANP	PG-N3B-PB-O3A
7	G	3920	ORN	NE-CD-CG-CB
7	A	1085	ORN	NE-CD-CG-CB
7	E	2920	ORN	NE-CD-CG-CB
6	E	2910	ANP	C5'-O5'-PA-O1A
7	G	3920	ORN	N-CA-CB-CG
7	A	1085	ORN	N-CA-CB-CG

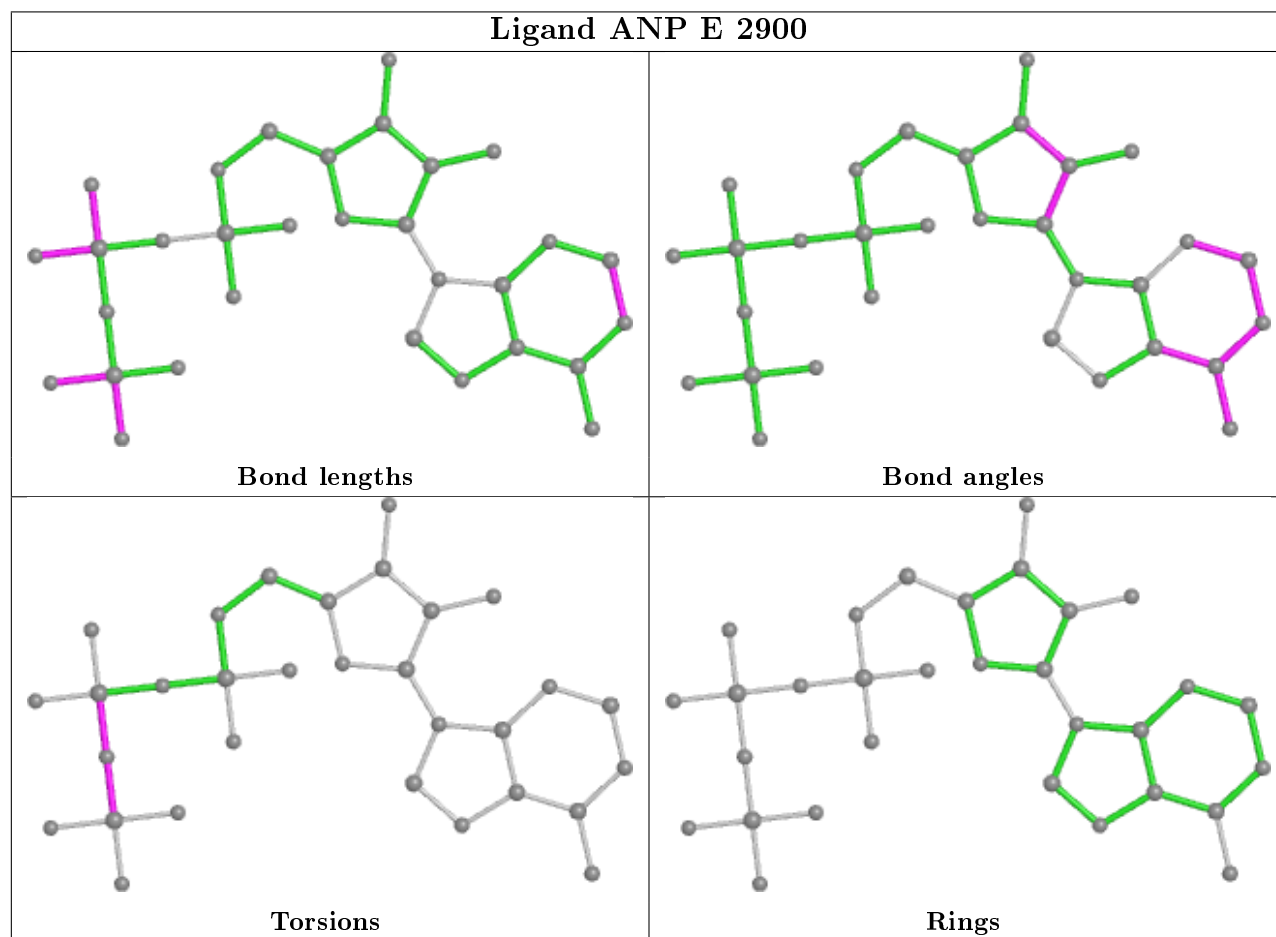
There are no ring outliers.

13 monomers are involved in 35 short contacts:

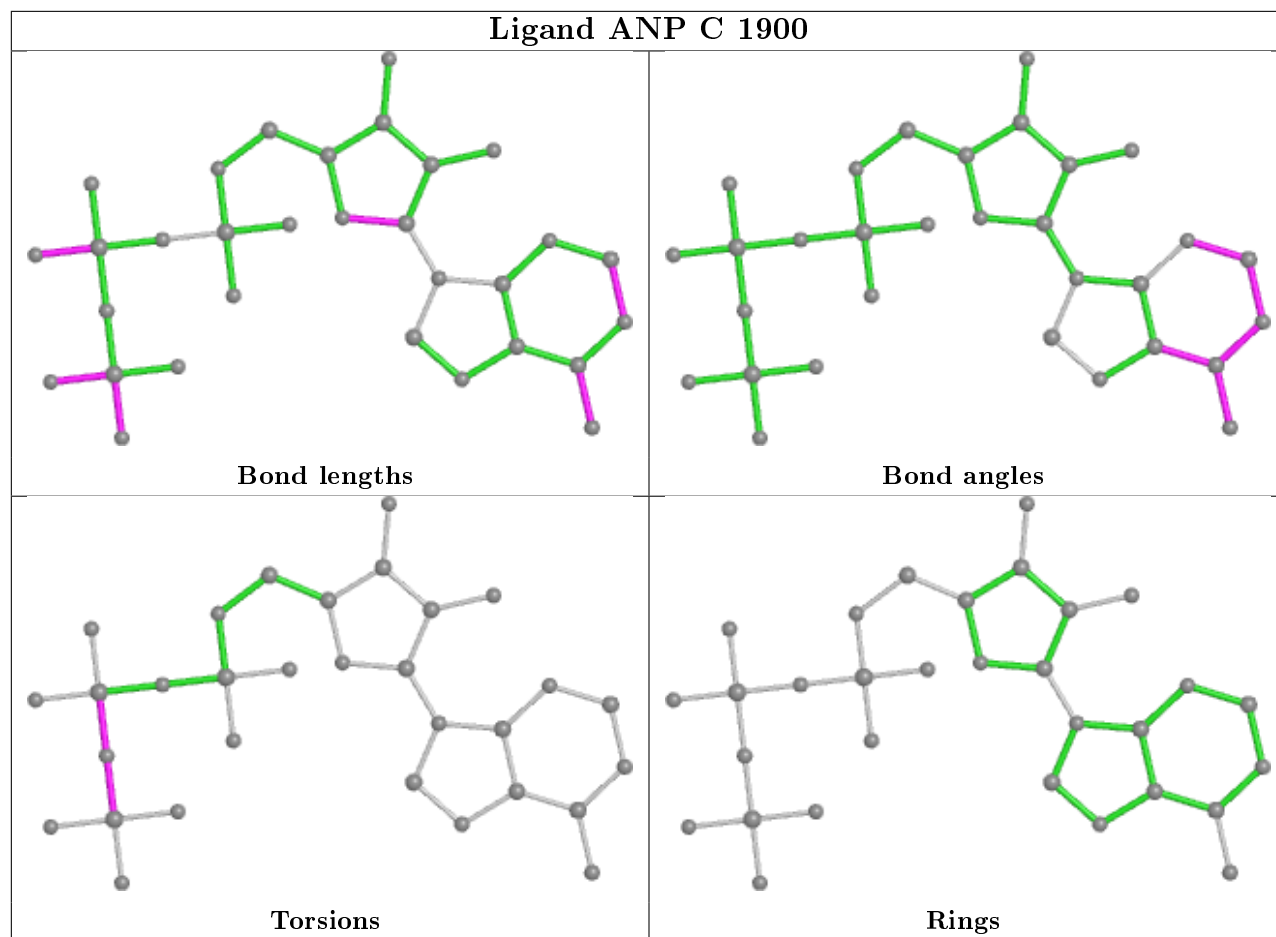
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1920	ORN	1	0
8	G	3950	NET	4	0
8	A	1086	NET	6	0
7	A	1085	ORN	1	0
6	C	1910	ANP	1	0
7	G	3920	ORN	1	0
6	E	2910	ANP	3	0
6	G	3910	ANP	2	0
8	E	2950	NET	6	0
6	A	1083	ANP	3	0
8	C	1950	NET	4	0
6	G	3900	ANP	2	0
7	E	2920	ORN	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

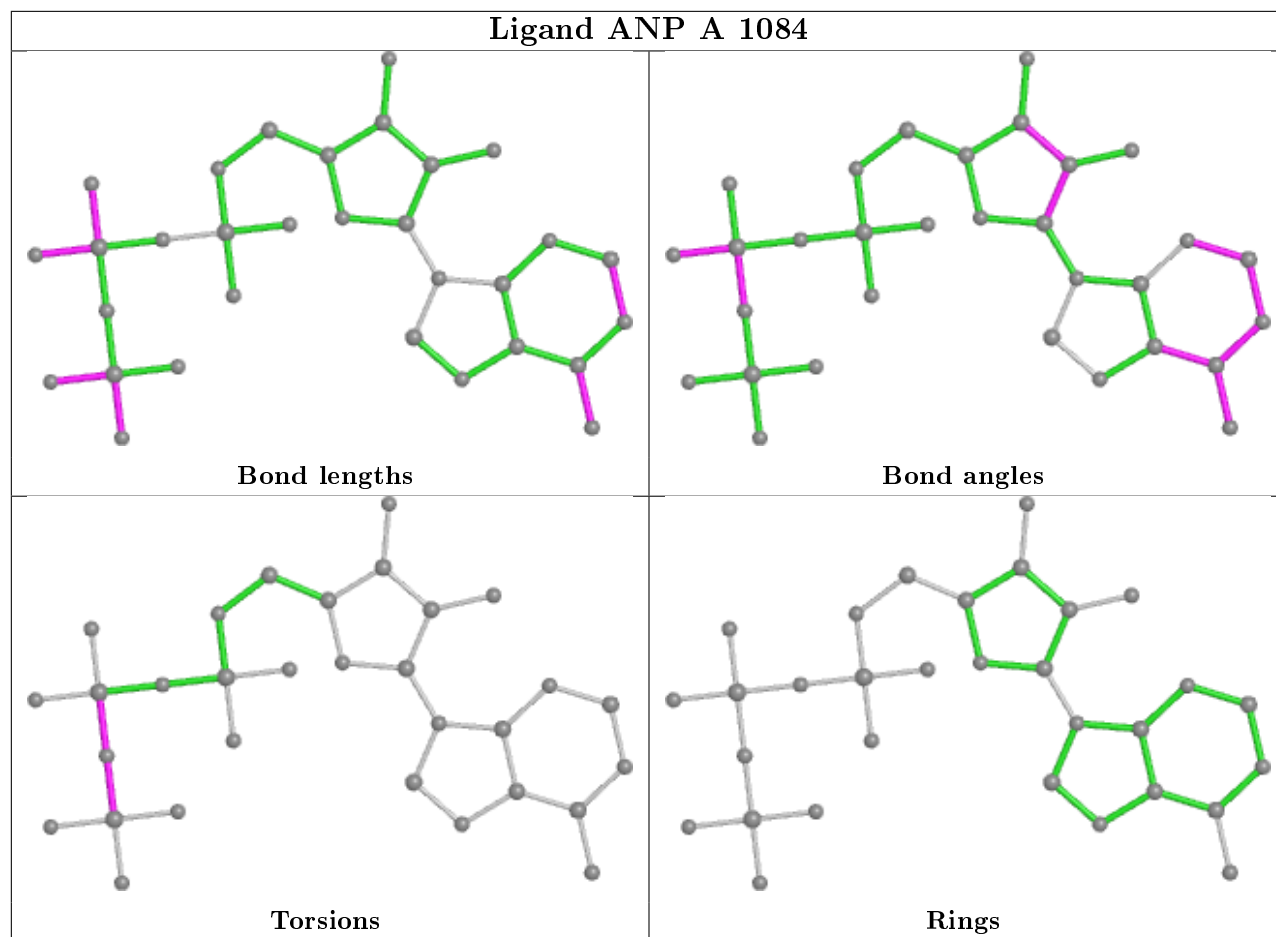
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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



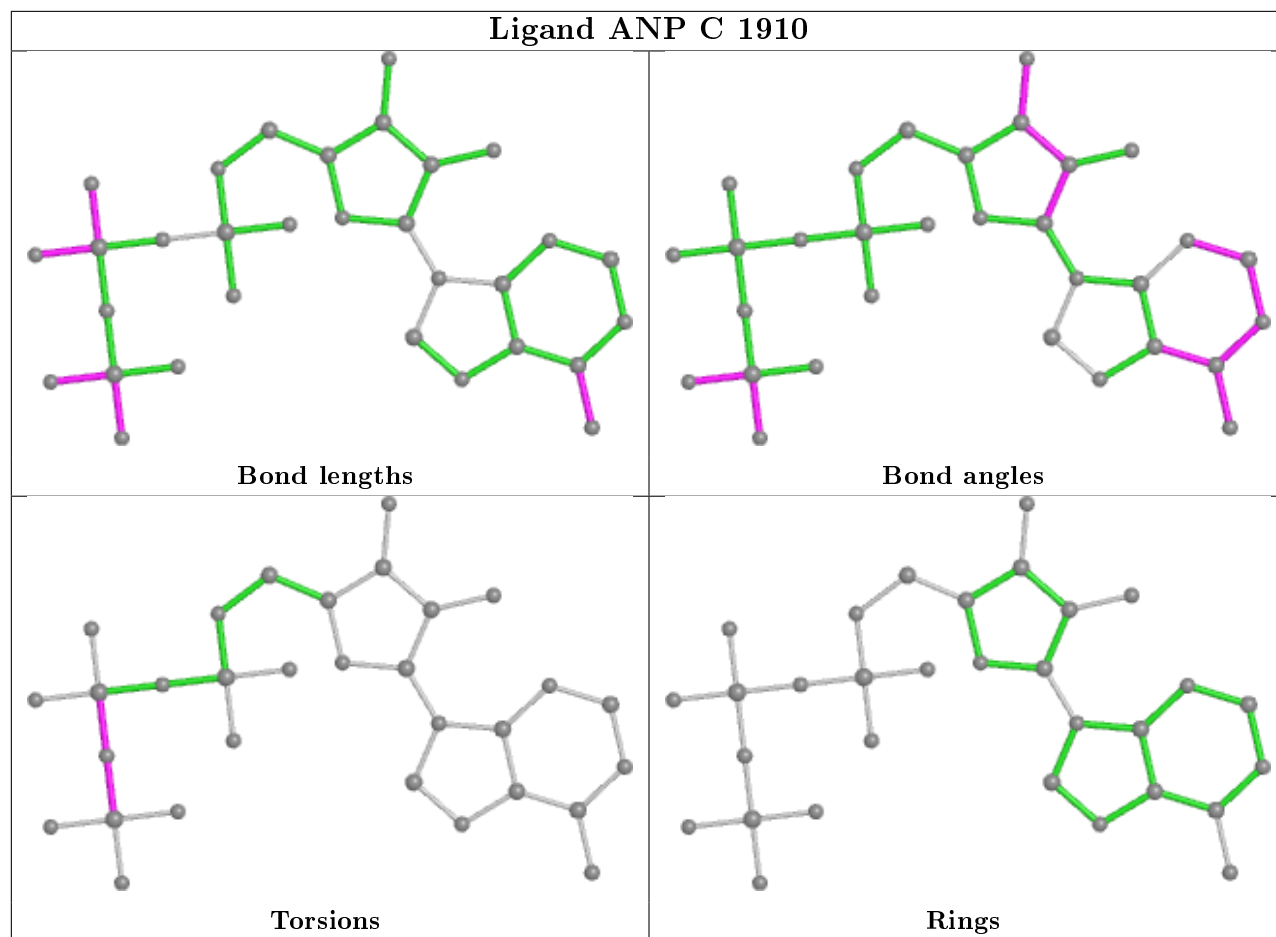


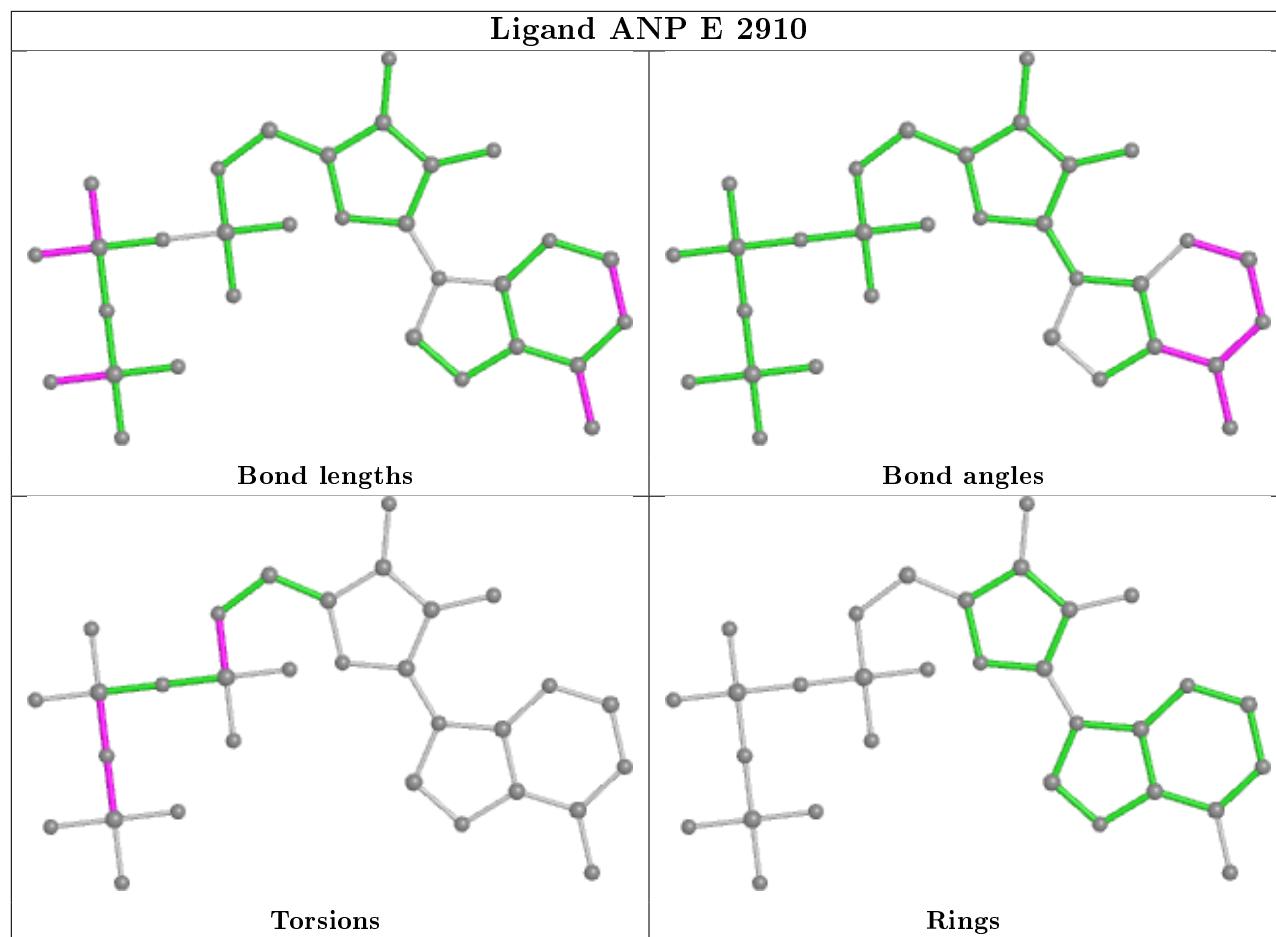


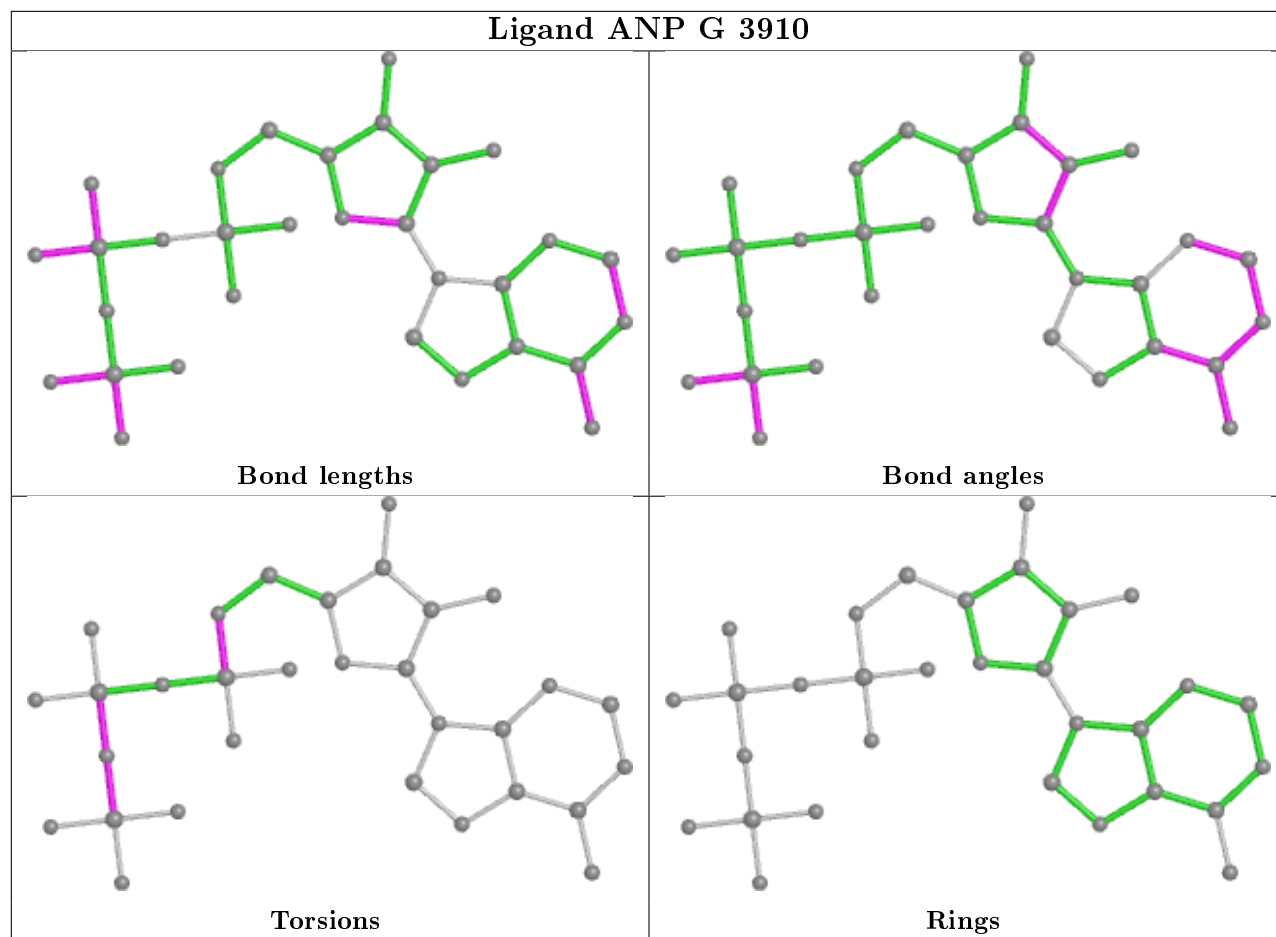
## Ligand ANP A 1084



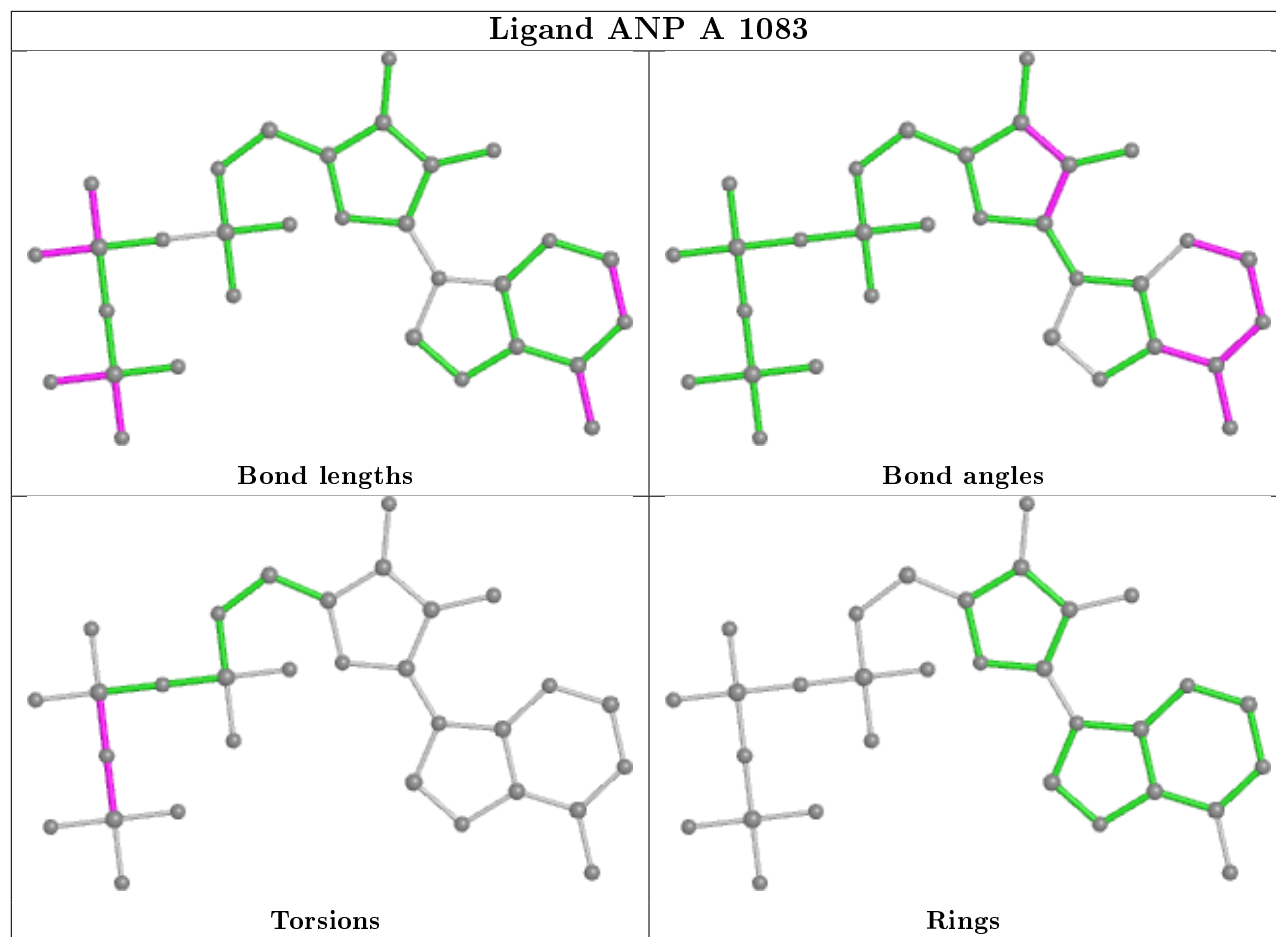
## Ligand ANP C 1910

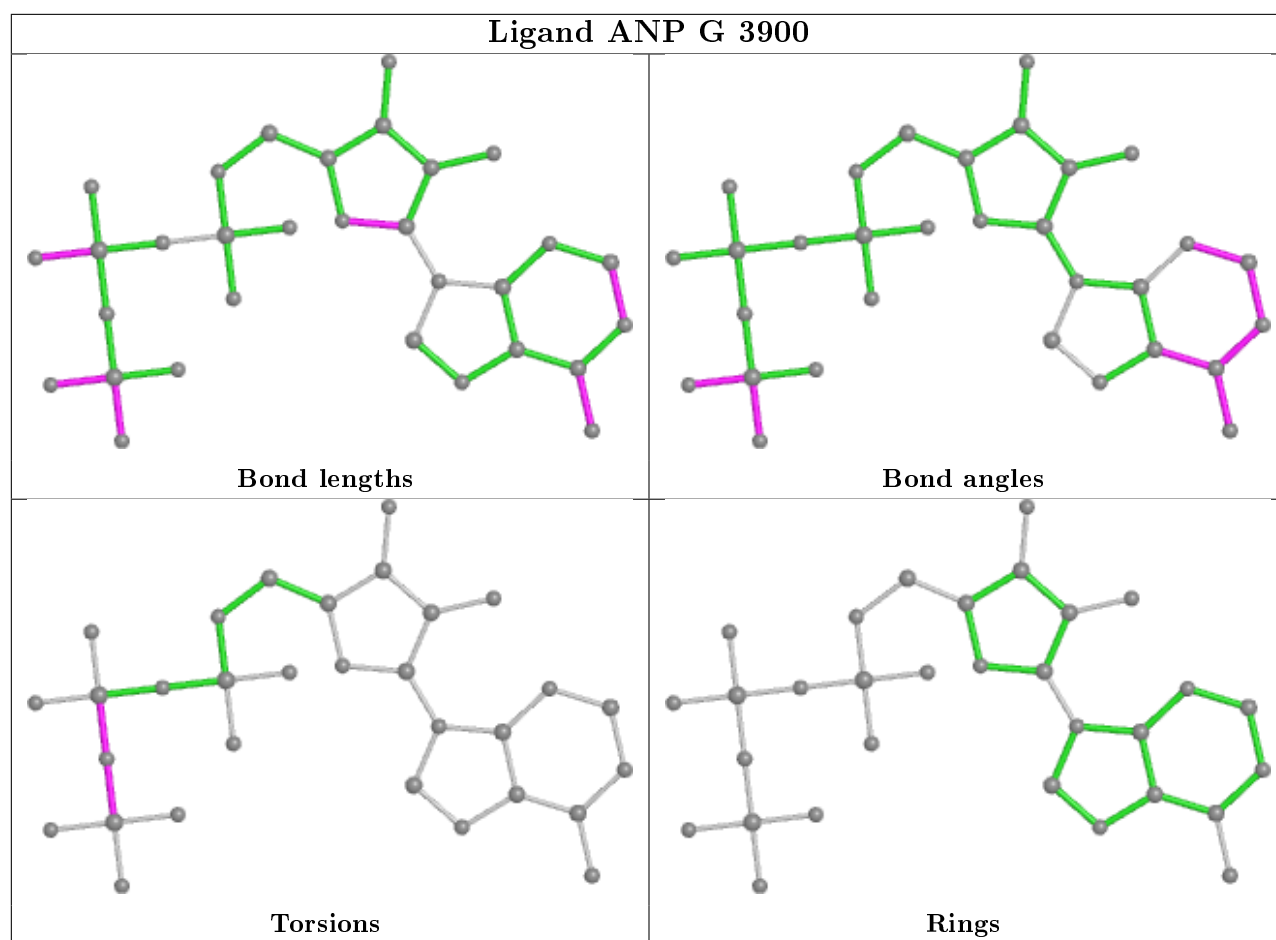






## Ligand ANP A 1083





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.