



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 6, 2017 – 09:58 PM EDT

PDB ID : 4XQ2  
Title : Ensemble refinement of cystathione gamma lyase (CalE6) D7G from *Micromonospora echinospora*  
Authors : Wang, F.; Yennamalli, R.M.; Singh, S.; Tan, K.; Thorson, J.S.; Phillips Jr., G.N.; Enzyme Discovery for Natural Product Biosynthesis (NatPro)  
Deposited on : unknown  
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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	<b>FAILED</b>
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

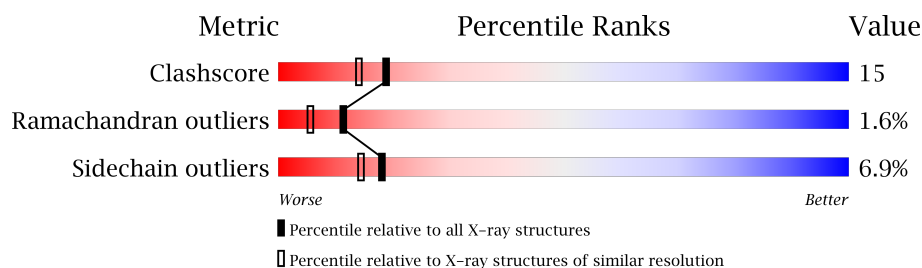
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.




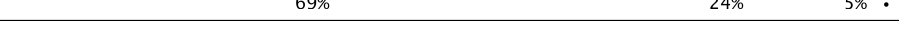
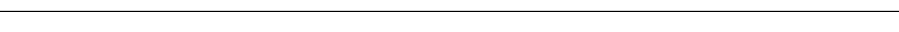


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	384	 71% 23% . .
1	1-B	384	 70% 24% . . .
1	1-C	384	 75% 20% . .
1	1-D	384	 69% 24% 5% .
1	1-E	384	 71% 24% . . .
1	1-F	384	 68% 27% . .
1	1-G	384	 73% 22% . . .


























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Mol	Chain	Length	Quality of chain
1	1-H	384	 69%25% . . .
1	10-A	384	 72%21% . . .
1	10-B	384	 68%27% . .
1	10-C	384	 70%26% . .
1	10-D	384	 68%26% . . .
1	10-E	384	 69%25% . . .
1	10-F	384	 67%26% . . .
1	10-G	384	 67%26%5% . .
1	10-H	384	 72%23% . .
1	2-A	384	 76%20% . .
1	2-B	384	 74%20% . .
1	2-C	384	 72%23% . .
1	2-D	384	 71%22%5% .
1	2-E	384	 72%24% . .
1	2-F	384	 75%21% . .
1	2-G	384	 77%18% . .
1	2-H	384	 70%23%5% . .
1	3-A	384	 73%21% . .
1	3-B	384	 74%21% . .
1	3-C	384	 70%23%5% .
1	3-D	384	 69%24%5% . .
1	3-E	384	 71%23% . .
1	3-F	384	 66%29% . .
1	3-G	384	 72%23% . .
1	3-H	384	 67%26% . .

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Mol	Chain	Length	Quality of chain
1	4-A	384	 71%23% . .
1	4-B	384	 72%21%5% . .
1	4-C	384	 72%23% . .
1	4-D	384	 68%26% . .
1	4-E	384	 67%26%5% .
1	4-F	384	 67%26%5% .
1	4-G	384	 71%23% . .
1	4-H	384	 71%24% . .
1	5-A	384	 71%23% . .
1	5-B	384	 66%28% . .
1	5-C	384	 70%25% . .
1	5-D	384	 74%20% . .
1	5-E	384	 66%25%6% . .
1	5-F	384	 73%23% . .
1	5-G	384	 75%19% . .
1	5-H	384	 72%22% . .
1	6-A	384	 75%20% . .
1	6-B	384	 69%24% . .
1	6-C	384	 71%24% . .
1	6-D	384	 69%25% . .
1	6-E	384	 75%18% . .
1	6-F	384	 70%23%5% .
1	6-G	384	 72%23% . .
1	6-H	384	 74%21% . .
1	7-A	384	 67%24%5% . .

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Mol	Chain	Length	Quality of chain
1	7-B	384	
1	7-C	384	
1	7-D	384	
1	7-E	384	
1	7-F	384	
1	7-G	384	
1	7-H	384	
1	8-A	384	
1	8-B	384	
1	8-C	384	
1	8-D	384	
1	8-E	384	
1	8-F	384	
1	8-G	384	
1	8-H	384	
1	9-A	384	
1	9-B	384	
1	9-C	384	
1	9-D	384	
1	9-E	384	
1	9-F	384	
1	9-G	384	
1	9-H	384	

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
2	MES	3-E	401	-	-	X	-
2	MES	4-C	401	-	-	X	-
2	MES	5-G	401	-	-	X	-
2	MES	6-F	401	-	-	X	-
2	MES	7-B	401	-	-	X	-
2	MES	7-H	401	-	-	X	-
2	MES	8-C	401	-	-	X	-
3	GOL	10-A	403	-	-	X	-
3	GOL	5-B	405	-	-	X	-
3	GOL	7-A	402	-	-	X	-
3	GOL	8-E	402	-	-	X	-
3	GOL	8-H	404	-	-	X	-
4	CL	10-E	404	-	-	X	-
4	CL	10-H	407	-	-	X	-
4	CL	2-H	406	-	-	X	-
4	CL	4-A	406	-	-	X	-
4	CL	5-D	405	-	-	X	-
4	CL	6-B	409	-	-	X	-
4	CL	6-D	405	-	-	X	-
4	CL	6-F	408	-	-	X	-
4	CL	7-F	408	-	-	X	-
5	FMT	3-F	407	-	-	X	-
5	FMT	7-F	407	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 243453 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 CalE6.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	1-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	2-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	3-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	4-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	5-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	6-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	7-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	8-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	9-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	10-A	376	Total	C	N	O	P	S	Se	0	0	0
			2839	1774	526	530	1	5	3			
1	1-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	2-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	3-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	4-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	5-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	6-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	7-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	8-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	9-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	10-B	378	Total	C	N	O	P	S	Se	0	0	0
			2846	1777	528	532	1	5	3			
1	1-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	2-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	3-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	4-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	5-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	6-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	7-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	8-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	9-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	10-C	379	Total	C	N	O	P	S	Se	0	0	0
			2837	1773	523	532	1	5	3			
1	1-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	2-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	3-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	4-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	5-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	6-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	7-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	8-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	9-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	10-D	376	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	519	524	1	5	3			
1	1-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	2-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	3-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	4-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	5-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	6-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	7-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	8-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	9-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	10-E	376	Total	C	N	O	P	S	Se	0	0	0
			2815	1764	514	528	1	5	3			
1	1-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	2-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	3-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	4-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	5-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	6-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	7-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	8-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	9-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	10-F	377	Total	C	N	O	P	S	Se	0	0	0
			2812	1760	518	525	1	5	3			
1	1-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	2-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	3-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	4-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	5-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	6-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	7-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	8-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	9-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	10-G	378	Total	C	N	O	P	S	Se	0	0	0
			2814	1761	516	528	1	5	3			
1	1-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	2-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	3-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	4-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	5-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	6-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	7-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	8-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			
1	9-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			

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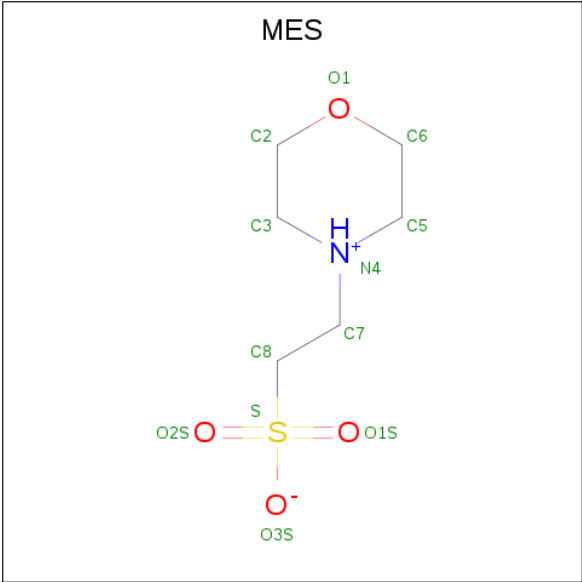
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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	10-H	378	Total	C	N	O	P	S	Se	0	0	0
			2831	1771	523	528	1	5	3			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8KNG3
A	-1	ASN	-	expression tag	UNP Q8KNG3
A	0	ALA	-	expression tag	UNP Q8KNG3
A	7	GLY	ASP	engineered mutation	UNP Q8KNG3
B	-2	SER	-	expression tag	UNP Q8KNG3
B	-1	ASN	-	expression tag	UNP Q8KNG3
B	0	ALA	-	expression tag	UNP Q8KNG3
B	7	GLY	ASP	engineered mutation	UNP Q8KNG3
C	-2	SER	-	expression tag	UNP Q8KNG3
C	-1	ASN	-	expression tag	UNP Q8KNG3
C	0	ALA	-	expression tag	UNP Q8KNG3
C	7	GLY	ASP	engineered mutation	UNP Q8KNG3
D	-2	SER	-	expression tag	UNP Q8KNG3
D	-1	ASN	-	expression tag	UNP Q8KNG3
D	0	ALA	-	expression tag	UNP Q8KNG3
D	7	GLY	ASP	engineered mutation	UNP Q8KNG3
E	-2	SER	-	expression tag	UNP Q8KNG3
E	-1	ASN	-	expression tag	UNP Q8KNG3
E	0	ALA	-	expression tag	UNP Q8KNG3
E	7	GLY	ASP	engineered mutation	UNP Q8KNG3
F	-2	SER	-	expression tag	UNP Q8KNG3
F	-1	ASN	-	expression tag	UNP Q8KNG3
F	0	ALA	-	expression tag	UNP Q8KNG3
F	7	GLY	ASP	engineered mutation	UNP Q8KNG3
G	-2	SER	-	expression tag	UNP Q8KNG3
G	-1	ASN	-	expression tag	UNP Q8KNG3
G	0	ALA	-	expression tag	UNP Q8KNG3
G	7	GLY	ASP	engineered mutation	UNP Q8KNG3
H	-2	SER	-	expression tag	UNP Q8KNG3
H	-1	ASN	-	expression tag	UNP Q8KNG3
H	0	ALA	-	expression tag	UNP Q8KNG3
H	7	GLY	ASP	engineered mutation	UNP Q8KNG3

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	2-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	3-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	4-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	5-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	6-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	7-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	8-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	9-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	10-A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	2-B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	4-B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	6-B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	8-B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	10-B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	3-C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	5-C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	6-C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	7-C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	8-C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	2-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	3-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	4-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	5-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	8-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	10-D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	2-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	3-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	4-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	5-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	6-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	7-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	8-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	9-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	10-E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	10-F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	2-G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	3-G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	6-G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	7-G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	1-H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	3-H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	4-H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	7-H	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL, FMT, CL) (formula:  $C_3H_8O_3$ ,  $CH_2O_2$ , Cl).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-A	1	Total	C	O	0	0
			6	3	3		
3	2-A	1	Total	C	O	0	0
			6	3	3		
3	3-A	1	Total	C	O	0	0
			6	3	3		
3	4-A	1	Total	C	O	0	0
			6	3	3		
3	5-A	1	Total	C	O	0	0
			6	3	3		
3	6-A	1	Total	C	O	0	0
			6	3	3		
3	7-A	1	Total	C	O	0	0
			6	3	3		
3	8-A	1	Total	C	O	0	0
			6	3	3		
3	9-A	1	Total	C	O	0	0
			6	3	3		
3	10-A	1	Total	C	O	0	0
			6	3	3		
3	1-A	1	Total	C	O	0	0
			6	3	3		
3	2-A	1	Total	C	O	0	0
			6	3	3		
3	3-A	1	Total	C	O	0	0
			6	3	3		
3	4-A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	5-A	1	Total	C	O	0	0
			6	3	3		
3	6-A	1	Total	C	O	0	0
			6	3	3		
3	7-A	1	Total	C	O	0	0
			6	3	3		
3	8-A	1	Total	C	O	0	0
			6	3	3		
3	9-A	1	Total	C	O	0	0
			6	3	3		
3	10-A	1	Total	C	O	0	0
			6	3	3		
3	1-A	1	Total	C	O	0	0
			6	3	3		
3	2-A	1	Total	C	O	0	0
			6	3	3		
3	3-A	1	Total	C	O	0	0
			6	3	3		
3	4-A	1	Total	C	O	0	0
			6	3	3		
3	5-A	1	Total	C	O	0	0
			6	3	3		
3	6-A	1	Total	C	O	0	0
			6	3	3		
3	7-A	1	Total	C	O	0	0
			6	3	3		
3	8-A	1	Total	C	O	0	0
			6	3	3		
3	9-A	1	Total	C	O	0	0
			6	3	3		
3	10-A	1	Total	C	O	0	0
			6	3	3		
3	1-B	1	Total	C	O	0	0
			6	3	3		
3	2-B	1	Total	C	O	0	0
			6	3	3		
3	4-B	1	Total	C	O	0	0
			6	3	3		
3	6-B	1	Total	C	O	0	0
			6	3	3		
3	8-B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	10-B	1	Total	C	O	0	0
			6	3	3		
3	1-B	1	Total	C	O	0	0
			6	3	3		
3	2-B	1	Total	C	O	0	0
			6	3	3		
3	3-B	1	Total	C	O	0	0
			6	3	3		
3	4-B	1	Total	C	O	0	0
			6	3	3		
3	5-B	1	Total	C	O	0	0
			6	3	3		
3	6-B	1	Total	C	O	0	0
			6	3	3		
3	7-B	1	Total	C	O	0	0
			6	3	3		
3	8-B	1	Total	C	O	0	0
			6	3	3		
3	9-B	1	Total	C	O	0	0
			6	3	3		
3	10-B	1	Total	C	O	0	0
			6	3	3		
3	1-B	1	Total	C	O	0	0
			6	3	3		
3	2-B	1	Total	C	O	0	0
			6	3	3		
3	3-B	1	Total	C	O	0	0
			6	3	3		
3	4-B	1	Total	C	O	0	0
			6	3	3		
3	5-B	1	Total	C	O	0	0
			6	3	3		
3	6-B	1	Total	C	O	0	0
			6	3	3		
3	7-B	1	Total	C	O	0	0
			6	3	3		
3	8-B	1	Total	C	O	0	0
			6	3	3		
3	9-B	1	Total	C	O	0	0
			6	3	3		
3	10-B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-B	1	Total	C	O	0	0
			6	3	3		
3	2-B	1	Total	C	O	0	0
			6	3	3		
3	3-B	1	Total	C	O	0	0
			6	3	3		
3	4-B	1	Total	C	O	0	0
			6	3	3		
3	5-B	1	Total	C	O	0	0
			6	3	3		
3	6-B	1	Total	C	O	0	0
			6	3	3		
3	7-B	1	Total	C	O	0	0
			6	3	3		
3	8-B	1	Total	C	O	0	0
			6	3	3		
3	9-B	1	Total	C	O	0	0
			6	3	3		
3	10-B	1	Total	C	O	0	0
			6	3	3		
3	1-B	1	Total	C	O	0	0
			6	3	3		
3	2-B	1	Total	C	O	0	0
			6	3	3		
3	3-B	1	Total	C	O	0	0
			6	3	3		
3	4-B	1	Total	C	O	0	0
			6	3	3		
3	5-B	1	Total	C	O	0	0
			6	3	3		
3	6-B	1	Total	C	O	0	0
			6	3	3		
3	7-B	1	Total	C	O	0	0
			6	3	3		
3	8-B	1	Total	C	O	0	0
			6	3	3		
3	9-B	1	Total	C	O	0	0
			6	3	3		
3	10-B	1	Total	C	O	0	0
			6	3	3		
3	1-B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	2-B	1	Total 6	C 3	O 3	0	0
3	3-B	1	Total 6	C 3	O 3	0	0
3	4-B	1	Total 6	C 3	O 3	0	0
3	5-B	1	Total 6	C 3	O 3	0	0
3	6-B	1	Total 6	C 3	O 3	0	0
3	7-B	1	Total 6	C 3	O 3	0	0
3	8-B	1	Total 6	C 3	O 3	0	0
3	9-B	1	Total 6	C 3	O 3	0	0
3	10-B	1	Total 6	C 3	O 3	0	0
3	1-B	1	Total 6	C 3	O 3	0	0
3	3-B	1	Total 6	C 3	O 3	0	0
3	5-B	1	Total 6	C 3	O 3	0	0
3	7-B	1	Total 6	C 3	O 3	0	0
3	8-B	1	Total 6	C 3	O 3	0	0
3	1-C	1	Total 6	C 3	O 3	0	0
3	2-C	1	Total 6	C 3	O 3	0	0
3	3-C	1	Total 6	C 3	O 3	0	0
3	4-C	1	Total 6	C 3	O 3	0	0
3	5-C	1	Total 6	C 3	O 3	0	0
3	6-C	1	Total 6	C 3	O 3	0	0
3	7-C	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	8-C	1	Total	C	O	0	0
			6	3	3		
3	9-C	1	Total	C	O	0	0
			6	3	3		
3	10-C	1	Total	C	O	0	0
			6	3	3		
3	1-D	1	Total	C	O	0	0
			6	3	3		
3	2-D	1	Total	C	O	0	0
			6	3	3		
3	3-D	1	Total	C	O	0	0
			6	3	3		
3	4-D	1	Total	C	O	0	0
			6	3	3		
3	5-D	1	Total	C	O	0	0
			6	3	3		
3	6-D	1	Total	C	O	0	0
			6	3	3		
3	7-D	1	Total	C	O	0	0
			6	3	3		
3	8-D	1	Total	C	O	0	0
			6	3	3		
3	9-D	1	Total	C	O	0	0
			6	3	3		
3	10-D	1	Total	C	O	0	0
			6	3	3		
3	1-D	1	Total	C	O	0	0
			6	3	3		
3	2-D	1	Total	C	O	0	0
			6	3	3		
3	3-D	1	Total	C	O	0	0
			6	3	3		
3	4-D	1	Total	C	O	0	0
			6	3	3		
3	5-D	1	Total	C	O	0	0
			6	3	3		
3	6-D	1	Total	C	O	0	0
			6	3	3		
3	7-D	1	Total	C	O	0	0
			6	3	3		
3	8-D	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	9-D	1	Total	C	O	0	0
			6	3	3		
3	10-D	1	Total	C	O	0	0
			6	3	3		
3	1-D	1	Total	C	O	0	0
			6	3	3		
3	5-D	1	Total	C	O	0	0
			6	3	3		
3	10-D	1	Total	C	O	0	0
			6	3	3		
3	1-E	1	Total	C	O	0	0
			6	3	3		
3	2-E	1	Total	C	O	0	0
			6	3	3		
3	3-E	1	Total	C	O	0	0
			6	3	3		
3	4-E	1	Total	C	O	0	0
			6	3	3		
3	5-E	1	Total	C	O	0	0
			6	3	3		
3	6-E	1	Total	C	O	0	0
			6	3	3		
3	7-E	1	Total	C	O	0	0
			6	3	3		
3	8-E	1	Total	C	O	0	0
			6	3	3		
3	9-E	1	Total	C	O	0	0
			6	3	3		
3	10-E	1	Total	C	O	0	0
			6	3	3		
3	1-E	1	Total	C	O	0	0
			6	3	3		
3	2-E	1	Total	C	O	0	0
			6	3	3		
3	3-E	1	Total	C	O	0	0
			6	3	3		
3	4-E	1	Total	C	O	0	0
			6	3	3		
3	5-E	1	Total	C	O	0	0
			6	3	3		
3	6-E	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	7-E	1	Total	C	O	0	0
			6	3	3		
3	8-E	1	Total	C	O	0	0
			6	3	3		
3	9-E	1	Total	C	O	0	0
			6	3	3		
3	10-E	1	Total	C	O	0	0
			6	3	3		
3	1-F	1	Total	C	O	0	0
			6	3	3		
3	10-F	1	Total	C	O	0	0
			6	3	3		
3	1-F	1	Total	C	O	0	0
			6	3	3		
3	3-F	1	Total	C	O	0	0
			6	3	3		
3	4-F	1	Total	C	O	0	0
			6	3	3		
3	6-F	1	Total	C	O	0	0
			6	3	3		
3	7-F	1	Total	C	O	0	0
			6	3	3		
3	8-F	1	Total	C	O	0	0
			6	3	3		
3	10-F	1	Total	C	O	0	0
			6	3	3		
3	1-F	1	Total	C	O	0	0
			6	3	3		
3	2-F	1	Total	C	O	0	0
			6	3	3		
3	3-F	1	Total	C	O	0	0
			6	3	3		
3	4-F	1	Total	C	O	0	0
			6	3	3		
3	5-F	1	Total	C	O	0	0
			6	3	3		
3	6-F	1	Total	C	O	0	0
			6	3	3		
3	7-F	1	Total	C	O	0	0
			6	3	3		
3	8-F	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	9-F	1	Total	C	O	0	0
			6	3	3		
3	10-F	1	Total	C	O	0	0
			6	3	3		
3	1-F	1	Total	C	O	0	0
			6	3	3		
3	2-F	1	Total	C	O	0	0
			6	3	3		
3	3-F	1	Total	C	O	0	0
			6	3	3		
3	4-F	1	Total	C	O	0	0
			6	3	3		
3	5-F	1	Total	C	O	0	0
			6	3	3		
3	6-F	1	Total	C	O	0	0
			6	3	3		
3	7-F	1	Total	C	O	0	0
			6	3	3		
3	8-F	1	Total	C	O	0	0
			6	3	3		
3	9-F	1	Total	C	O	0	0
			6	3	3		
3	10-F	1	Total	C	O	0	0
			6	3	3		
3	1-F	1	Total	C	O	0	0
			6	3	3		
3	2-F	1	Total	C	O	0	0
			6	3	3		
3	3-F	1	Total	C	O	0	0
			6	3	3		
3	5-F	1	Total	C	O	0	0
			6	3	3		
3	6-F	1	Total	C	O	0	0
			6	3	3		
3	7-F	1	Total	C	O	0	0
			6	3	3		
3	8-F	1	Total	C	O	0	0
			6	3	3		
3	9-F	1	Total	C	O	0	0
			6	3	3		
3	10-F	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-F	1	Total	C	O	0	0
			6	3	3		
3	2-F	1	Total	C	O	0	0
			6	3	3		
3	3-F	1	Total	C	O	0	0
			6	3	3		
3	6-F	1	Total	C	O	0	0
			6	3	3		
3	7-F	1	Total	C	O	0	0
			6	3	3		
3	1-G	1	Total	C	O	0	0
			6	3	3		
3	2-G	1	Total	C	O	0	0
			6	3	3		
3	3-G	1	Total	C	O	0	0
			6	3	3		
3	4-G	1	Total	C	O	0	0
			6	3	3		
3	5-G	1	Total	C	O	0	0
			6	3	3		
3	6-G	1	Total	C	O	0	0
			6	3	3		
3	7-G	1	Total	C	O	0	0
			6	3	3		
3	8-G	1	Total	C	O	0	0
			6	3	3		
3	9-G	1	Total	C	O	0	0
			6	3	3		
3	10-G	1	Total	C	O	0	0
			6	3	3		
3	1-G	1	Total	C	O	0	0
			6	3	3		
3	2-G	1	Total	C	O	0	0
			6	3	3		
3	3-G	1	Total	C	O	0	0
			6	3	3		
3	4-G	1	Total	C	O	0	0
			6	3	3		
3	5-G	1	Total	C	O	0	0
			6	3	3		
3	6-G	1	Total	C	O	0	0
			6	3	3		

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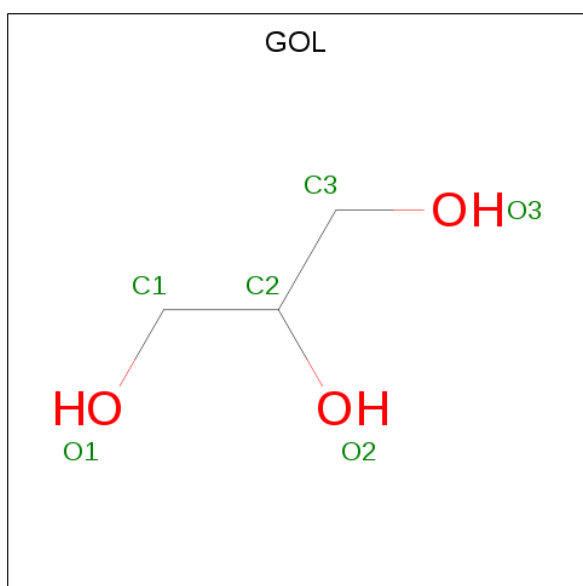
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	7-G	1	Total	C	O	0	0
			6	3	3		
3	8-G	1	Total	C	O	0	0
			6	3	3		
3	9-G	1	Total	C	O	0	0
			6	3	3		
3	10-G	1	Total	C	O	0	0
			6	3	3		
3	1-G	1	Total	C	O	0	0
			6	3	3		
3	2-G	1	Total	C	O	0	0
			6	3	3		
3	3-G	1	Total	C	O	0	0
			6	3	3		
3	4-G	1	Total	C	O	0	0
			6	3	3		
3	5-G	1	Total	C	O	0	0
			6	3	3		
3	7-G	1	Total	C	O	0	0
			6	3	3		
3	8-G	1	Total	C	O	0	0
			6	3	3		
3	1-G	1	Total	C	O	0	0
			6	3	3		
3	3-G	1	Total	C	O	0	0
			6	3	3		
3	1-H	1	Total	C	O	0	0
			6	3	3		
3	2-H	1	Total	C	O	0	0
			6	3	3		
3	3-H	1	Total	C	O	0	0
			6	3	3		
3	4-H	1	Total	C	O	0	0
			6	3	3		
3	5-H	1	Total	C	O	0	0
			6	3	3		
3	6-H	1	Total	C	O	0	0
			6	3	3		
3	7-H	1	Total	C	O	0	0
			6	3	3		
3	8-H	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	9-H	1	Total	C	O	0	0
			6	3	3		
3	10-H	1	Total	C	O	0	0
			6	3	3		
3	1-H	1	Total	C	O	0	0
			6	3	3		
3	2-H	1	Total	C	O	0	0
			6	3	3		
3	3-H	1	Total	C	O	0	0
			6	3	3		
3	4-H	1	Total	C	O	0	0
			6	3	3		
3	5-H	1	Total	C	O	0	0
			6	3	3		
3	6-H	1	Total	C	O	0	0
			6	3	3		
3	7-H	1	Total	C	O	0	0
			6	3	3		
3	8-H	1	Total	C	O	0	0
			6	3	3		
3	9-H	1	Total	C	O	0	0
			6	3	3		
3	10-H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: GOL, FMT, CL) (formula:  $C_3H_8O_3$ ,  $CH_2O_2$ , Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	9-H	2	Total Cl 2 2	0	0
4	7-C	1	Total Cl 1 1	0	0
4	2-F	1	Total Cl 1 1	0	0
4	1-B	1	Total Cl 1 1	0	0
4	9-D	2	Total Cl 3 3	0	0
4	6-C	1	Total Cl 1 1	0	0
4	5-A	1	Total Cl 2 2	0	0
4	8-A	2	Total Cl 2 2	0	0
4	2-H	2	Total Cl 2 2	0	0
4	7-F	1	Total Cl 1 1	0	0
4	4-D	2	Total Cl 3 3	0	0
4	3-H	2	Total Cl 2 2	0	0
4	4-H	1	Total Cl 1 1	0	0
4	1-D	2	Total Cl 2 2	0	0
4	7-B	1	Total Cl 1 1	0	0
4	4-A	2	Total Cl 2 2	0	0
4	3-C	1	Total Cl 1 1	0	0
4	7-H	1	Total Cl 1 1	0	0
4	2-C	1	Total Cl 1 1	0	0
4	1-A	2	Total Cl 2 2	0	0
4	9-C	1	Total Cl 1 1	0	0
4	5-D	2	Total Cl 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	8-B	1	Total 1	Cl 1	0	0
4	7-A	1	Total 2	Cl 2	0	0
4	10-C	2	Total 2	Cl 2	0	0
4	6-D	2	Total 3	Cl 3	0	0
4	3-B	1	Total 1	Cl 1	0	0
4	1-G	1	Total 1	Cl 1	0	0
4	5-C	2	Total 2	Cl 2	0	0
4	3-G	1	Total 1	Cl 1	0	0
4	4-G	1	Total 2	Cl 2	0	0
4	7-D	2	Total 3	Cl 3	0	0
4	2-D	2	Total 3	Cl 3	0	0
4	3-F	1	Total 1	Cl 1	0	0
4	10-D	2	Total 2	Cl 2	0	0
4	6-A	1	Total 1	Cl 1	0	0
4	8-C	1	Total 1	Cl 1	0	0
4	6-H	2	Total 2	Cl 2	0	0
4	8-H	2	Total 2	Cl 2	0	0
4	3-A	1	Total 2	Cl 2	0	0
4	5-B	1	Total 1	Cl 1	0	0
4	1-H	2	Total 2	Cl 2	0	0
4	8-D	2	Total 3	Cl 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-E	1	Total	Cl	0	0
			1	1		
4	4-C	1	Total	Cl	0	0
			1	1		
4	1-C	2	Total	Cl	0	0
			2	2		
4	10-E	1	Total	Cl	0	0
			1	1		
4	6-B	1	Total	Cl	0	0
			2	2		
4	3-D	2	Total	Cl	0	0
			3	3		
4	10-H	2	Total	Cl	0	0
			2	2		
4	7-G	1	Total	Cl	0	0
			2	2		
4	2-A	2	Total	Cl	0	0
			2	2		
4	5-H	2	Total	Cl	0	0
			2	2		
4	10-A	2	Total	Cl	0	0
			2	2		
4	9-A	1	Total	Cl	0	0
			2	2		
4	6-F	1	Total	Cl	0	0
			1	1		
4	1-F	1	Total	Cl	0	0
			1	1		

- Molecule 5 is FORMIC ACID (three-letter code: GOL, FMT, CL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>, CH<sub>2</sub>O<sub>2</sub>, Cl).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	1-C	1	Total	C	O	0	0
			3	1	2		
5	5-C	1	Total	C	O	0	0
			3	1	2		
5	6-C	1	Total	C	O	0	0
			3	1	2		
5	7-C	1	Total	C	O	0	0
			3	1	2		
5	9-C	1	Total	C	O	0	0
			3	1	2		
5	10-C	1	Total	C	O	0	0
			3	1	2		
5	1-F	1	Total	C	O	0	0
			3	1	2		
5	2-F	1	Total	C	O	0	0
			3	1	2		
5	3-F	1	Total	C	O	0	0
			3	1	2		
5	6-F	1	Total	C	O	0	0
			3	1	2		
5	7-F	1	Total	C	O	0	0
			3	1	2		
5	1-G	1	Total	C	O	0	0
			3	1	2		
5	3-G	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1-A	180	Total O 180 180	0	0
6	2-A	190	Total O 190 190	0	0
6	3-A	183	Total O 183 183	0	0
6	4-A	184	Total O 184 184	0	0
6	5-A	197	Total O 197 197	0	0
6	6-A	179	Total O 179 179	0	0
6	7-A	192	Total O 192 192	0	0
6	8-A	183	Total O 183 183	0	0
6	9-A	188	Total O 188 188	0	0
6	10-A	173	Total O 173 173	0	0
6	1-B	198	Total O 198 198	0	0
6	2-B	189	Total O 189 189	0	0
6	3-B	183	Total O 183 183	0	0
6	4-B	189	Total O 189 189	0	0
6	5-B	189	Total O 189 189	0	0
6	6-B	195	Total O 195 195	0	0
6	7-B	196	Total O 196 196	0	0
6	8-B	185	Total O 185 185	0	0
6	9-B	198	Total O 198 198	0	0
6	10-B	195	Total O 195 195	0	0
6	1-C	178	Total O 178 178	0	0
6	2-C	178	Total O 178 178	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	3-C	181	Total 181	O 181	0	0
6	4-C	176	Total 176	O 176	0	0
6	5-C	178	Total 178	O 178	0	0
6	6-C	174	Total 174	O 174	0	0
6	7-C	196	Total 196	O 196	0	0
6	8-C	183	Total 183	O 183	0	0
6	9-C	178	Total 178	O 178	0	0
6	10-C	188	Total 188	O 188	0	0
6	1-D	183	Total 183	O 183	0	0
6	2-D	159	Total 159	O 159	0	0
6	3-D	188	Total 188	O 188	0	0
6	4-D	179	Total 179	O 179	0	0
6	5-D	179	Total 179	O 179	0	0
6	6-D	161	Total 161	O 161	0	0
6	7-D	177	Total 177	O 177	0	0
6	8-D	179	Total 179	O 179	0	0
6	9-D	179	Total 179	O 179	0	0
6	10-D	177	Total 177	O 177	0	0
6	1-E	178	Total 178	O 178	0	0
6	2-E	177	Total 177	O 177	0	0
6	3-E	196	Total 196	O 196	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	4-E	197	Total 197	O 197	0	0
6	5-E	173	Total 173	O 173	0	0
6	6-E	191	Total 191	O 191	0	0
6	7-E	180	Total 180	O 180	0	0
6	8-E	194	Total 194	O 194	0	0
6	9-E	181	Total 181	O 181	0	0
6	10-E	182	Total 182	O 182	0	0
6	1-F	178	Total 178	O 178	0	0
6	2-F	175	Total 175	O 175	0	0
6	3-F	159	Total 159	O 159	0	0
6	4-F	177	Total 177	O 177	0	0
6	5-F	166	Total 166	O 166	0	0
6	6-F	189	Total 189	O 189	0	0
6	7-F	179	Total 179	O 179	0	0
6	8-F	162	Total 162	O 162	0	0
6	9-F	176	Total 176	O 176	0	0
6	10-F	167	Total 167	O 167	0	0
6	1-G	186	Total 186	O 186	0	0
6	2-G	175	Total 175	O 175	0	0
6	3-G	183	Total 183	O 183	0	0
6	4-G	185	Total 185	O 185	0	0

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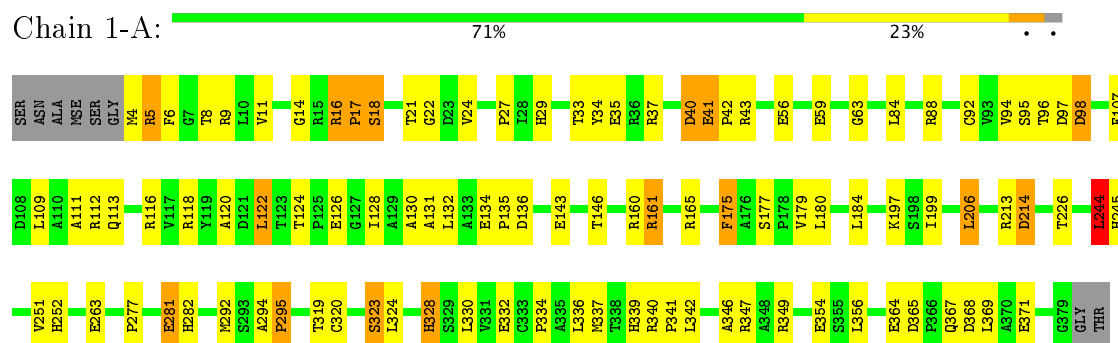
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	5-G	172	Total 172	O 172	0	0
6	6-G	176	Total 176	O 176	0	0
6	7-G	187	Total 187	O 187	0	0
6	8-G	179	Total 179	O 179	0	0
6	9-G	197	Total 197	O 197	0	0
6	10-G	182	Total 182	O 182	0	0
6	1-H	172	Total 172	O 172	0	0
6	2-H	185	Total 185	O 185	0	0
6	3-H	163	Total 163	O 163	0	0
6	4-H	184	Total 184	O 184	0	0
6	5-H	183	Total 183	O 183	0	0
6	6-H	184	Total 184	O 184	0	0
6	7-H	183	Total 183	O 183	0	0
6	8-H	191	Total 191	O 191	0	0
6	9-H	168	Total 168	O 168	0	0
6	10-H	194	Total 194	O 194	0	0

### 3 Residue-property plots

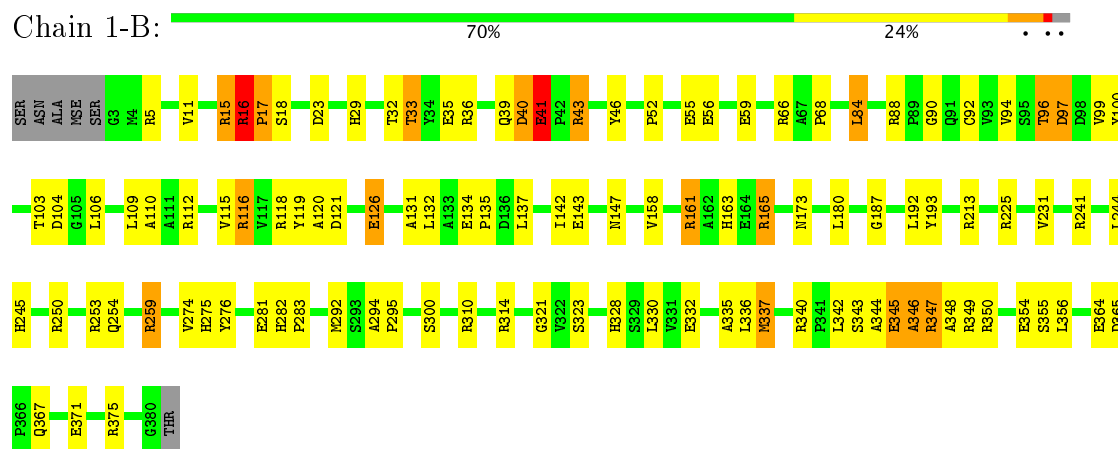
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS failed to run properly.

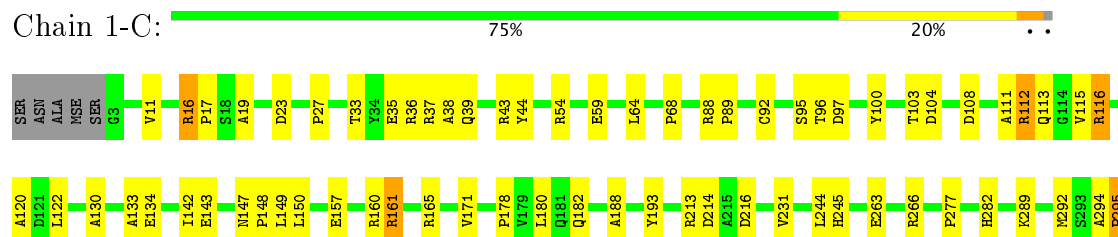
#### • Molecule 1: CalE6

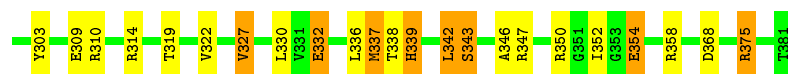


#### • Molecule 1: CalE6



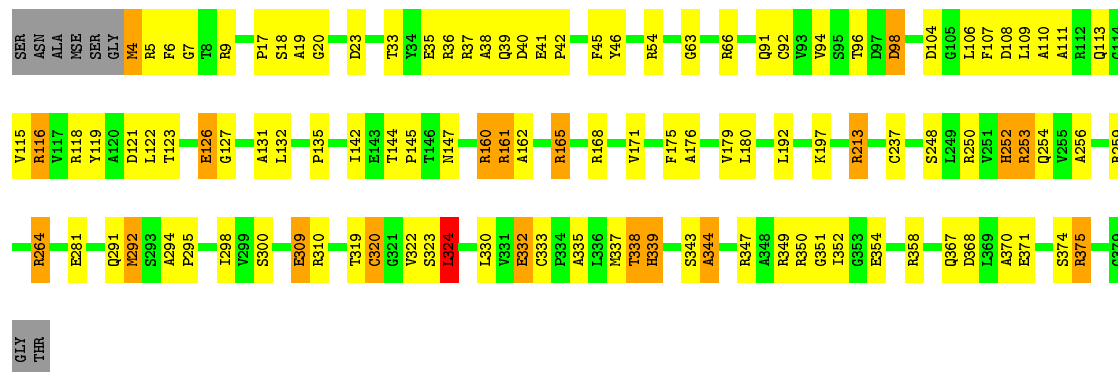
#### • Molecule 1: CalE6





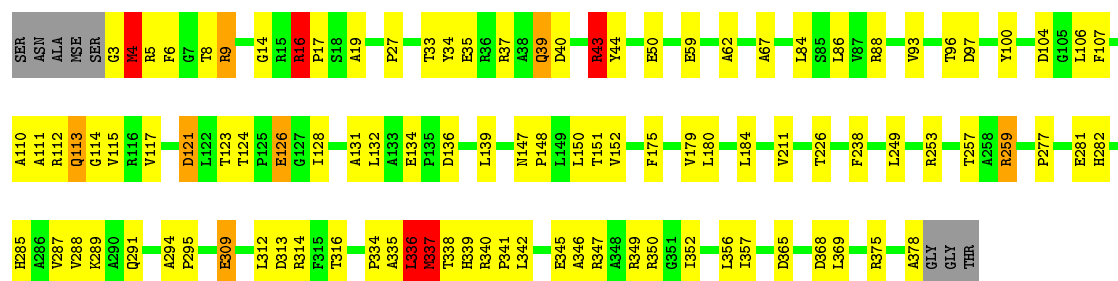
• Molecule 1: CalE6

Chain 1-D: 69% 24% 5%



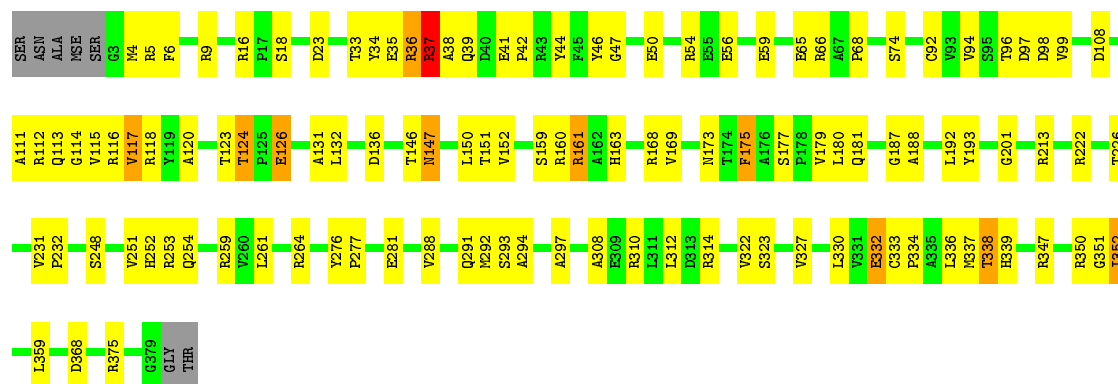
• Molecule 1: CalE6

Chain 1-E: 71% 24% ...



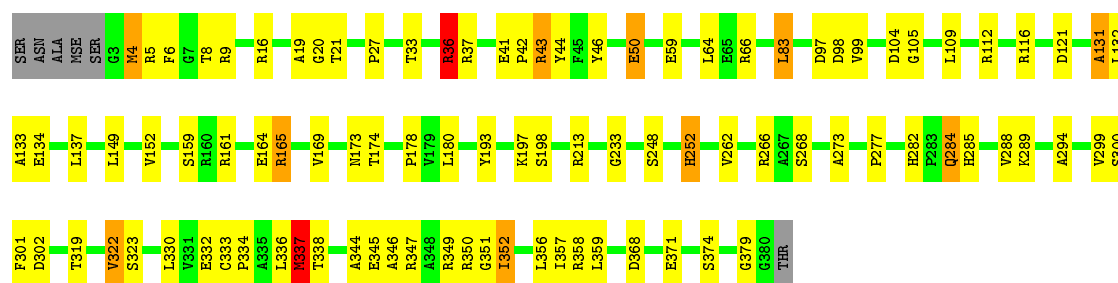
• Molecule 1: CalE6

Chain 1-F: 68% 27% ..



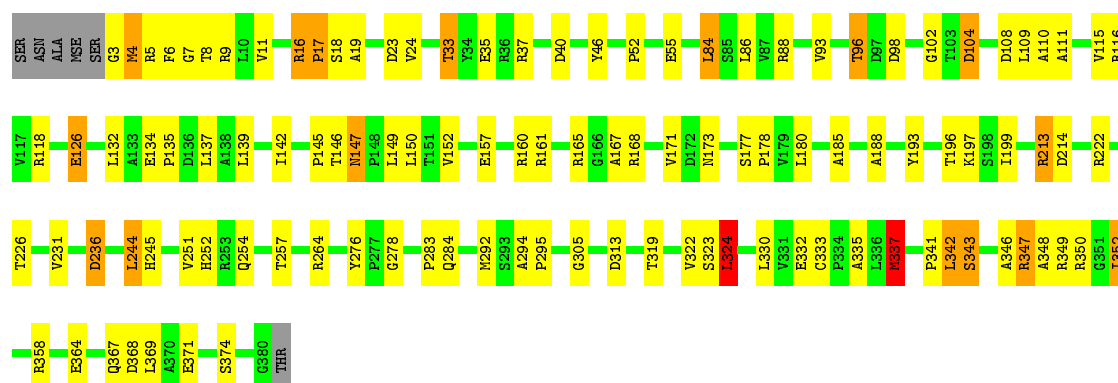
• Molecule 1: CalE6

Chain 1-G: 73% 22% ...



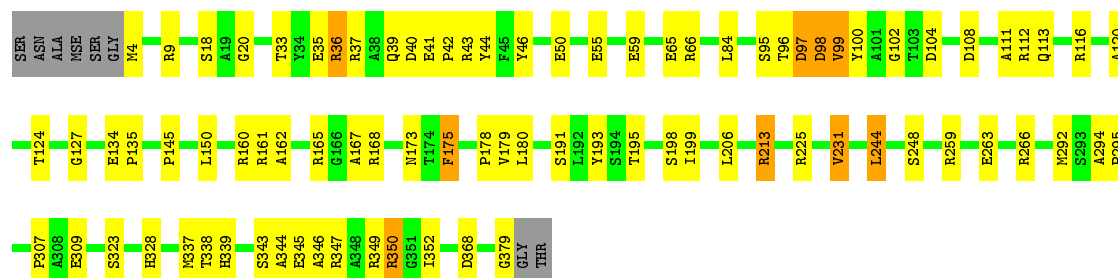
- Molecule 1: CalE6

Chain 1-H: 69% 25% . .



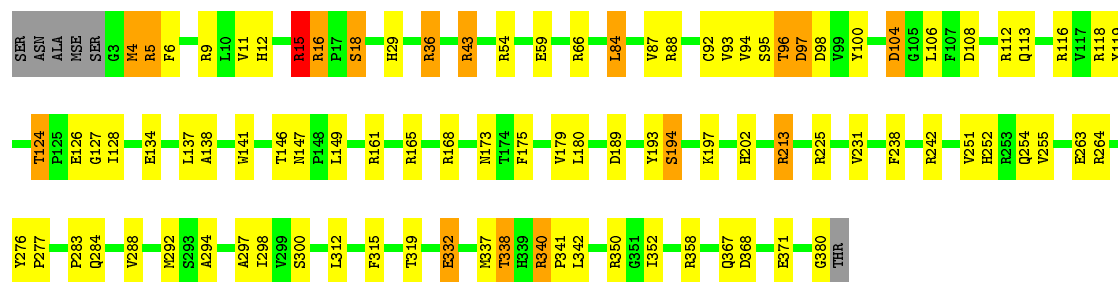
- Molecule 1: CalE6

Chain 2-A: 76% 20% . .



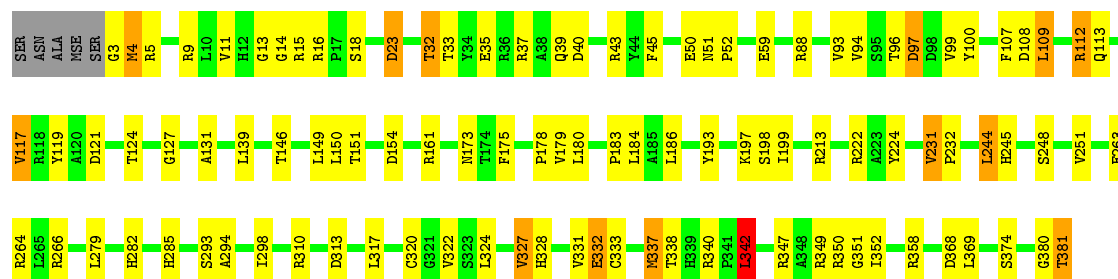
- Molecule 1: CalE6

Chain 2-B: 74% 20% . .



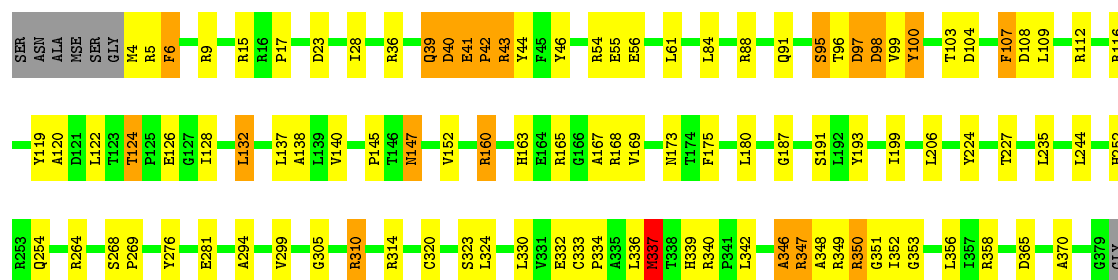
- Molecule 1: CalE6

Chain 2-C:  72% 23% ..



• Molecule 1: CalE6

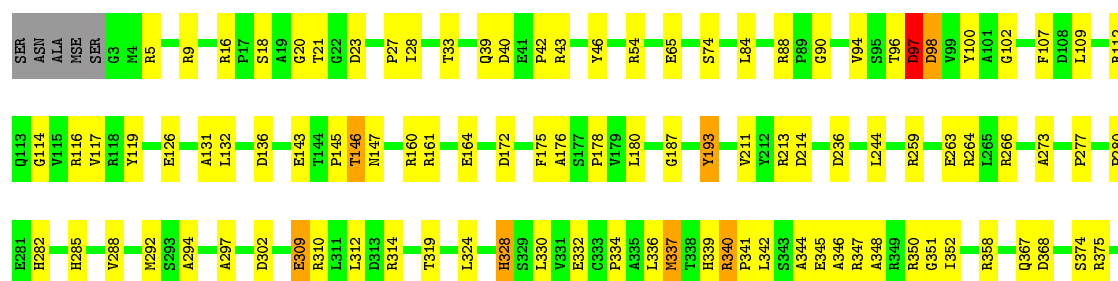
Chain 2-D:  71% 22% 5% .



THR


• Molecule 1: CalE6

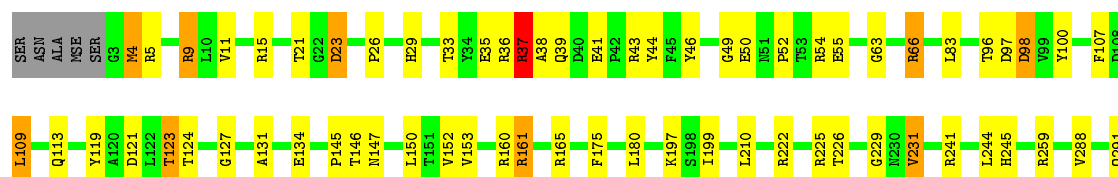
Chain 2-E:  72% 24% ..



A378  
GLY  
GLY  
THR

• Molecule 1: CalE6

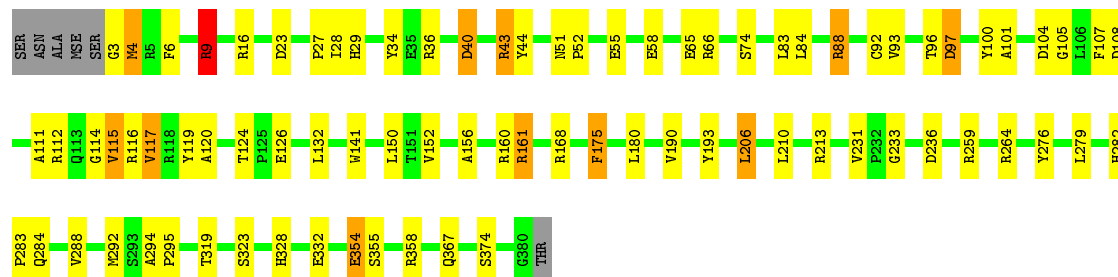
Chain 2-F:  75% 21% ..





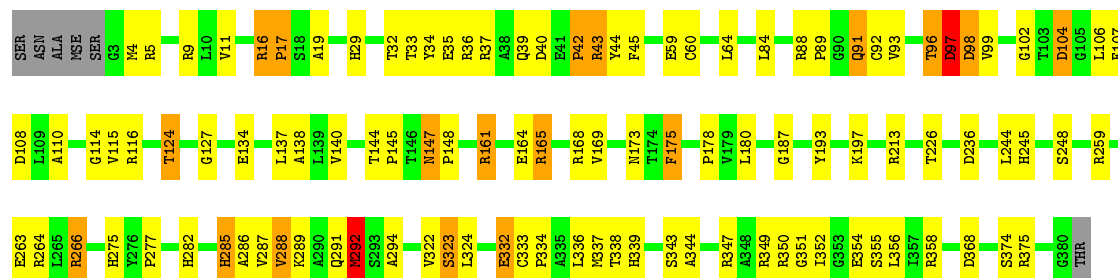
• Molecule 1: CalE6

Chain 2-G: 77% 18% . .



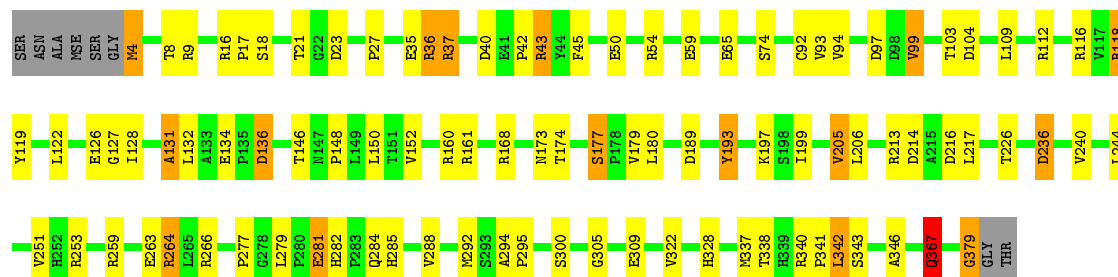
• Molecule 1: CalE6

Chain 2-H: 70% 23% 5% . .



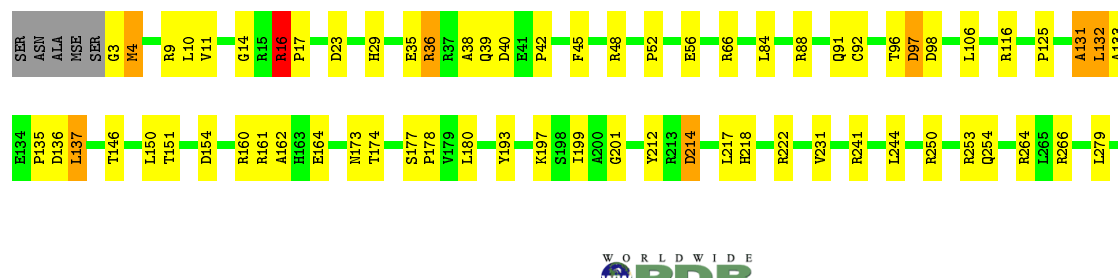
• Molecule 1: CalE6

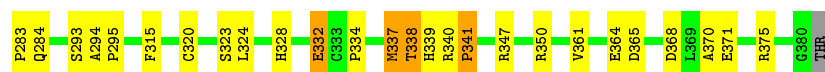
Chain 3-A: 73% 21% . .



• Molecule 1: CalE6

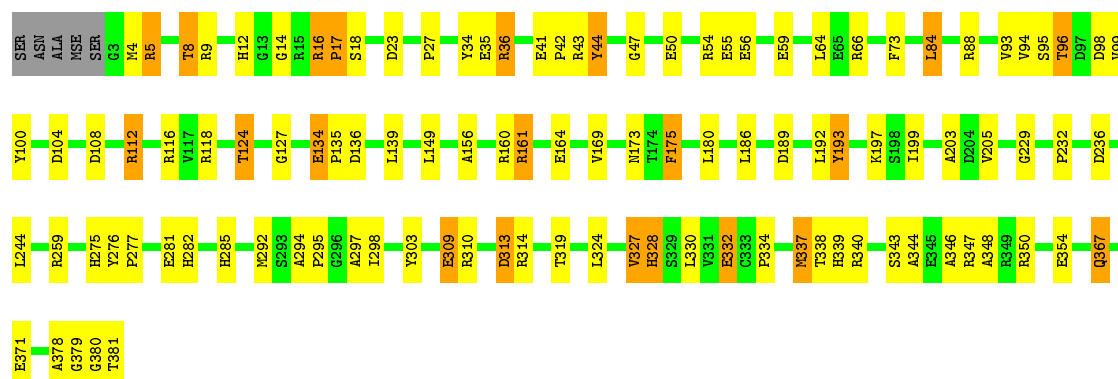
Chain 3-B: 74% 21% . .





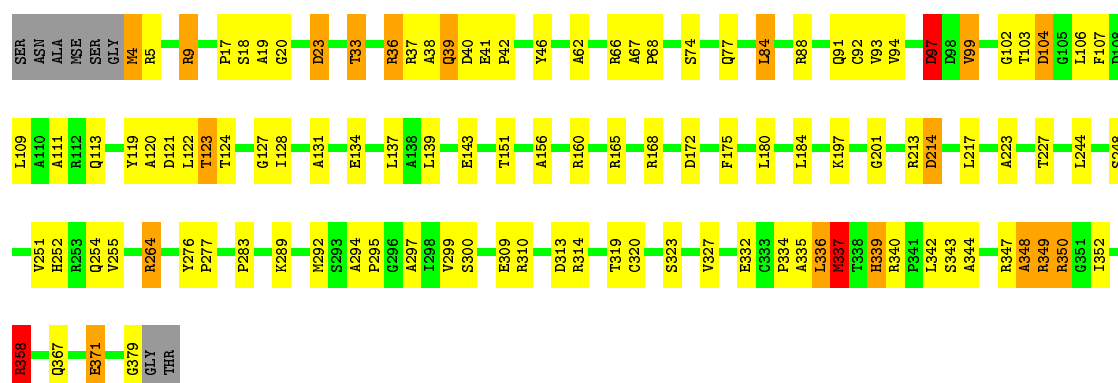
• Molecule 1: CalE6

Chain 3-C: 70% 23% 5%



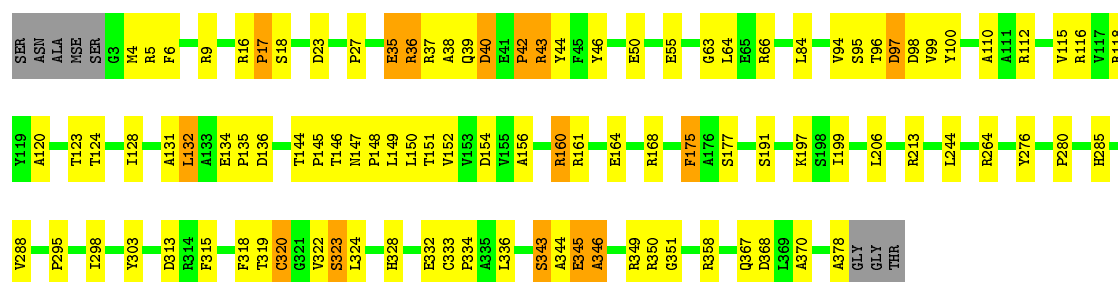
• Molecule 1: CalE6

Chain 3-D: 69% 24% 5%



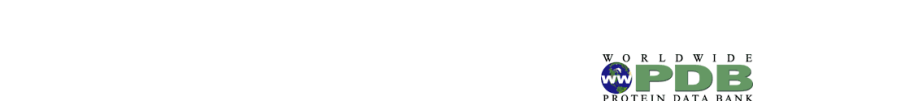
• Molecule 1: CalE6

Chain 3-E: 71% 23%

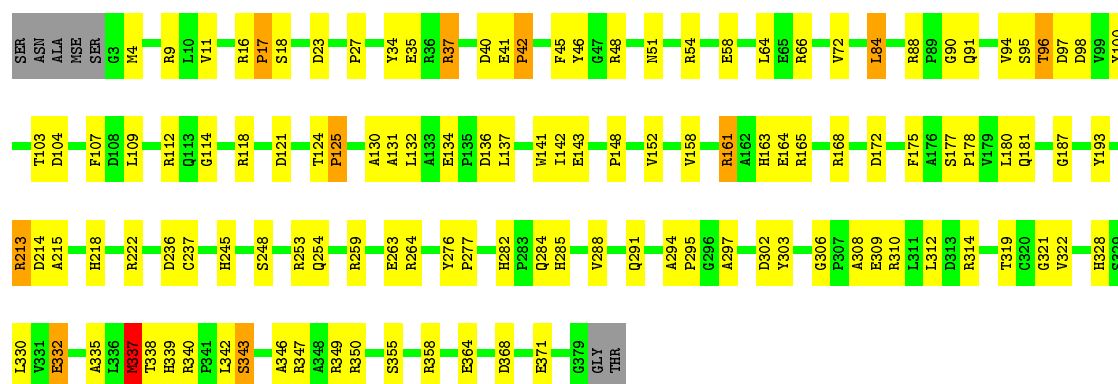


• Molecule 1: CalE6

Chain 3-F: 66% 29%

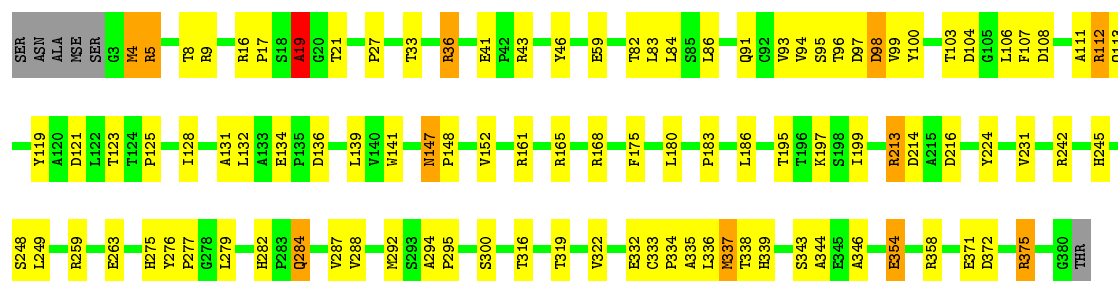






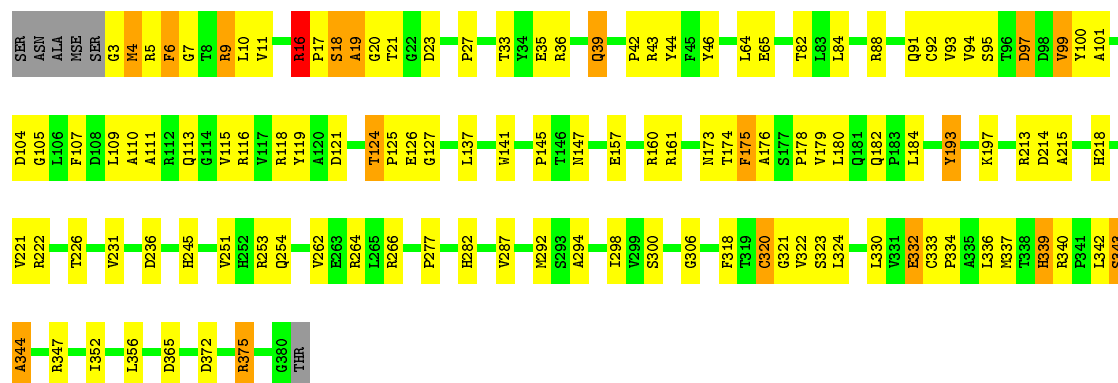
• Molecule 1: CalE6

Chain 3-G: 72% 23%



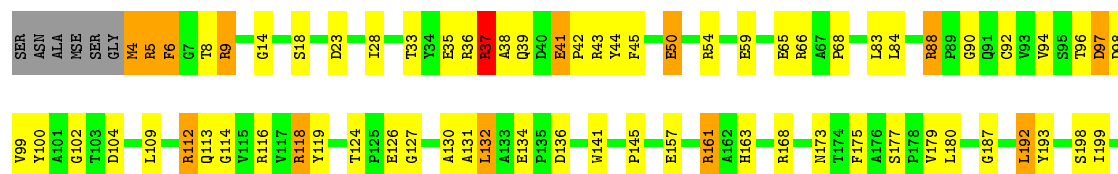
• Molecule 1: CalE6

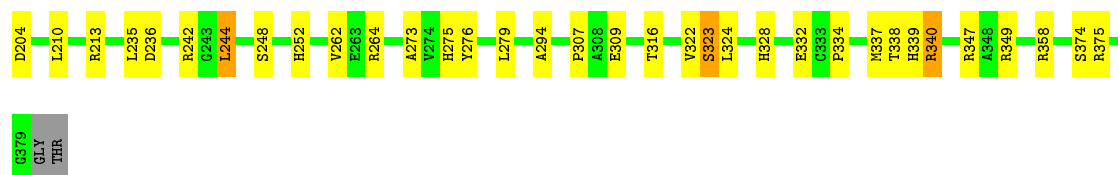
Chain 3-H: 67% 26%



• Molecule 1: CalE6

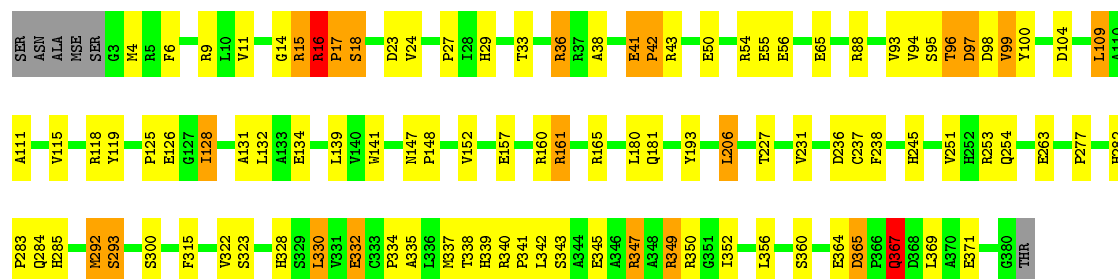
Chain 4-A: 71% 23%





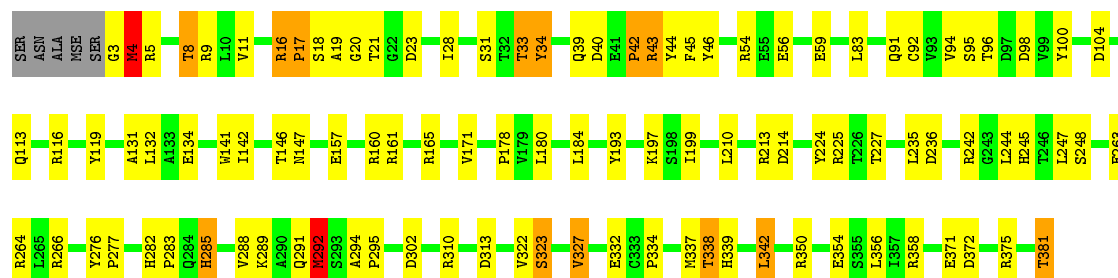
- Molecule 1: CalE6

Chain 4-B: 72% 21% 5% ..



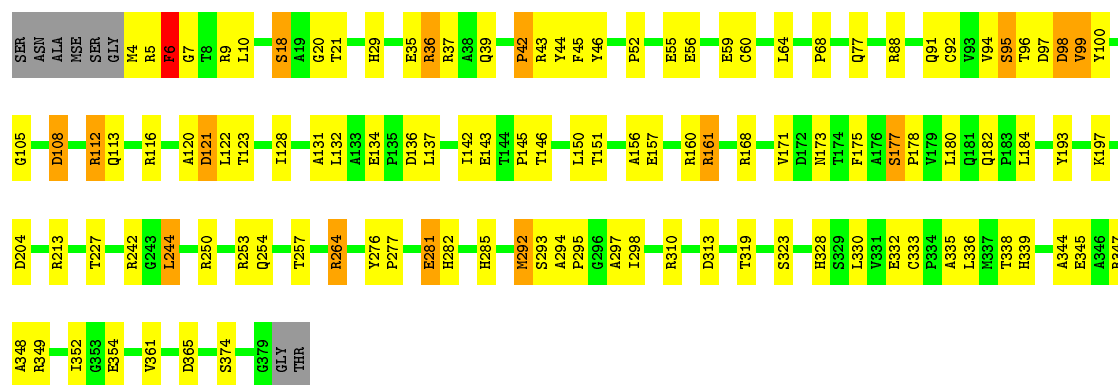
- Molecule 1: CalE6

Chain 4-C: 72% 23% ..



- Molecule 1: CalE6

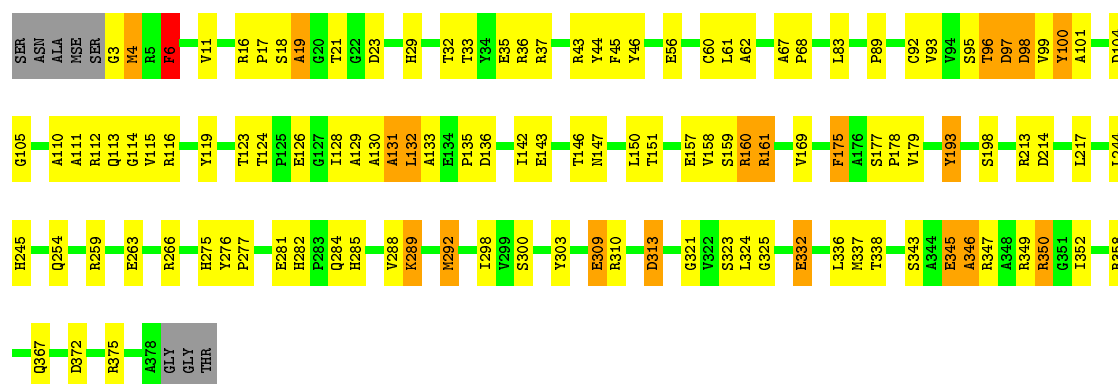
Chain 4-D: 68% 26% ..



- Molecule 1: CalE6

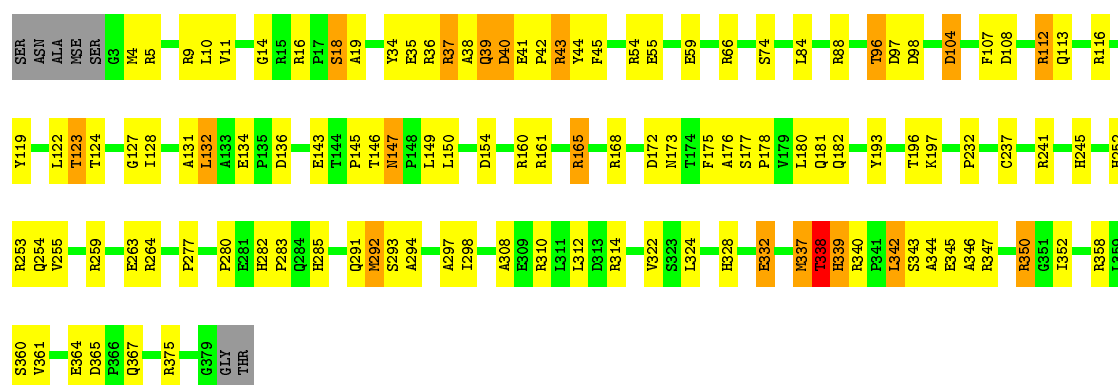
Chain 4-E: 67% 26% 5% ..





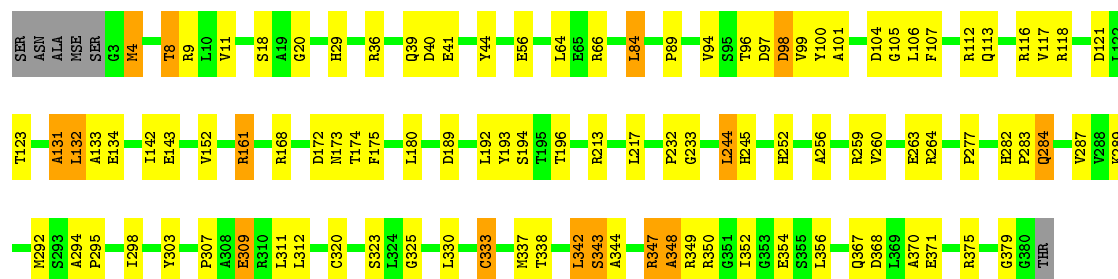
• Molecule 1: CalE6

Chain 4-F: 67% 26% 5% .



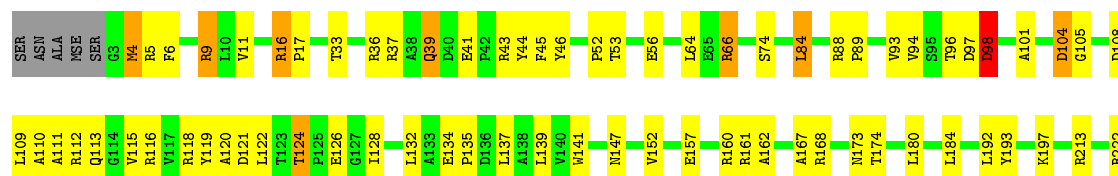
• Molecule 1: CalE6

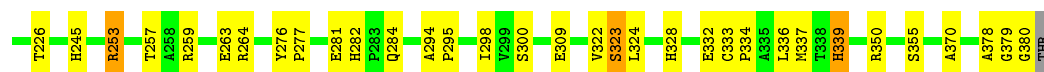
Chain 4-G: 71% 23% . .



• Molecule 1: CalE6

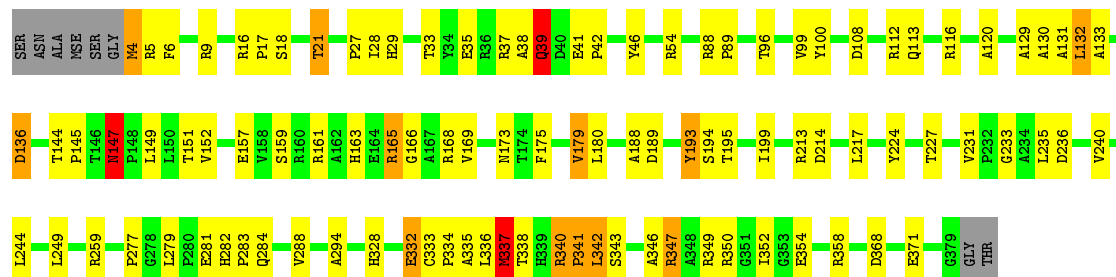
Chain 4-H: 71% 24% . .





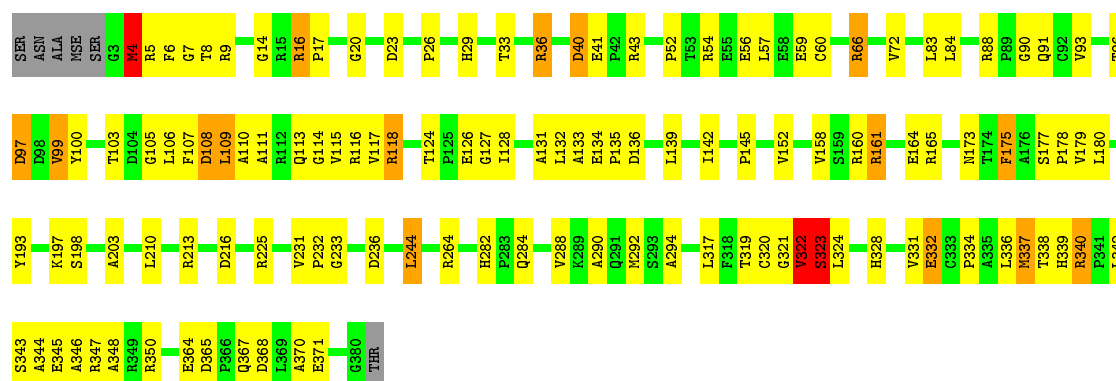
• Molecule 1: CalE6

Chain 5-A: 71% 23% . . .



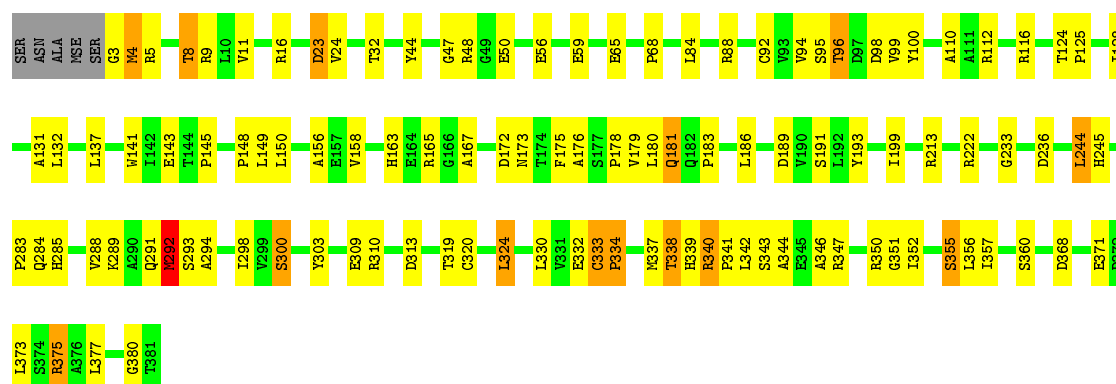
• Molecule 1: CalE6

Chain 5-B: 66% 28% . . .



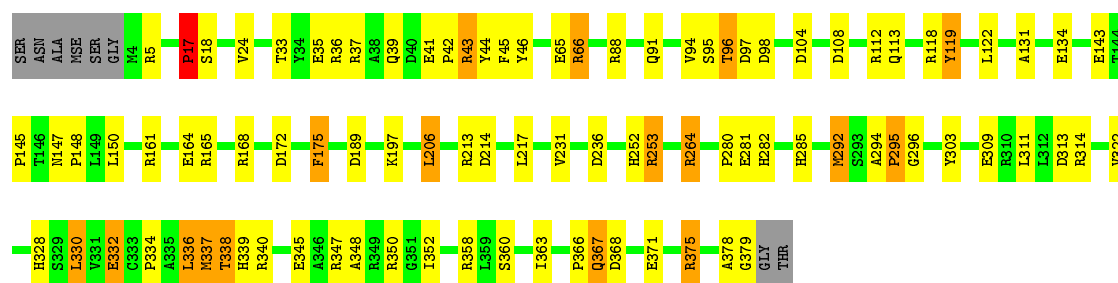
• Molecule 1: CalE6

Chain 5-C: 70% 25% . .



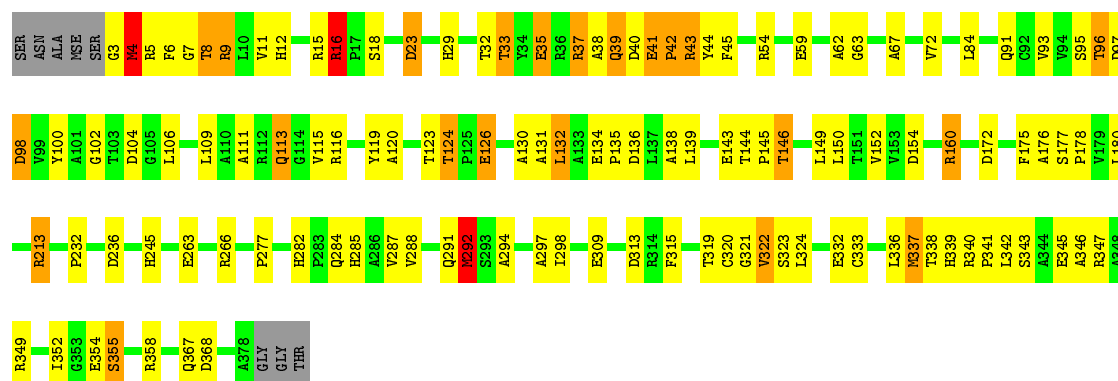
• Molecule 1: CalE6

Chain 5-D: 74% 20% . .



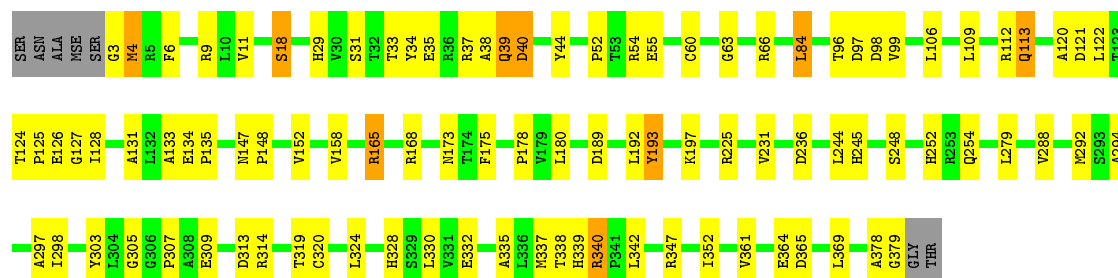
- Molecule 1: CalE6

Chain 5-E: 66% 25% 6% ..



- Molecule 1: CalE6

Chain 5-F: 73% 23% ..

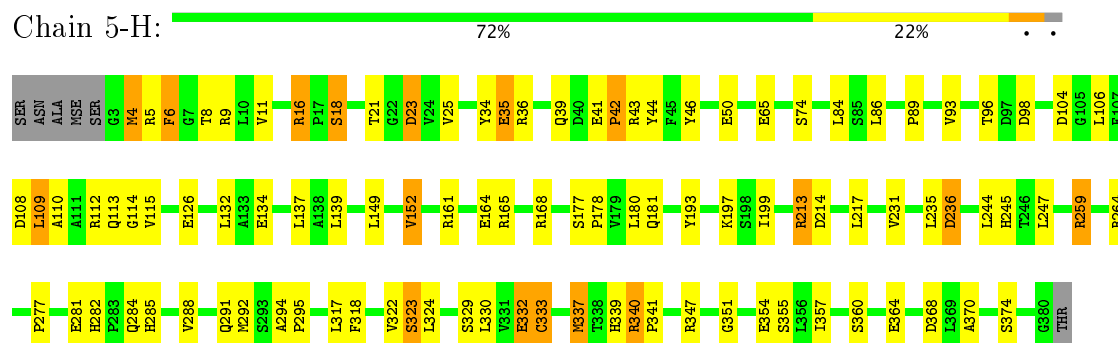


- Molecule 1: CalE6

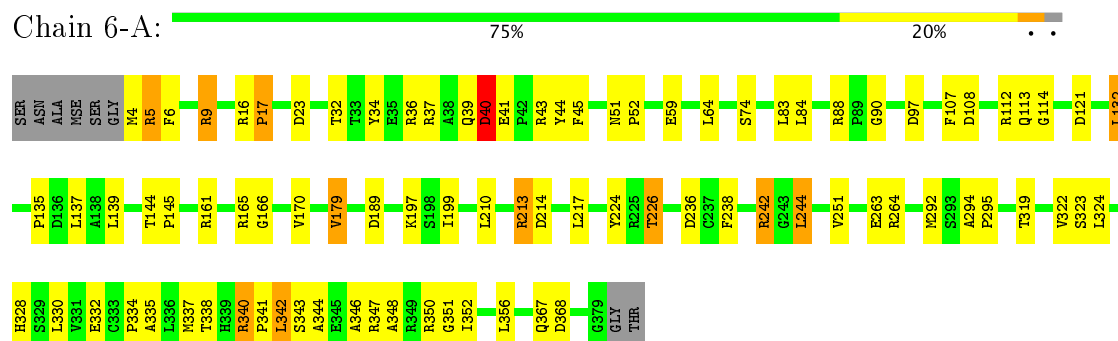
Chain 5-G: 75% 19% ..



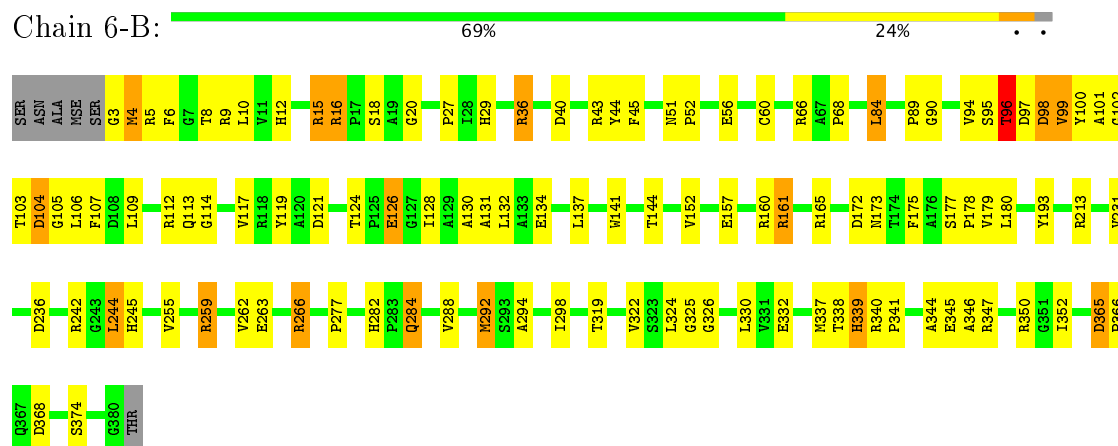
- Molecule 1: CalE6



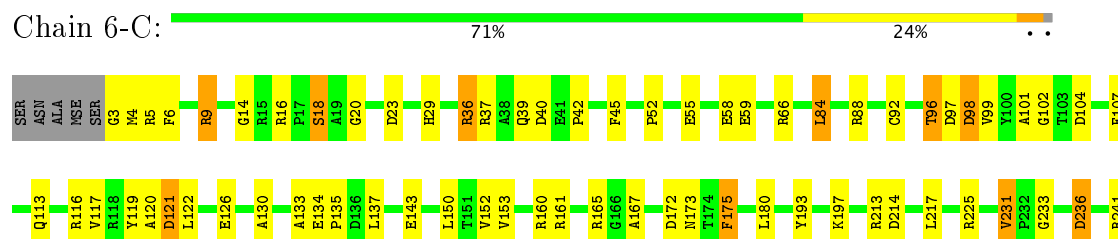
- Molecule 1: CalE6

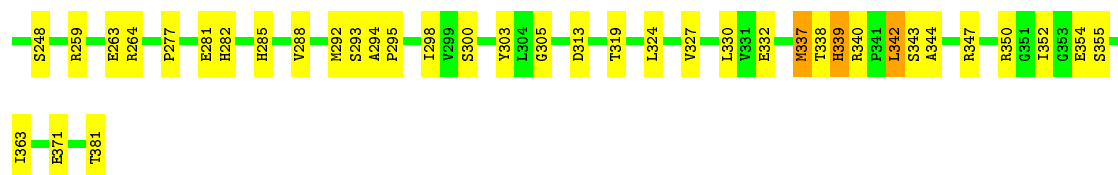


- Molecule 1: CalE6



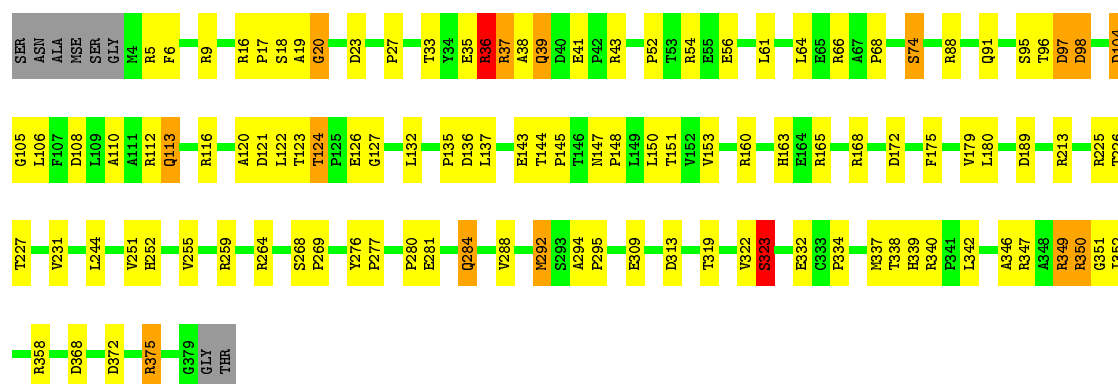
- Molecule 1: CalE6





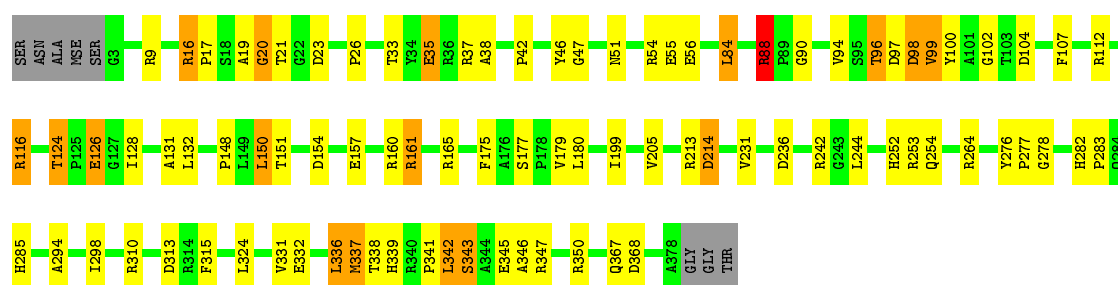
- Molecule 1: CalE6

Chain 6-D: 69% 25%



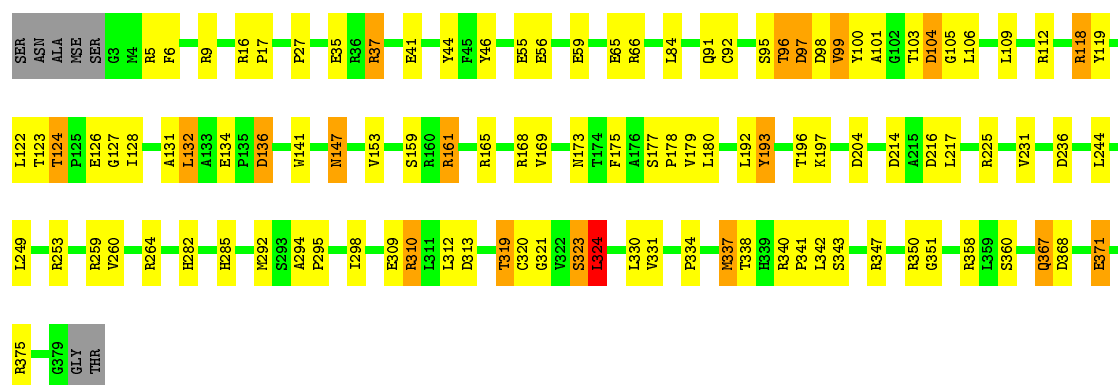
- Molecule 1: CalE6

Chain 6-E: 75% 18%

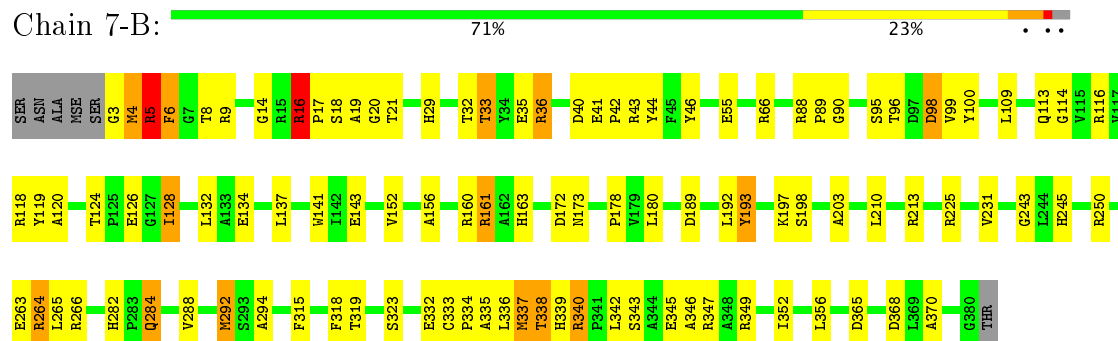


- Molecule 1: CalE6

Chain 6-F: 70% 23% 5%

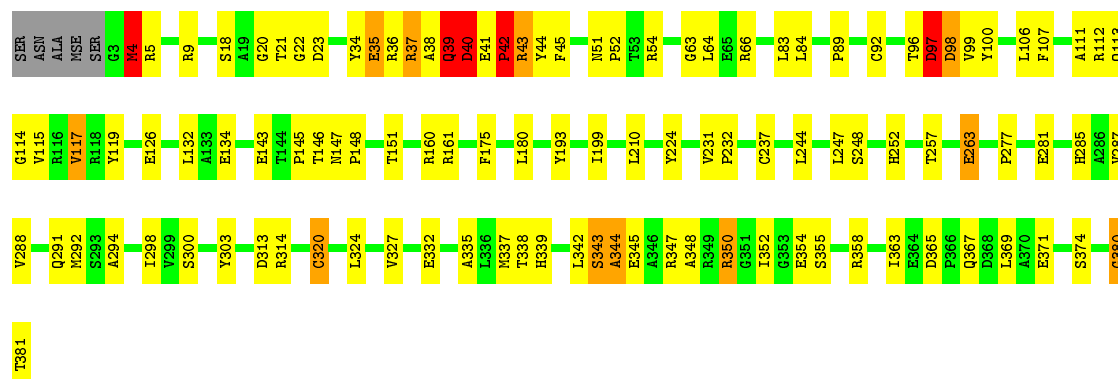


- Molecule 1: CalE6

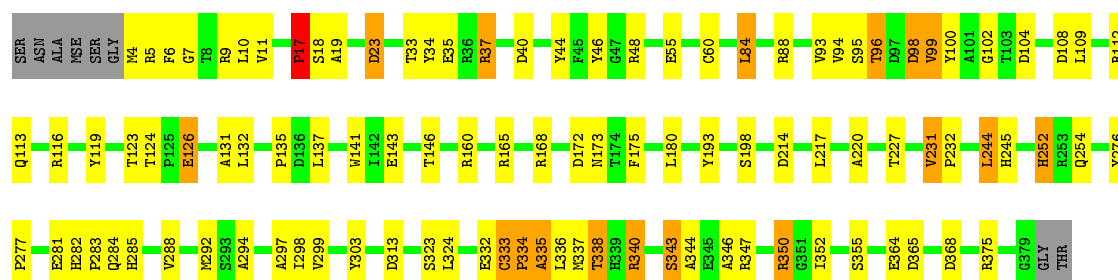




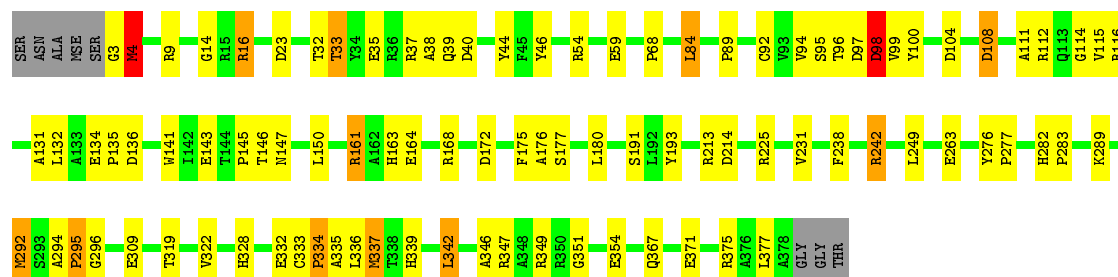
- Molecule 1: CalE6

Chain 7-C: 

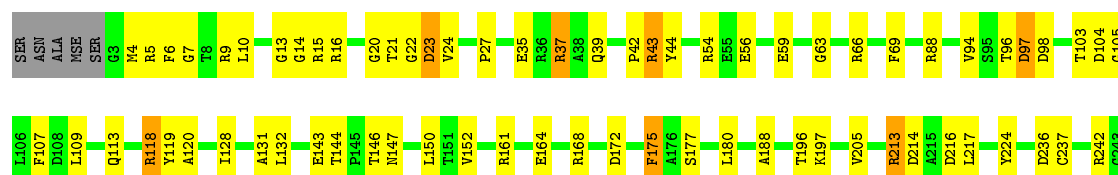
- Molecule 1: CalE6

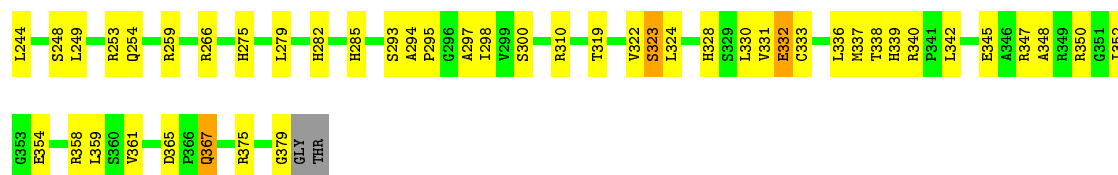
Chain 7-D: 

- Molecule 1: CalE6

Chain 7-E: 

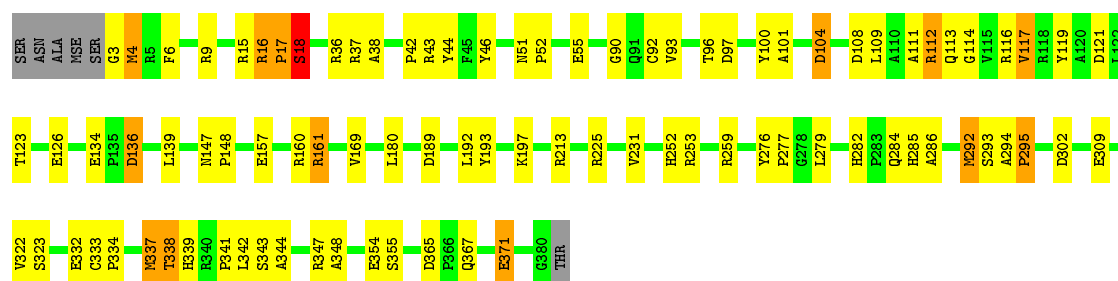
- Molecule 1: CalE6

Chain 7-F: 



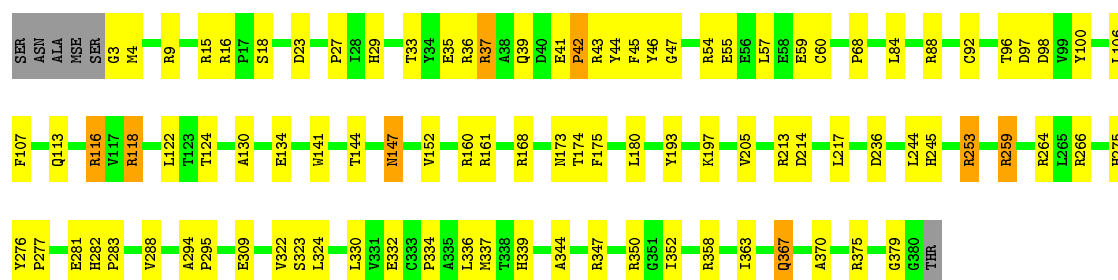
• Molecule 1: CalE6

Chain 7-G: 75% 20%



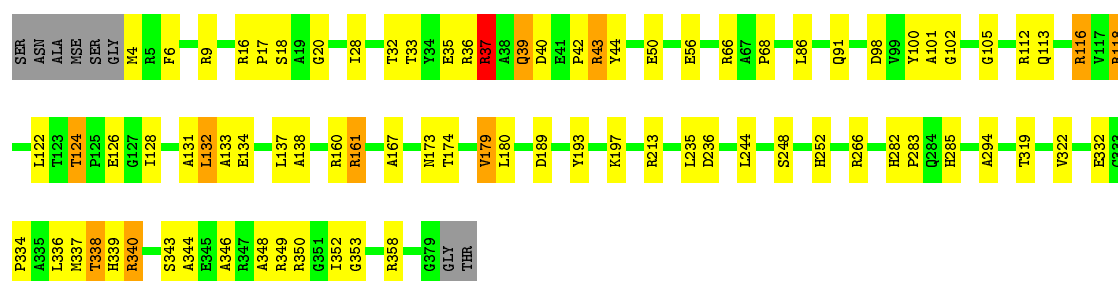
• Molecule 1: CalE6

Chain 7-H: 73% 23%



• Molecule 1: CalE6

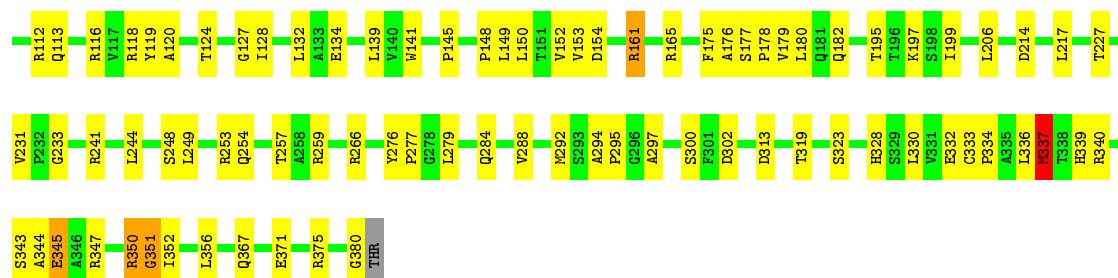
Chain 8-A: 77% 18%



• Molecule 1: CalE6

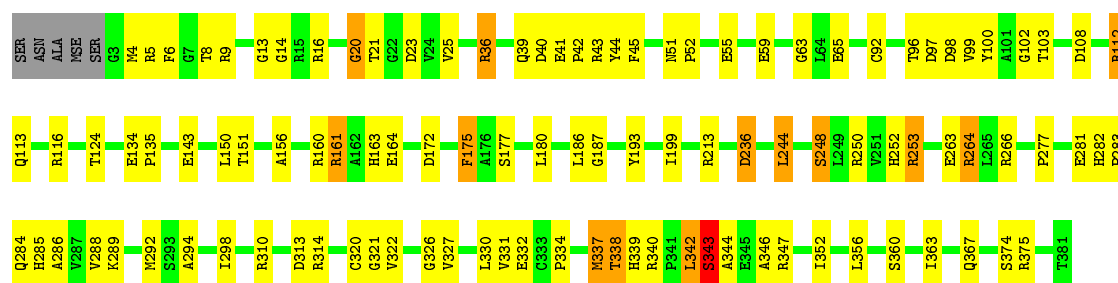
Chain 8-B: 68% 28%





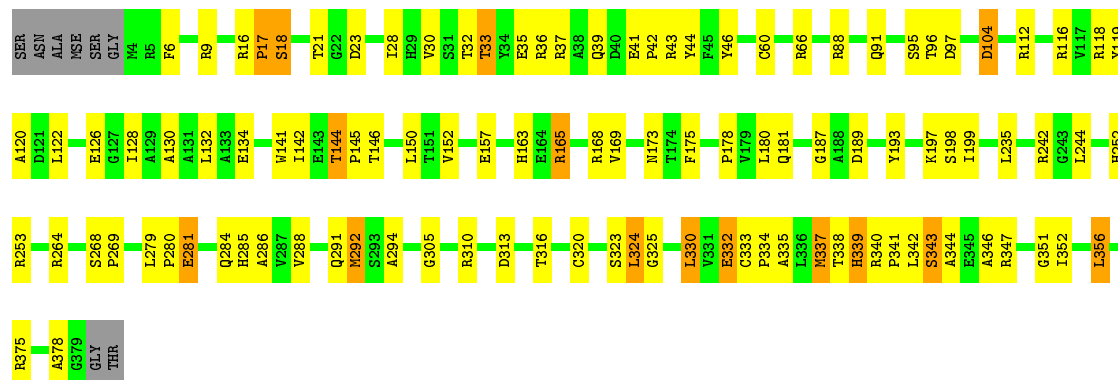
• Molecule 1: CalE6

Chain 8-C: 71% 24%



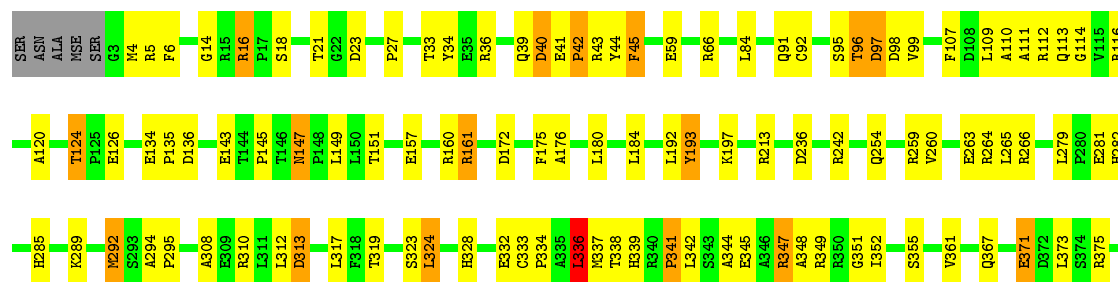
• Molecule 1: CalE6

Chain 8-D: 70% 24%



• Molecule 1: CalE6

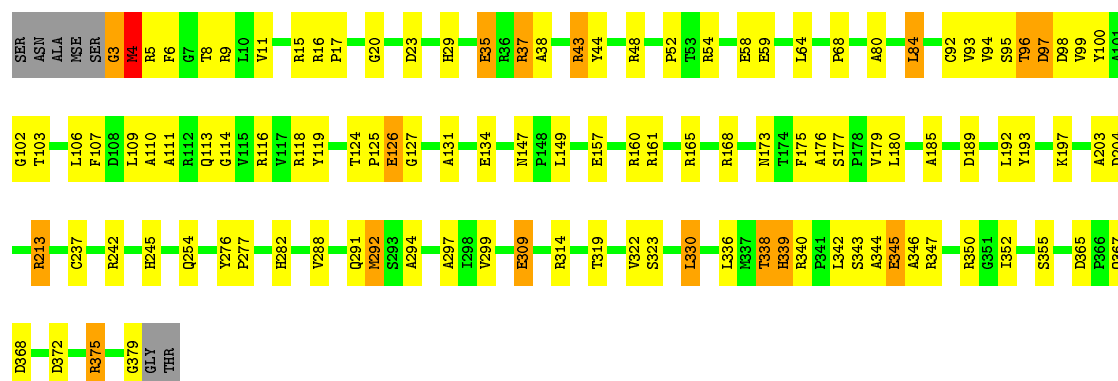
Chain 8-E: 70% 24%






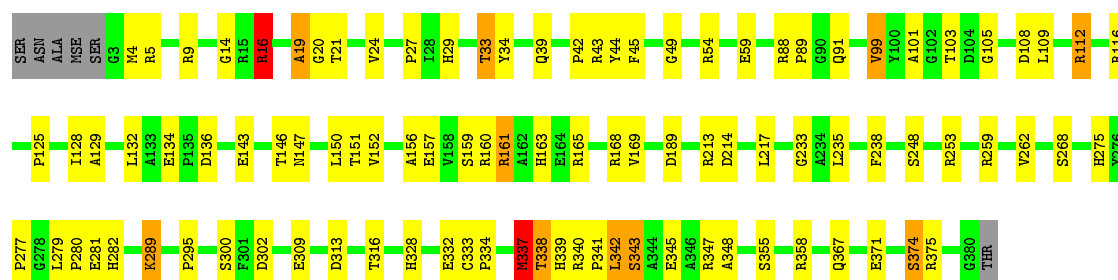
• Molecule 1: CalE6

Chain 8-F:  69% 25%




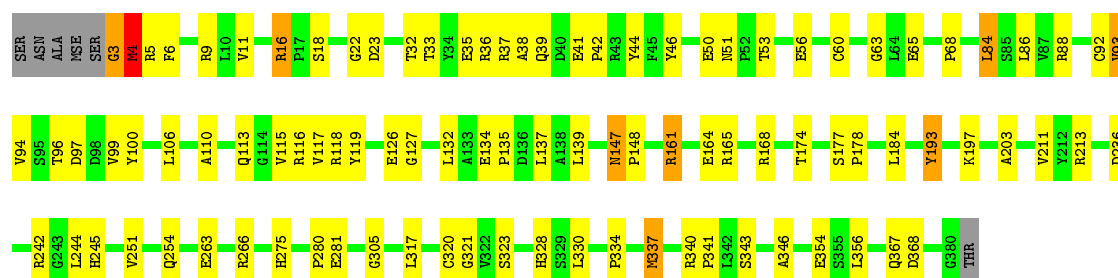
• Molecule 1: CalE6

Chain 8-G:  73% 22%



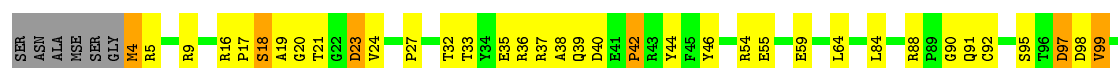
• Molecule 1: CalE6

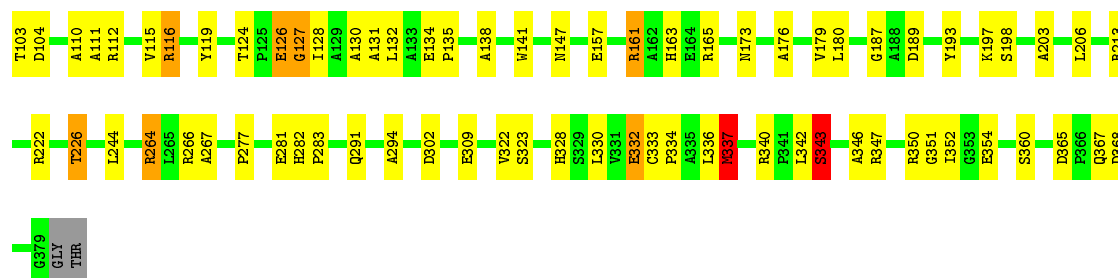
Chain 8-H:  73% 23%



• Molecule 1: CalE6

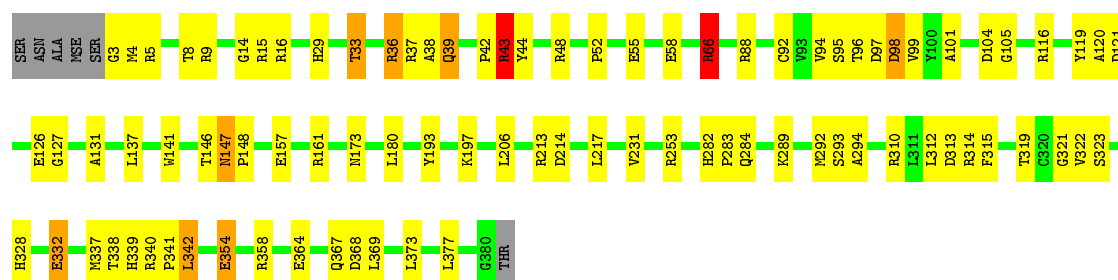
Chain 9-A:  70% 24%





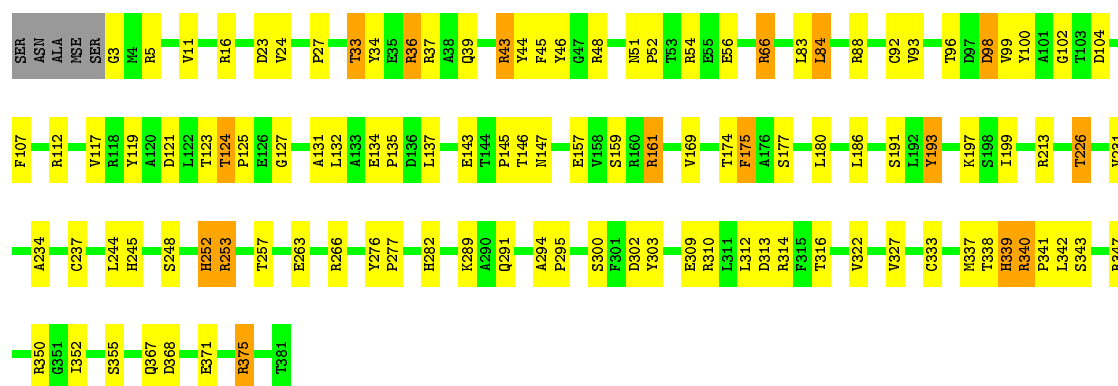
- Molecule 1: CalE6

Chain 9-B: 75% 21% ...



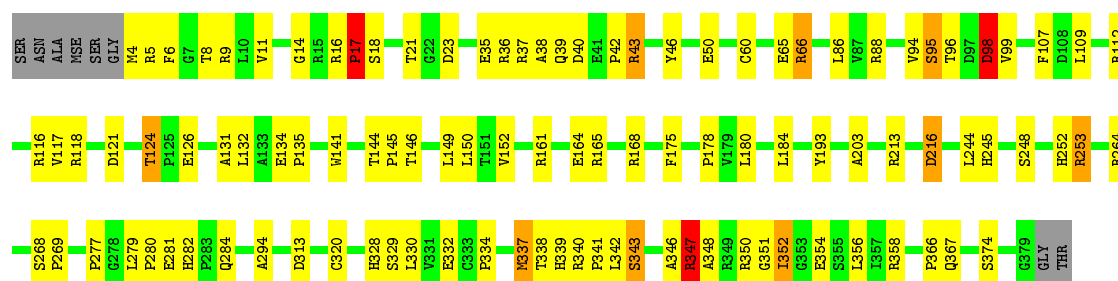
- Molecule 1: CalE6

Chain 9-C: 70% 25% ..



- Molecule 1: CalE6

Chain 9-D: 71% 24% ...



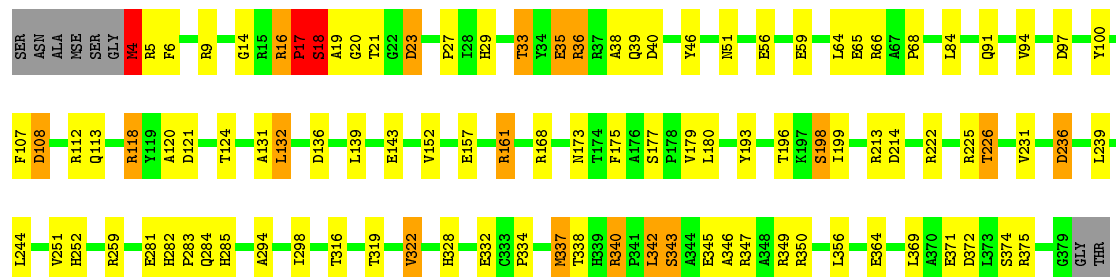
- Molecule 1: CalE6

SER	ASN	MSE	ALA	SER	G3	F6	M4	G7	R16	T8	P17	L10	R16	P17	T21	D22	D23	E29	Y34	E35	R36	R37	D40	E41	P42	R43	Y44	F45	Y46	E50	N51	P52	E55	E59	E65	L84	V87	R88	P89	G90	C92	V93	V94	S95	Y100	E103														
	G102		G105		L109		R112		Q113		R116		R118		Y119		A120		T124		L132		A133		E134		P135		D136		L137		L149		E157		Y158		S159		R161		A162		E163		R165	G166	A167	R168	N173	L180	L192	Y193	T196	I199	L210	R213	V231	L235
	G105		L109		R112		Q113		R116		R118		Y119		A120		T124		L132		A133		E134		P135		D136		L137		L149		E157		Y158		S159		R161		A162		E163		R165		G166	A167	R168	N173	L180	L192	Y193	T196	I199	L210	R213	V231	L235	
	G105		L109		R112		Q113		R116		R118		Y119		A120		T124		L132		A133		E134		P135		D136		L137		L149		E157		Y158		S159		R161		A162		E163		R165		G166	A167	R168	N173	L180	L192	Y193	T196	I199	L210	R213	V231	L235	
	G105		L109		R112		Q113		R116		R118		Y119		A120		T124		L132		A133		E134		P135		D136		L137		L149		E157		Y158		S159		R161		A162		E163		R165		G166	A167	R168	N173	L180	L192	Y193	T196	I199	L210	R213	V231	L235	
	G105		L109		R112		Q113		R116		R118		Y119		A120		T124		L132		A133		E134		P135		D136		L137		L149		E157		Y158		S159		R161		A162		E163		R165		G166	A167	R168	N173	L180	L192	Y193	T196	I199	L210	R213	V231	L235	
	G105		L109		R112		Q113		R116		R118		Y119		A120		T124		L132		A133		E134		P135		D136		L137		L149		E157		Y158		S159		R161		A162		E163		R165		G166	A167	R168	N173	L180	L192	Y193	T196	I199	L210	R213	V231	L235	
	G105		L109		R112		Q113		R116		R118		Y119		A120		T124		L132		A133		E134		P135		D136		L137		L149		E157		Y158		S159		R161		A162		E163		R165		G166	A167	R168	N173	L180	L192	Y193	T196	I199	L210	R213	V231	L235	
	G105		L109		R112		Q113		R116		R118		Y119		A120		T124		L132		A133		E134		P135		D136		L137		L149		E157		Y158		S159		R161		A162		E163		R165		G166	A167	R168	N173	L180	L192	Y193	T196	I199	L210	R213	V231	L235	
	G105		L109		R112		Q113		R116		R118		Y119		A120		T124		L132		A133		E134		P135		D136		L137		L149		E157		Y158		S159		R161		A162		E163		R165		G166	A167	R168	N173	L180	L192	Y193	T196	I199	L210	R213	V231	L235	



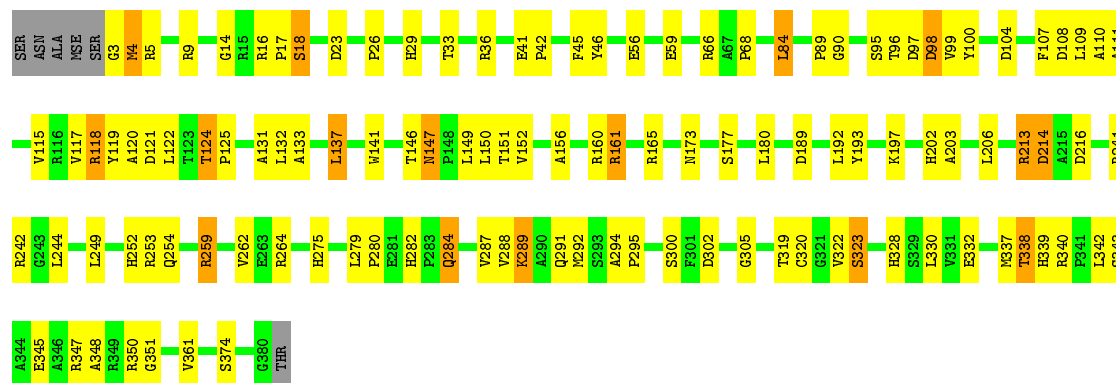
• Molecule 1: CalE6

Chain 10-A: 72% 21% . .



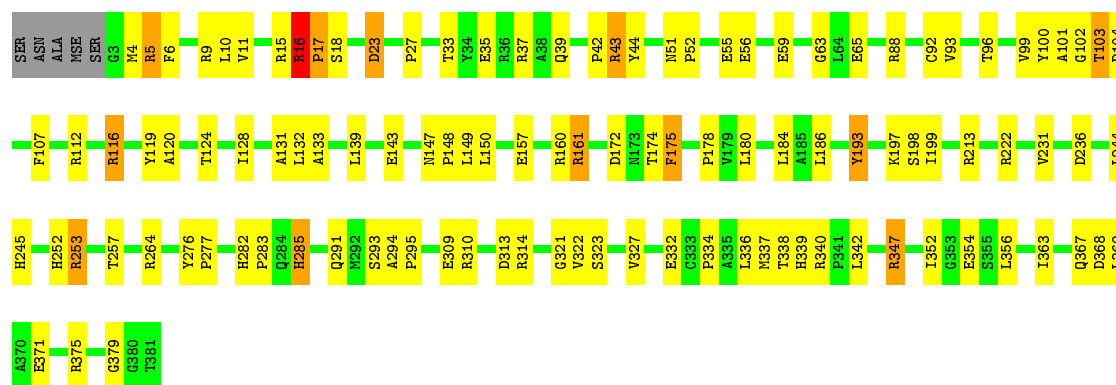
• Molecule 1: CalE6

Chain 10-B: 68% 27% . .



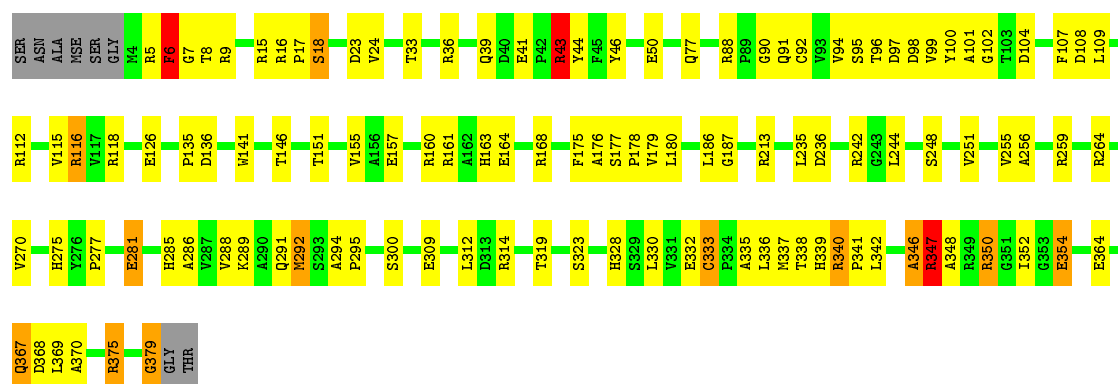
• Molecule 1: CalE6

Chain 10-C: 70% 26% . .



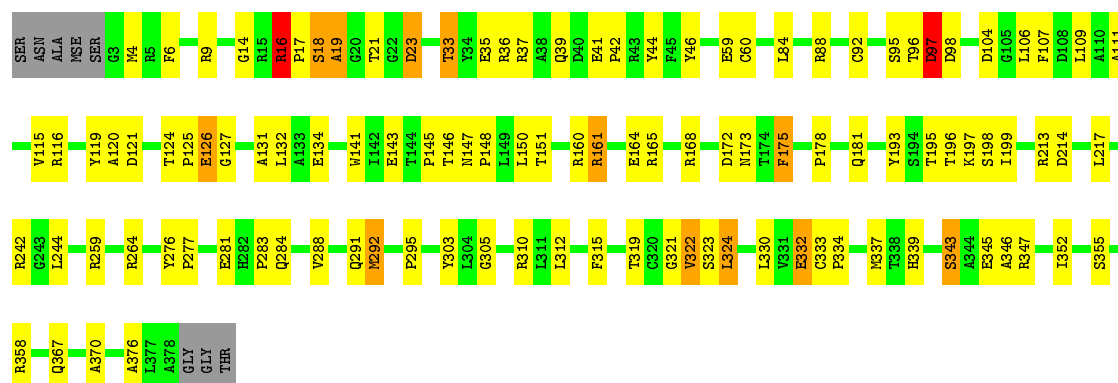
• Molecule 1: CalE6

Chain 10-D: 68% 26% . .



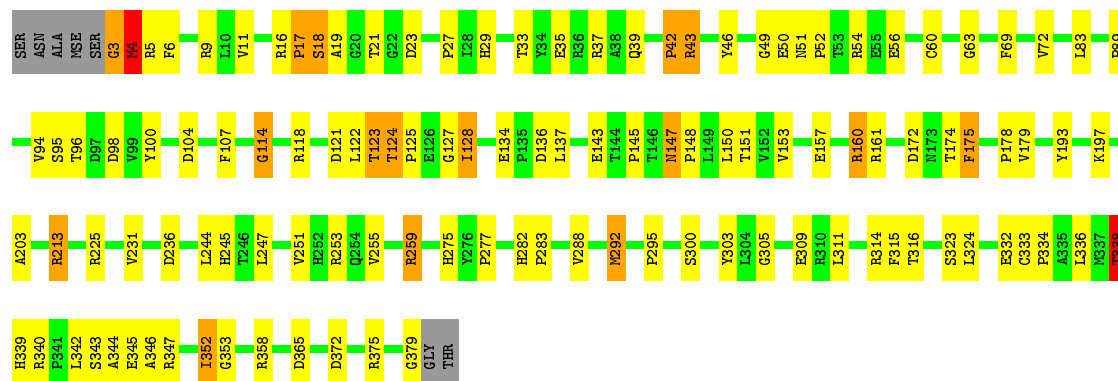
• Molecule 1: CalE6

Chain 10-E: 69% 25% ..



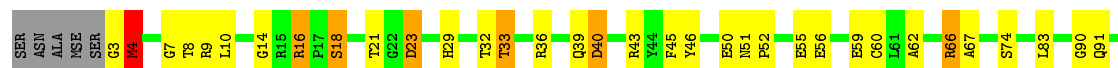
• Molecule 1: CalE6

Chain 10-F: 67% 26% ..

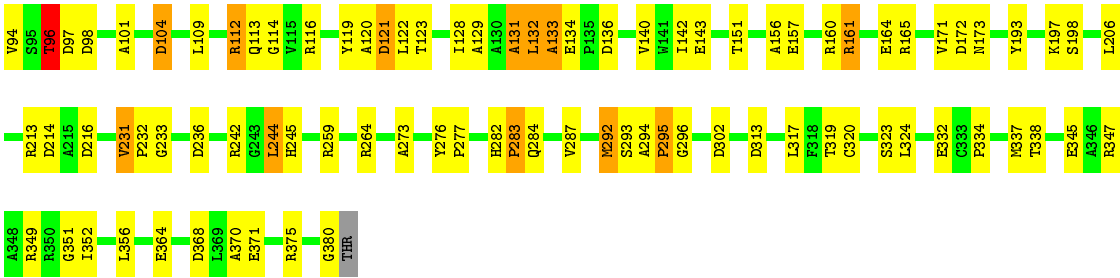


• Molecule 1: CalE6

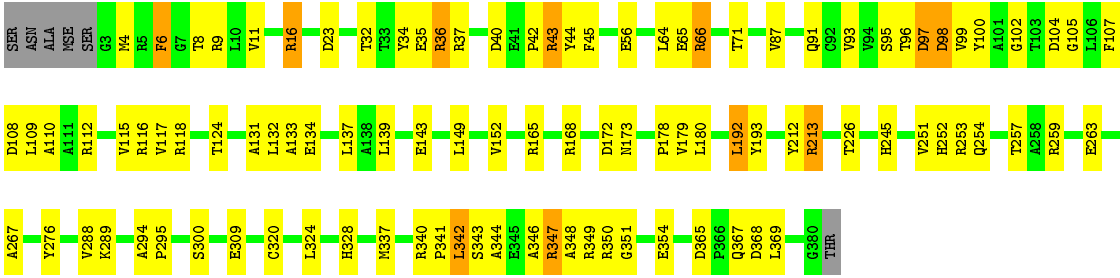
Chain 10-G: 67% 26% 5% ..







● Molecule 1: CalE6



## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.85Å 146.98Å 349.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.97 – 2.10	Depositor
% Data completeness (in resolution range)	100.0 (33.97-2.10)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 2.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.ENSEMBLE_REFINEMENT: DEV_1839)	Depositor
R, $R_{free}$	0.143 , 0.183	Depositor
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.192	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
Total number of atoms	243453	wwPDB-V
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-V

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FMT, LLP, MES, CL

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	1-A	0.50	3/2868 (0.1%)	0.63	1/3906 (0.0%)
1	1-B	0.45	0/2874	0.64	0/3912
1	1-C	0.43	0/2865	0.62	0/3903
1	1-D	0.51	1/2841 (0.0%)	0.65	2/3874 (0.1%)
1	1-E	0.47	0/2843	0.68	3/3874 (0.1%)
1	1-F	0.40	0/2840	0.59	0/3871
1	1-G	0.42	0/2842	0.62	2/3874 (0.1%)
1	1-H	0.44	0/2859	0.64	2/3893 (0.1%)
1	2-A	0.42	0/2868	0.63	0/3906
1	2-B	0.43	0/2874	0.64	3/3912 (0.1%)
1	2-C	0.45	0/2865	0.64	2/3903 (0.1%)
1	2-D	0.42	0/2841	0.66	3/3874 (0.1%)
1	2-E	0.44	0/2843	0.63	2/3874 (0.1%)
1	2-F	0.42	0/2840	0.59	0/3871
1	2-G	0.40	0/2842	0.63	3/3874 (0.1%)
1	2-H	0.44	0/2859	0.63	1/3893 (0.0%)
1	3-A	0.45	1/2868 (0.0%)	0.61	1/3906 (0.0%)
1	3-B	0.42	0/2874	0.63	1/3912 (0.0%)
1	3-C	0.45	0/2865	0.64	1/3903 (0.0%)
1	3-D	0.44	0/2841	0.72	7/3874 (0.2%)
1	3-E	0.46	1/2843 (0.0%)	0.63	0/3874
1	3-F	0.44	1/2840 (0.0%)	0.61	1/3871 (0.0%)
1	3-G	0.41	0/2842	0.64	3/3874 (0.1%)
1	3-H	0.43	0/2859	0.63	0/3893
1	4-A	0.44	1/2868 (0.0%)	0.61	0/3906
1	4-B	0.47	1/2874 (0.0%)	0.65	3/3912 (0.1%)
1	4-C	0.47	2/2865 (0.1%)	0.64	1/3903 (0.0%)
1	4-D	0.48	2/2841 (0.1%)	0.60	0/3874
1	4-E	0.44	0/2843	0.64	0/3874
1	4-F	0.42	0/2840	0.61	0/3871
1	4-G	0.43	0/2842	0.62	1/3874 (0.0%)
1	4-H	0.43	0/2859	0.60	0/3893

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	5-A	0.46	0/2868	0.63	3/3906 (0.1%)
1	5-B	0.49	1/2874 (0.0%)	0.64	2/3912 (0.1%)
1	5-C	0.47	1/2865 (0.0%)	0.66	2/3903 (0.1%)
1	5-D	0.44	0/2841	0.64	0/3874
1	5-E	0.53	2/2843 (0.1%)	0.68	3/3874 (0.1%)
1	5-F	0.45	1/2840 (0.0%)	0.63	2/3871 (0.1%)
1	5-G	0.42	0/2842	0.62	1/3874 (0.0%)
1	5-H	0.43	0/2859	0.62	0/3893
1	6-A	0.45	2/2868 (0.1%)	0.60	0/3906
1	6-B	0.44	0/2874	0.62	1/3912 (0.0%)
1	6-C	0.46	1/2865 (0.0%)	0.61	1/3903 (0.0%)
1	6-D	0.43	0/2841	0.65	0/3874
1	6-E	0.43	0/2843	0.68	4/3874 (0.1%)
1	6-F	0.42	0/2840	0.61	1/3871 (0.0%)
1	6-G	0.41	0/2842	0.61	1/3874 (0.0%)
1	6-H	0.47	0/2859	0.63	1/3893 (0.0%)
1	7-A	0.45	0/2868	0.64	2/3906 (0.1%)
1	7-B	0.43	0/2874	0.63	2/3912 (0.1%)
1	7-C	0.50	1/2865 (0.0%)	0.70	4/3903 (0.1%)
1	7-D	0.46	1/2841 (0.0%)	0.70	4/3874 (0.1%)
1	7-E	0.46	1/2843 (0.0%)	0.62	2/3874 (0.1%)
1	7-F	0.44	0/2840	0.65	0/3871
1	7-G	0.43	0/2842	0.65	2/3874 (0.1%)
1	7-H	0.42	0/2859	0.61	0/3893
1	8-A	0.44	0/2868	0.61	0/3906
1	8-B	0.43	0/2874	0.65	1/3912 (0.0%)
1	8-C	0.44	0/2865	0.62	0/3903
1	8-D	0.44	0/2841	0.64	2/3874 (0.1%)
1	8-E	0.47	1/2843 (0.0%)	0.64	1/3874 (0.0%)
1	8-F	0.43	0/2840	0.62	2/3871 (0.1%)
1	8-G	0.41	0/2842	0.61	1/3874 (0.0%)
1	8-H	0.42	0/2859	0.63	1/3893 (0.0%)
1	9-A	0.44	0/2868	0.63	1/3906 (0.0%)
1	9-B	0.48	2/2874 (0.1%)	0.66	4/3912 (0.1%)
1	9-C	0.48	1/2865 (0.0%)	0.64	1/3903 (0.0%)
1	9-D	0.41	0/2841	0.63	0/3874
1	9-E	0.42	0/2843	0.64	0/3874
1	9-F	0.45	1/2840 (0.0%)	0.65	2/3871 (0.1%)
1	9-G	0.41	0/2842	0.62	2/3874 (0.1%)
1	9-H	0.43	0/2859	0.60	0/3893
1	10-A	0.45	0/2868	0.63	0/3906
1	10-B	0.44	0/2874	0.62	2/3912 (0.1%)
1	10-C	0.45	1/2865 (0.0%)	0.65	0/3903

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	10-D	0.43	0/2841	0.67	1/3874 (0.0%)
1	10-E	0.46	0/2843	0.63	2/3874 (0.1%)
1	10-F	0.42	0/2840	0.63	0/3871
1	10-G	0.44	0/2842	0.64	0/3874
1	10-H	0.41	0/2859	0.61	1/3893 (0.0%)
All	All	0.44	30/228320 (0.0%)	0.63	105/311070 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2-C	0	1
1	2-D	0	2
1	2-E	0	1
1	2-G	0	1
1	3-A	0	1
1	3-B	0	1
1	3-C	0	1
1	3-H	0	1
1	4-B	0	1
1	4-C	0	2
1	4-E	0	1
1	5-A	0	3
1	5-D	0	1
1	5-F	0	1
1	5-G	0	1
1	6-E	0	1
1	6-F	0	1
1	6-G	0	1
1	7-A	0	1
1	7-B	0	1
1	7-C	0	1
1	7-D	0	2
1	7-E	0	1
1	7-H	0	1
1	8-B	0	1
1	8-C	0	2
1	8-E	0	2
1	8-F	0	2
1	8-H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	9-C	0	1
1	9-E	0	1
1	9-F	0	1
1	10-A	0	1
1	10-C	0	1
1	10-D	0	1
1	10-E	0	1
1	10-F	0	1
All	All	0	45

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-B	322	VAL	CB-CG2	-11.16	1.29	1.52
1	1-D	344	ALA	CA-CB	-11.10	1.29	1.52
1	1-A	281	GLU	CB-CG	-9.85	1.33	1.52
1	9-C	66	ARG	CG-CD	-8.89	1.29	1.51
1	5-E	146	THR	CB-CG2	-8.80	1.23	1.52
1	4-D	45	PHE	CE2-CZ	8.65	1.53	1.37
1	4-D	45	PHE	CE1-CZ	8.13	1.52	1.37
1	4-C	34	TYR	CE1-CZ	8.06	1.49	1.38
1	5-C	292	MSE	CG-SE	7.72	2.21	1.95
1	5-E	355	SER	CB-OG	-7.53	1.32	1.42
1	4-A	4	MSE	SE-CE	-6.81	1.55	1.95
1	9-B	43	ARG	CD-NE	-6.70	1.35	1.46
1	10-C	16	ARG	CG-CD	-6.36	1.36	1.51
1	3-E	320	CYS	CB-SG	-6.32	1.71	1.82
1	7-C	320	CYS	CB-SG	-6.29	1.71	1.82
1	7-D	17	PRO	CA-C	-6.27	1.40	1.52
1	4-C	34	TYR	CD1-CE1	6.21	1.48	1.39
1	5-F	165	ARG	CG-CD	-5.88	1.37	1.51
1	9-B	43	ARG	CB-CG	-5.82	1.36	1.52
1	1-A	281	GLU	CG-CD	5.79	1.60	1.51
1	6-C	236	ASP	CB-CG	-5.68	1.39	1.51
1	7-E	4	MSE	CG-SE	5.65	2.14	1.95
1	6-A	9	ARG	CB-CG	-5.37	1.38	1.52
1	8-E	45	PHE	CE2-CZ	5.36	1.47	1.37
1	9-F	342	LEU	CG-CD1	-5.35	1.32	1.51
1	4-B	367	GLN	CB-CG	-5.22	1.38	1.52
1	1-A	18	SER	CA-CB	5.18	1.60	1.52
1	3-F	337	MSE	CB-CG	5.04	1.67	1.52
1	6-A	226	THR	CB-CG2	-5.04	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-A	367	GLN	CB-CG	-5.01	1.39	1.52

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-A	4	MSE	CB-CG-SE	-10.95	79.84	112.70
1	3-D	97	ASP	CB-CG-OD1	-10.80	108.58	118.30
1	7-D	37	ARG	CG-CD-NE	10.78	134.44	111.80
1	9-A	337	MSE	CB-CG-SE	-10.36	81.63	112.70
1	7-C	97	ASP	CB-CG-OD1	-9.41	109.83	118.30
1	7-D	37	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	6-E	214	ASP	CB-CG-OD2	-8.84	110.35	118.30
1	7-C	4	MSE	CB-CG-SE	-8.74	86.48	112.70
1	2-D	337	MSE	CB-CG-SE	8.57	138.41	112.70
1	5-C	292	MSE	CB-CG-SE	8.37	137.80	112.70
1	2-H	292	MSE	CG-SE-CE	-8.30	80.63	98.90
1	5-B	337	MSE	CB-CG-SE	-8.28	87.86	112.70
1	9-F	289	LYS	N-CA-CB	-8.26	95.73	110.60
1	3-D	9	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	6-E	214	ASP	CB-CG-OD1	7.96	125.47	118.30
1	10-D	379	GLY	N-CA-C	7.54	131.94	113.10
1	3-D	97	ASP	CB-CG-OD2	7.46	125.01	118.30
1	7-C	380	GLY	N-CA-C	7.43	131.68	113.10
1	8-B	337	MSE	CB-CG-SE	-7.30	90.79	112.70
1	7-G	337	MSE	CA-CB-CG	-7.28	100.93	113.30
1	3-G	19	ALA	N-CA-CB	-7.27	99.93	110.10
1	3-D	358	ARG	NE-CZ-NH1	-7.26	116.67	120.30
1	1-H	324	LEU	CA-CB-CG	7.07	131.56	115.30
1	1-E	16	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	5-E	292	MSE	CG-SE-CE	6.88	114.04	98.90
1	2-G	126	GLU	CB-CA-C	-6.85	96.71	110.40
1	2-G	9	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	7-B	16	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	4-B	4	MSE	CB-CG-SE	6.80	133.11	112.70
1	6-E	336	LEU	CA-CB-CG	6.80	130.95	115.30
1	9-B	43	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	3-D	9	ARG	NE-CZ-NH1	-6.75	116.92	120.30
1	2-C	97	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	9-B	66	ARG	NE-CZ-NH2	6.61	123.60	120.30
1	7-D	37	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	8-D	292	MSE	CB-CG-SE	6.43	131.99	112.70
1	10-B	4	MSE	CA-CB-CG	-6.38	102.45	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-D	344	ALA	N-CA-CB	-6.32	101.25	110.10
1	7-G	337	MSE	CB-CA-C	6.26	122.93	110.40
1	2-D	324	LEU	CA-CB-CG	6.20	129.57	115.30
1	3-G	337	MSE	CG-SE-CE	-6.20	85.26	98.90
1	1-H	337	MSE	CB-CG-SE	-6.19	94.13	112.70
1	5-E	16	ARG	CA-CB-CG	6.18	127.01	113.40
1	5-F	165	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	7-E	4	MSE	CA-CB-CG	6.11	123.68	113.30
1	8-E	336	LEU	CB-CG-CD1	6.08	121.34	111.00
1	4-C	292	MSE	CB-CG-SE	-6.01	94.68	112.70
1	3-G	4	MSE	CB-CG-SE	5.99	130.68	112.70
1	3-D	358	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	5-F	165	ARG	CG-CD-NE	5.96	124.31	111.80
1	2-C	97	ASP	CB-CG-OD2	5.93	123.64	118.30
1	5-A	4	MSE	CA-CB-CG	5.90	123.33	113.30
1	2-B	43	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	2-B	5	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	5-E	292	MSE	CB-CA-C	-5.82	98.76	110.40
1	6-G	312	LEU	CB-CG-CD1	-5.80	101.14	111.00
1	3-D	337	MSE	CB-CG-SE	5.79	130.07	112.70
1	5-A	337	MSE	CG-SE-CE	-5.77	86.21	98.90
1	6-H	16	ARG	CB-CG-CD	5.76	126.58	111.60
1	6-E	88	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	1-E	4	MSE	CG-SE-CE	-5.73	86.30	98.90
1	9-G	4	MSE	CB-CG-SE	5.68	129.75	112.70
1	3-F	337	MSE	CA-CB-CG	5.65	122.90	113.30
1	7-C	97	ASP	CB-CG-OD2	5.62	123.36	118.30
1	5-G	337	MSE	CG-SE-CE	5.54	111.09	98.90
1	3-B	16	ARG	C-N-CA	-5.52	98.81	122.00
1	2-E	337	MSE	N-CA-C	5.46	125.75	111.00
1	5-A	340	ARG	CG-CD-NE	5.44	123.22	111.80
1	5-B	4	MSE	CB-CG-SE	-5.43	96.41	112.70
1	8-H	3	GLY	N-CA-C	-5.39	99.61	113.10
1	4-G	4	MSE	CG-SE-CE	5.38	110.75	98.90
1	2-G	9	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	7-A	292	MSE	CG-SE-CE	-5.35	87.14	98.90
1	7-E	337	MSE	CG-SE-CE	-5.33	87.17	98.90
1	8-F	345	GLU	CB-CA-C	-5.30	99.80	110.40
1	8-G	337	MSE	CB-CG-SE	-5.30	96.80	112.70
1	1-D	324	LEU	CA-CB-CG	5.29	127.47	115.30
1	7-B	16	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	1-E	337	MSE	N-CA-C	5.27	125.22	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-A	18	SER	N-CA-CB	5.26	118.39	110.50
1	6-B	15	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	3-C	292	MSE	CA-CB-CG	5.25	122.23	113.30
1	9-G	281	GLU	N-CA-CB	5.25	120.05	110.60
1	4-B	367	GLN	CA-CB-CG	-5.24	101.86	113.40
1	6-C	337	MSE	CA-CB-CG	5.22	122.18	113.30
1	2-E	337	MSE	CB-CG-SE	5.20	128.30	112.70
1	5-C	292	MSE	CB-CA-C	5.20	120.80	110.40
1	1-G	4	MSE	CA-CB-CG	5.17	122.09	113.30
1	8-F	96	THR	CA-CB-CG2	-5.17	105.17	112.40
1	3-A	379	GLY	CA-C-O	-5.16	111.31	120.60
1	9-C	66	ARG	CG-CD-NE	5.15	122.62	111.80
1	1-G	36	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	9-F	292	MSE	CB-CA-C	5.12	120.63	110.40
1	2-D	100	TYR	CB-CG-CD1	5.10	124.06	121.00
1	2-B	15	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	10-E	97	ASP	CB-CA-C	-5.09	100.21	110.40
1	7-D	17	PRO	N-CA-C	5.08	125.31	112.10
1	10-B	4	MSE	CG-SE-CE	-5.07	87.75	98.90
1	4-B	15	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	10-E	16	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	9-B	342	LEU	CA-CB-CG	5.02	126.86	115.30
1	9-B	342	LEU	N-CA-C	-5.02	97.45	111.00
1	6-F	324	LEU	CA-CB-CG	5.01	126.83	115.30
1	10-H	192	LEU	CA-CB-CG	5.01	126.82	115.30
1	8-D	324	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	10-A	4	MSE	Peptide
1	10-C	193	TYR	Peptide
1	10-D	15	ARG	Peptide
1	10-E	96	THR	Peptide
1	10-F	3	GLY	Peptide
1	2-C	32	THR	Peptide
1	2-D	336	LEU	Peptide
1	2-D	41	GLU	Peptide
1	2-E	193	TYR	Peptide
1	2-G	193	TYR	Peptide
1	3-A	193	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	3-B	4	MSE	Peptide
1	3-C	193	TYR	Peptide
1	3-H	193	TYR	Peptide
1	4-B	193	TYR	Peptide
1	4-C	291	GLN	Peptide
1	4-C	4	MSE	Peptide
1	4-E	193	TYR	Peptide
1	5-A	147	ASN	Peptide
1	5-A	193	TYR	Peptide
1	5-A	342	LEU	Peptide
1	5-D	17	PRO	Peptide
1	5-F	193	TYR	Peptide
1	5-G	193	TYR	Peptide
1	6-E	341	PRO	Peptide
1	6-F	193	TYR	Peptide
1	6-G	336	LEU	Peptide
1	7-A	193	TYR	Peptide
1	7-B	193	TYR	Peptide
1	7-C	193	TYR	Peptide
1	7-D	17	PRO	Peptide
1	7-D	340	ARG	Peptide
1	7-E	193	TYR	Peptide
1	7-H	15	ARG	Peptide
1	8-B	336	LEU	Peptide
1	8-C	193	TYR	Peptide
1	8-C	5	ARG	Peptide
1	8-E	193	TYR	Peptide
1	8-E	97	ASP	Peptide
1	8-F	3	GLY	Peptide
1	8-F	97	ASP	Peptide
1	8-H	193	TYR	Peptide
1	9-C	193	TYR	Peptide
1	9-E	193	TYR	Peptide
1	9-F	4	MSE	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	2839	0	2834	78	0
1	1-B	2846	0	2838	83	0
1	1-C	2837	0	2819	68	0
1	1-D	2812	0	2791	100	0
1	1-E	2815	0	2794	90	0
1	1-F	2812	0	2787	92	0
1	1-G	2814	0	2786	86	0
1	1-H	2831	0	2818	91	0
1	2-A	2839	0	2834	67	0
1	2-B	2846	0	2837	89	0
1	2-C	2837	0	2818	86	0
1	2-D	2812	0	2791	87	0
1	2-E	2815	0	2794	84	0
1	2-F	2812	0	2786	75	0
1	2-G	2814	0	2786	58	0
1	2-H	2831	0	2817	93	0
1	3-A	2839	0	2833	85	0
1	3-B	2846	0	2838	80	0
1	3-C	2837	0	2818	100	0
1	3-D	2812	0	2791	90	0
1	3-E	2815	0	2793	84	0
1	3-F	2812	0	2786	88	0
1	3-G	2814	0	2786	86	0
1	3-H	2831	0	2817	97	0
1	4-A	2839	0	2833	98	0
1	4-B	2846	0	2837	95	0
1	4-C	2837	0	2819	87	0
1	4-D	2812	0	2791	85	0
1	4-E	2815	0	2794	104	0
1	4-F	2812	0	2786	95	0
1	4-G	2814	0	2786	87	0
1	4-H	2831	0	2818	89	0
1	5-A	2839	0	2833	102	0
1	5-B	2846	0	2838	115	0
1	5-C	2837	0	2818	102	0
1	5-D	2812	0	2790	79	0
1	5-E	2815	0	2794	117	0
1	5-F	2812	0	2787	84	0
1	5-G	2814	0	2786	79	0
1	5-H	2831	0	2817	100	0
1	6-A	2839	0	2834	68	0
1	6-B	2846	0	2837	90	0
1	6-C	2837	0	2818	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6-D	2812	0	2790	91	0
1	6-E	2815	0	2794	79	0
1	6-F	2812	0	2786	87	0
1	6-G	2814	0	2785	81	0
1	6-H	2831	0	2817	70	0
1	7-A	2839	0	2833	110	0
1	7-B	2846	0	2837	99	0
1	7-C	2837	0	2818	90	0
1	7-D	2812	0	2790	85	0
1	7-E	2815	0	2793	87	0
1	7-F	2812	0	2786	94	0
1	7-G	2814	0	2786	87	0
1	7-H	2831	0	2817	75	0
1	8-A	2839	0	2834	75	0
1	8-B	2846	0	2838	94	0
1	8-C	2837	0	2818	85	0
1	8-D	2812	0	2791	92	0
1	8-E	2815	0	2793	100	0
1	8-F	2812	0	2787	100	0
1	8-G	2814	0	2786	79	0
1	8-H	2831	0	2817	79	0
1	9-A	2839	0	2834	85	0
1	9-B	2846	0	2837	78	0
1	9-C	2837	0	2818	99	0
1	9-D	2812	0	2790	92	0
1	9-E	2815	0	2794	96	0
1	9-F	2812	0	2786	104	0
1	9-G	2814	0	2785	79	0
1	9-H	2831	0	2817	75	0
1	10-A	2839	0	2833	86	0
1	10-B	2846	0	2837	113	0
1	10-C	2837	0	2818	90	0
1	10-D	2812	0	2790	92	0
1	10-E	2815	0	2794	97	0
1	10-F	2812	0	2787	86	0
1	10-G	2814	0	2786	92	0
1	10-H	2831	0	2818	83	0
2	1-A	12	0	12	1	0
2	1-B	12	0	12	0	0
2	1-C	12	0	12	1	0
2	1-D	12	0	12	3	0
2	1-E	12	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1-F	12	0	12	2	0
2	1-G	12	0	12	2	0
2	1-H	12	0	12	2	0
2	2-A	12	0	13	0	0
2	2-B	12	0	12	3	0
2	2-C	12	0	12	5	0
2	2-D	12	0	12	2	0
2	2-E	12	0	12	4	0
2	2-F	12	0	12	3	0
2	2-G	12	0	12	2	0
2	2-H	12	0	12	2	0
2	3-A	12	0	12	0	0
2	3-B	12	0	12	1	0
2	3-C	12	0	12	2	0
2	3-D	12	0	12	1	0
2	3-E	12	0	12	6	0
2	3-F	12	0	12	2	0
2	3-G	12	0	12	3	0
2	3-H	12	0	12	5	0
2	4-A	12	0	12	4	0
2	4-B	12	0	12	5	0
2	4-C	12	0	12	8	0
2	4-D	12	0	12	3	0
2	4-E	12	0	12	4	0
2	4-F	12	0	12	2	0
2	4-G	12	0	12	1	0
2	4-H	12	0	12	2	0
2	5-A	12	0	12	0	0
2	5-B	12	0	12	3	0
2	5-C	12	0	12	3	0
2	5-D	12	0	12	2	0
2	5-E	12	0	12	5	0
2	5-F	12	0	12	2	0
2	5-G	12	0	12	6	0
2	5-H	12	0	12	1	0
2	6-A	12	0	12	0	0
2	6-B	12	0	12	3	0
2	6-C	12	0	12	1	0
2	6-D	12	0	12	3	0
2	6-E	12	0	12	3	0
2	6-F	12	0	12	8	0
2	6-G	12	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-H	12	0	12	4	0
2	7-A	12	0	12	0	0
2	7-B	12	0	12	6	0
2	7-C	12	0	12	2	0
2	7-D	12	0	12	2	0
2	7-E	12	0	12	2	0
2	7-F	12	0	12	1	0
2	7-G	12	0	12	3	0
2	7-H	12	0	12	6	0
2	8-A	12	0	12	2	0
2	8-B	12	0	12	2	0
2	8-C	12	0	12	8	0
2	8-D	12	0	12	3	0
2	8-E	12	0	12	0	0
2	8-F	12	0	12	1	0
2	8-G	12	0	12	1	0
2	8-H	12	0	12	2	0
2	9-A	12	0	12	1	0
2	9-B	12	0	12	2	0
2	9-C	12	0	12	2	0
2	9-D	12	0	12	3	0
2	9-E	12	0	12	2	0
2	9-F	12	0	12	0	0
2	9-G	12	0	12	0	0
2	9-H	12	0	12	3	0
2	10-A	12	0	12	2	0
2	10-B	12	0	12	5	0
2	10-C	12	0	12	2	0
2	10-D	12	0	12	0	0
2	10-E	12	0	12	2	0
2	10-F	12	0	12	5	0
2	10-G	12	0	12	0	0
2	10-H	12	0	12	5	0
3	1-A	18	0	24	2	0
3	1-B	42	0	48	5	0
3	1-C	6	0	9	0	0
3	1-D	18	0	23	0	0
3	1-E	12	0	16	2	0
3	1-F	36	0	39	3	0
3	1-G	24	0	24	4	0
3	1-H	12	0	16	4	0
3	2-A	18	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2-B	36	0	47	2	0
3	2-C	18	0	16	2	0
3	2-D	12	0	16	1	0
3	2-E	24	0	24	3	0
3	2-F	24	0	33	0	0
3	2-G	18	0	24	2	0
3	2-H	18	0	24	4	0
3	3-A	24	0	24	2	0
3	3-B	36	0	48	5	0
3	3-C	12	0	16	0	0
3	3-D	12	0	16	1	0
3	3-E	18	0	16	6	0
3	3-F	30	0	40	4	0
3	3-G	24	0	24	4	0
3	3-H	12	0	16	1	0
3	4-A	18	0	24	3	0
3	4-B	36	0	48	4	0
3	4-C	18	0	16	2	0
3	4-D	12	0	16	3	0
3	4-E	18	0	16	1	0
3	4-F	18	0	25	1	0
3	4-G	30	0	24	3	0
3	4-H	18	0	24	4	0
3	5-A	24	0	24	5	0
3	5-B	36	0	48	7	0
3	5-C	6	0	9	0	0
3	5-D	18	0	24	3	0
3	5-E	24	0	24	3	0
3	5-F	18	0	25	3	0
3	5-G	24	0	24	2	0
3	5-H	18	0	24	4	0
3	6-A	24	0	24	2	0
3	6-B	36	0	48	2	0
3	6-C	6	0	9	1	0
3	6-D	18	0	24	4	0
3	6-E	18	0	16	2	0
3	6-F	30	0	40	7	0
3	6-G	12	0	17	3	0
3	6-H	24	0	32	0	0
3	7-A	24	0	24	6	0
3	7-B	36	0	48	1	0
3	7-C	6	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	7-D	18	0	24	2	0
3	7-E	18	0	16	4	0
3	7-F	30	0	40	5	0
3	7-G	18	0	24	2	0
3	7-H	18	0	24	1	0
3	8-A	18	0	24	2	0
3	8-B	42	0	48	4	0
3	8-C	12	0	16	1	0
3	8-D	12	0	16	1	0
3	8-E	18	0	16	6	0
3	8-F	24	0	33	5	0
3	8-G	24	0	24	2	0
3	8-H	18	0	24	4	0
3	9-A	24	0	24	0	0
3	9-B	30	0	40	0	0
3	9-C	12	0	16	2	0
3	9-D	18	0	24	5	0
3	9-E	24	0	24	1	0
3	9-F	18	0	25	2	0
3	9-G	18	0	24	3	0
3	9-H	24	0	32	4	0
3	10-A	18	0	24	5	0
3	10-B	36	0	48	3	0
3	10-C	12	0	16	1	0
3	10-D	18	0	24	3	0
3	10-E	12	0	16	1	0
3	10-F	30	0	40	2	0
3	10-G	18	0	24	4	0
3	10-H	24	0	32	4	0
4	1-A	2	0	0	0	0
4	1-B	1	0	8	0	0
4	1-C	2	0	0	0	0
4	1-D	2	0	0	0	0
4	1-E	1	0	0	0	0
4	1-F	1	0	1	0	0
4	1-G	1	0	1	0	0
4	1-H	2	0	0	0	0
4	2-A	2	0	0	1	0
4	2-B	1	0	0	0	0
4	2-C	1	0	1	0	0
4	2-D	3	0	0	1	0
4	2-E	1	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	2-F	1	0	0	0	0
4	2-G	1	0	0	1	0
4	2-H	2	0	0	2	0
4	3-A	2	0	8	2	0
4	3-B	1	0	0	0	0
4	3-C	1	0	0	0	0
4	3-D	3	0	0	0	0
4	3-E	1	0	8	0	0
4	3-F	1	0	0	0	0
4	3-G	1	0	1	2	0
4	3-H	2	0	0	0	0
4	4-A	2	0	0	2	0
4	4-B	1	0	0	0	0
4	4-C	1	0	1	1	0
4	4-D	3	0	0	1	0
4	4-E	1	0	8	1	0
4	4-F	1	0	0	0	0
4	4-G	2	0	9	4	0
4	4-H	1	0	0	0	0
4	5-A	2	0	8	4	0
4	5-B	1	0	0	0	0
4	5-C	2	0	0	1	0
4	5-D	2	0	0	2	0
4	5-E	1	0	8	0	0
4	5-F	1	0	0	0	0
4	5-G	1	0	1	0	0
4	5-H	2	0	0	1	0
4	6-A	1	0	8	1	0
4	6-B	2	0	0	2	0
4	6-C	1	0	0	0	0
4	6-D	3	0	0	3	0
4	6-E	1	0	8	0	0
4	6-F	1	0	0	3	0
4	6-G	1	0	0	0	0
4	6-H	2	0	0	1	0
4	7-A	2	0	8	1	0
4	7-B	1	0	0	0	0
4	7-C	1	0	0	0	0
4	7-D	3	0	0	0	0
4	7-E	1	0	8	0	0
4	7-F	1	0	0	2	0
4	7-G	2	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	7-H	1	0	0	0	0
4	8-A	2	0	0	1	0
4	8-B	1	0	8	0	0
4	8-C	1	0	0	0	0
4	8-D	3	0	0	0	0
4	8-E	1	0	8	2	0
4	8-F	1	0	0	0	0
4	8-G	1	0	1	1	0
4	8-H	2	0	0	0	0
4	9-A	2	0	8	0	0
4	9-B	1	0	0	0	0
4	9-C	1	0	0	0	0
4	9-D	3	0	0	0	0
4	9-E	1	0	8	1	0
4	9-F	1	0	0	0	0
4	9-G	1	0	0	0	0
4	9-H	2	0	0	1	0
4	10-A	2	0	0	1	0
4	10-B	1	0	0	0	0
4	10-C	2	0	0	1	0
4	10-D	2	0	0	0	0
4	10-E	1	0	0	2	0
4	10-F	1	0	0	1	0
4	10-G	1	0	0	0	0
4	10-H	2	0	0	3	0
5	1-C	3	0	0	0	0
5	1-F	3	0	8	0	0
5	1-G	3	0	8	0	0
5	2-C	3	0	8	1	0
5	2-F	3	0	0	0	0
5	2-G	3	0	1	0	0
5	3-C	3	0	1	0	0
5	3-F	3	0	1	2	0
5	3-G	3	0	8	0	0
5	4-C	3	0	8	1	0
5	4-F	3	0	0	0	0
5	4-G	3	0	8	0	0
5	5-C	3	0	0	0	0
5	5-F	3	0	0	0	0
5	5-G	3	0	8	1	0
5	6-C	3	0	0	1	0
5	6-F	3	0	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	6-G	3	0	0	0	0
5	7-C	3	0	0	0	0
5	7-F	3	0	1	2	0
5	7-G	3	0	1	0	0
5	8-C	3	0	1	0	0
5	8-F	3	0	0	1	0
5	8-G	3	0	8	0	0
5	9-C	3	0	1	0	0
5	9-F	3	0	0	0	0
5	9-G	3	0	1	0	0
5	10-C	3	0	1	0	0
5	10-F	3	0	1	1	0
5	10-G	3	0	1	0	0
6	1-A	180	0	0	15	0
6	1-B	198	0	0	14	0
6	1-C	178	0	0	14	0
6	1-D	183	0	0	26	0
6	1-E	178	0	0	11	0
6	1-F	178	0	0	14	0
6	1-G	186	0	0	15	0
6	1-H	172	0	0	14	0
6	2-A	190	0	0	11	0
6	2-B	189	0	0	18	0
6	2-C	178	0	0	22	0
6	2-D	159	0	0	12	0
6	2-E	177	0	0	19	0
6	2-F	175	0	0	14	0
6	2-G	175	0	0	14	0
6	2-H	185	0	0	15	0
6	3-A	183	0	0	23	0
6	3-B	183	0	0	13	0
6	3-C	181	0	0	26	0
6	3-D	188	0	0	17	0
6	3-E	196	0	0	15	0
6	3-F	159	0	0	10	0
6	3-G	183	0	0	10	0
6	3-H	163	0	0	15	0
6	4-A	184	0	0	15	0
6	4-B	189	0	0	20	0
6	4-C	176	0	0	14	0
6	4-D	179	0	0	9	0
6	4-E	197	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	4-F	177	0	0	32	0
6	4-G	185	0	0	21	0
6	4-H	184	0	0	17	0
6	5-A	197	0	0	25	0
6	5-B	189	0	0	11	0
6	5-C	178	0	0	26	0
6	5-D	179	0	0	12	0
6	5-E	173	0	0	27	0
6	5-F	166	0	0	15	0
6	5-G	172	0	0	11	0
6	5-H	183	0	0	21	0
6	6-A	179	0	0	12	0
6	6-B	195	0	0	16	0
6	6-C	174	0	0	22	0
6	6-D	161	0	0	8	0
6	6-E	191	0	0	21	0
6	6-F	189	0	0	14	0
6	6-G	176	0	0	11	0
6	6-H	184	0	0	12	0
6	7-A	192	0	0	18	0
6	7-B	196	0	0	10	0
6	7-C	196	0	0	22	0
6	7-D	177	0	0	14	0
6	7-E	180	0	0	20	0
6	7-F	179	0	0	19	0
6	7-G	187	0	0	20	0
6	7-H	183	0	0	13	0
6	8-A	183	0	0	13	0
6	8-B	185	0	0	21	0
6	8-C	183	0	0	24	0
6	8-D	179	0	0	19	0
6	8-E	194	0	0	25	0
6	8-F	162	0	0	18	0
6	8-G	179	0	0	14	0
6	8-H	191	0	0	14	0
6	9-A	188	0	0	20	0
6	9-B	198	0	0	18	0
6	9-C	178	0	0	22	0
6	9-D	179	0	0	14	0
6	9-E	181	0	0	19	0
6	9-F	176	0	0	18	0
6	9-G	197	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	9-H	168	0	0	20	0
6	10-A	173	0	0	9	0
6	10-B	195	0	0	26	0
6	10-C	188	0	0	27	0
6	10-D	177	0	0	15	0
6	10-E	182	0	0	21	0
6	10-F	167	0	0	11	0
6	10-G	182	0	0	10	0
6	10-H	194	0	0	22	0
All	All	243453	0	227856	6730	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 15.

All (6730) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:MSE:CG	1:E:4:MSE:SE	2.14	1.44
1:C:292:MSE:CG	1:C:292:MSE:SE	2.21	1.37
1:A:4:MSE:HB3	1:A:8:THR:HB	1.26	1.15
1:B:5:ARG:NH1	1:C:368:ASP:OD1	1.83	1.12
1:H:333:CYS:H	1:H:337:MSE:SE	1.84	1.10
1:E:259:ARG:NH1	6:E:655:HOH:O	1.82	1.09
1:G:333:CYS:H	1:G:337:MSE:HE3	1.09	1.08
5:C:404:CL:CL	6:C:659:HOH:O	2.08	1.06
1:E:9:ARG:NH2	1:E:63:GLY:O	1.86	1.06
1:D:292:MSE:SE	1:D:295:PRO:HA	2.05	1.05
1:F:4:MSE:HB3	1:F:9:ARG:HG2	1.36	1.05
1:G:333:CYS:N	1:G:337:MSE:HE3	1.71	1.05
1:B:6:PHE:HA	1:B:9:ARG:HE	1.22	1.05
1:G:9:ARG:HH22	1:G:66:ARG:HE	1.04	1.03
1:G:36:ARG:NH2	4:G:407:CL:CL	2.28	1.03
1:G:333:CYS:H	1:G:337:MSE:SE	1.92	1.01
1:E:16:ARG:NH1	6:E:655:HOH:O	1.90	1.01
1:B:3:GLY:N	6:B:674:HOH:O	1.94	1.01
1:F:199:ILE:HG23	1:F:244:LEU:HD21	1.40	1.00
1:G:4:MSE:SE	1:G:9:ARG:HA	2.11	1.00
1:G:168:ARG:NE	4:G:407:CL:CL	2.31	0.99
1:E:285:HIS:HB3	6:E:657:HOH:O	1.62	0.99
1:D:322:VAL:HG13	1:D:337:MSE:SE	2.12	0.98
1:F:332:GLU:HB2	1:F:337:MSE:HE2	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:MSE:SE	6:F:645:HOH:O	2.32	0.98
1:G:292:MSE:HE1	1:G:295:PRO:HA	1.46	0.97
1:E:66:ARG:NH1	6:E:666:HOH:O	1.97	0.96
1:E:4:MSE:HB2	1:E:8:THR:HB	1.48	0.96
1:E:213:ARG:HH11	3:E:402:GOL:H2	1.29	0.96
1:E:345:GLU:HA	6:E:694:HOH:O	1.65	0.96
3:F:403:GOL:O3	4:F:408:CL:CL	2.22	0.95
1:G:275:HIS:HB2	1:G:300:SER:HB2	1.49	0.95
1:B:16:ARG:NH1	1:B:56:GLU:OE1	1.99	0.95
1:C:285:HIS:HB2	6:C:651:HOH:O	1.67	0.94
1:E:168:ARG:NH2	4:E:404:CL:CL	2.36	0.94
1:A:336:LEU:O	1:A:340:ARG:NH2	2.01	0.94
1:H:91:GLN:NE2	6:H:686:HOH:O	2.00	0.94
1:H:43:ARG:NH2	6:H:668:HOH:O	2.00	0.93
1:E:3:GLY:N	6:E:657:HOH:O	2.02	0.93
1:C:147:ASN:HD21	1:C:358:ARG:HH11	1.14	0.93
1:D:259:ARG:NH1	6:D:621:HOH:O	2.01	0.93
1:H:97:ASP:HB2	6:H:683:HOH:O	1.66	0.93
1:C:116:ARG:NH2	6:C:501:HOH:O	2.01	0.92
1:F:97:ASP:HB3	6:F:671:HOH:O	1.68	0.92
1:E:264:ARG:HD3	6:E:507:HOH:O	1.69	0.92
1:A:285:HIS:ND1	6:A:670:HOH:O	2.02	0.92
1:G:332:GLU:O	1:G:358:ARG:N	2.01	0.92
1:D:98:ASP:O	6:D:573:HOH:O	1.86	0.91
1:B:339:HIS:O	1:B:347:ARG:NH1	2.03	0.91
1:F:147:ASN:ND2	6:F:563:HOH:O	2.01	0.91
1:G:348:ALA:O	1:G:350:ARG:N	2.03	0.91
1:C:4:MSE:SE	1:C:9:ARG:HA	2.19	0.91
1:A:334:PRO:HB3	1:A:339:HIS:CD2	2.06	0.91
1:A:214:ASP:HB2	4:A:405:CL:CL	2.07	0.91
1:C:285:HIS:HB2	6:C:657:HOH:O	1.68	0.91
1:G:380:GLY:HA2	6:G:669:HOH:O	1.71	0.91
1:H:104:ASP:OD1	1:H:119:TYR:OH	1.88	0.91
1:G:36:ARG:NH2	4:G:409:CL:CL	2.41	0.91
1:G:338:THR:HG22	2:G:401:MES:H82	1.52	0.91
1:C:9:ARG:NH2	1:C:63:GLY:O	2.03	0.91
4:A:405:GOL:H11	1:B:102:GLY:HA2	1.52	0.91
1:E:340:ARG:O	1:E:342:LEU:N	2.04	0.90
1:D:336:LEU:HB3	1:D:337:MSE:SE	2.21	0.90
1:H:97:ASP:O	1:H:350:ARG:NH2	2.03	0.90
1:A:37:ARG:NH2	1:B:315:PHE:O	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:ARG:NH1	6:F:663:HOH:O	2.02	0.90
1:A:214:ASP:HB3	6:A:689:HOH:O	1.70	0.90
1:G:43:ARG:NH1	6:G:1395:HOH:O	2.04	0.90
1:A:285:HIS:ND1	6:A:672:HOH:O	2.05	0.90
1:E:97:ASP:HB2	6:E:669:HOH:O	1.72	0.90
1:C:332:GLU:HB2	1:C:337:MSE:SE	2.21	0.90
1:F:42:PRO:HD2	6:F:665:HOH:O	1.71	0.90
1:D:313:ASP:HB3	6:D:673:HOH:O	1.71	0.90
1:H:347:ARG:NH2	1:H:354:GLU:OE1	2.04	0.90
1:F:118:ARG:NH2	1:F:134:GLU:OE2	2.04	0.90
1:A:350:ARG:HB2	6:A:667:HOH:O	1.70	0.89
1:G:358:ARG:NH1	2:G:401:MES:O2S	2.05	0.89
1:B:4:MSE:SE	6:B:659:HOH:O	2.40	0.89
1:B:322:VAL:HG13	1:B:337:MSE:HE2	1.53	0.89
1:C:147:ASN:HD21	1:C:358:ARG:HD2	1.35	0.89
1:H:283:PRO:O	6:H:665:HOH:O	1.88	0.89
1:A:54:ARG:NH1	6:A:640:HOH:O	2.05	0.89
1:C:9:ARG:NH2	1:C:63:GLY:O	2.06	0.89
1:A:121:ASP:OD1	6:A:670:HOH:O	1.89	0.89
1:E:214:ASP:HB3	6:E:652:HOH:O	1.72	0.89
1:D:286:ALA:HB3	6:D:666:HOH:O	1.71	0.89
1:D:313:ASP:HB3	6:D:677:HOH:O	1.71	0.88
1:G:236:ASP:OD2	6:G:654:HOH:O	1.92	0.88
1:A:336:LEU:O	1:A:340:ARG:NH2	2.07	0.88
1:B:288:VAL:HG13	1:B:292:MSE:HE3	1.54	0.88
1:D:332:GLU:OE1	1:D:358:ARG:NH2	2.07	0.88
1:A:134:GLU:O	1:A:165:ARG:NH1	2.07	0.88
1:A:35:GLU:HG2	1:A:38:ALA:HB2	1.53	0.88
1:F:214:ASP:OD1	6:F:645:HOH:O	1.89	0.88
1:H:288:VAL:HA	1:H:292:MSE:SE	2.23	0.88
1:C:354:GLU:HG3	6:C:671:HOH:O	1.73	0.88
1:C:367:GLN:NE2	1:C:371:GLU:OE2	2.07	0.88
1:C:16:ARG:NH2	1:C:59:GLU:OE1	2.06	0.87
1:B:97:ASP:O	1:B:350:ARG:NH1	2.06	0.87
1:H:16:ARG:HG3	6:H:660:HOH:O	1.74	0.87
1:D:342:LEU:HD13	1:D:350:ARG:HD3	1.56	0.87
1:E:347:ARG:HB3	1:E:352:ILE:HB	1.56	0.87
1:D:168:ARG:HH22	3:D:403:GOL:H2	1.38	0.87
1:E:16:ARG:HB3	6:E:655:HOH:O	1.73	0.87
1:A:316:THR:OG1	1:A:375:ARG:NH1	2.07	0.87
1:A:37:ARG:HH22	1:B:320:CYS:H	1.17	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:CYS:SG	6:D:654:HOH:O	2.33	0.87
1:D:334:PRO:HA	1:D:338:THR:HB	1.57	0.87
1:F:165:ARG:HD2	6:F:659:HOH:O	1.75	0.86
1:B:118:ARG:NH2	1:B:119:TYR:O	2.07	0.86
1:A:334:PRO:HB3	1:A:339:HIS:HD2	1.40	0.86
1:A:94:VAL:HG11	1:A:131:ALA:HB1	1.57	0.86
1:B:4:MSE:SE	6:B:667:HOH:O	2.42	0.86
1:E:263:GLU:OE2	1:E:266:ARG:NH1	2.09	0.86
1:C:97:ASP:HB3	6:C:671:HOH:O	1.75	0.86
1:C:343:SER:HB3	1:C:346:ALA:HB3	1.58	0.86
1:B:132:LEU:O	1:B:165:ARG:NE	2.08	0.86
1:D:168:ARG:NH2	3:D:404:GOL:O3	2.09	0.86
1:F:365:ASP:OD2	6:F:664:HOH:O	1.94	0.86
1:A:263:GLU:OE1	6:A:501:HOH:O	1.94	0.86
1:E:282:HIS:HB3	1:E:285:HIS:HB2	1.57	0.86
1:D:6:PHE:O	1:D:8:THR:N	2.08	0.86
1:B:16:ARG:NH1	6:B:671:HOH:O	2.07	0.85
1:C:259:ARG:NH1	6:C:652:HOH:O	2.08	0.85
1:B:338:THR:HG22	2:B:401:MES:H32	1.58	0.85
1:C:6:PHE:HA	1:C:9:ARG:HE	1.39	0.85
1:C:98:ASP:N	1:C:98:ASP:OD2	2.08	0.85
1:A:337:MSE:HE3	1:B:36:ARG:HD2	1.59	0.85
1:E:264:ARG:NH1	1:E:367:GLN:OE1	2.10	0.85
1:A:35:GLU:O	1:A:39:GLN:NE2	2.09	0.85
1:A:42:PRO:HB2	6:A:662:HOH:O	1.76	0.85
1:F:38:ALA:O	6:F:668:HOH:O	1.93	0.85
1:E:168:ARG:NH2	3:E:405:CL:CL	2.47	0.85
1:E:17:PRO:HD3	6:E:679:HOH:O	1.75	0.85
1:B:189:ASP:HA	1:B:213:ARG:HH22	1.40	0.85
1:B:43:ARG:HD3	6:B:664:HOH:O	1.76	0.85
1:D:54:ARG:NH1	6:D:611:HOH:O	2.10	0.85
1:E:9:ARG:NH2	6:E:623:HOH:O	2.08	0.85
1:B:214:ASP:HB3	1:B:217:LEU:HB3	1.59	0.85
1:E:288:VAL:O	1:E:292:MSE:HB2	1.77	0.84
1:C:354:GLU:HG2	6:C:670:HOH:O	1.75	0.84
1:B:365:ASP:H	1:C:8:THR:HG22	1.42	0.84
1:D:168:ARG:NH2	3:D:404:GOL:O3	2.10	0.84
1:D:35:GLU:OE2	1:D:37:ARG:NH2	2.10	0.84
1:F:4:MSE:HB3	1:F:9:ARG:HG2	1.59	0.84
1:D:97:ASP:OD1	6:D:665:HOH:O	1.95	0.84
1:F:5:ARG:NH1	1:G:371:GLU:OE2	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:ARG:HH12	1:G:66:ARG:HE	1.23	0.84
1:F:358:ARG:NH1	2:F:401:MES:O1S	2.11	0.84
1:G:97:ASP:O	6:G:1480:HOH:O	1.95	0.84
1:H:157:GLU:OE1	1:H:160:ARG:NH1	2.11	0.84
1:G:16:ARG:NH2	1:G:59:GLU:OE1	2.10	0.84
1:E:378:ALA:O	6:E:682:HOH:O	1.95	0.84
1:F:4:MSE:O	6:F:659:HOH:O	1.94	0.84
1:B:101:ALA:O	1:B:105:GLY:N	2.10	0.84
1:B:213:ARG:NH1	6:B:629:HOH:O	2.10	0.84
1:B:6:PHE:HB2	1:B:9:ARG:HH11	1.42	0.84
1:E:371:GLU:OE1	6:E:672:HOH:O	1.93	0.84
1:F:5:ARG:NH1	1:G:371:GLU:OE1	2.10	0.84
1:F:310:ARG:HE	1:F:314:ARG:HH12	1.22	0.84
1:A:379:GLY:HA3	6:A:684:HOH:O	1.78	0.83
1:A:199:ILE:HG23	1:A:244:LEU:HD21	1.58	0.83
1:F:20:GLY:O	1:F:22:GLY:N	2.12	0.83
1:E:314:ARG:NH1	1:E:378:ALA:O	2.11	0.83
1:H:264:ARG:NH2	1:H:374:SER:OG	2.11	0.83
1:C:36:ARG:NH1	6:C:619:HOH:O	2.07	0.83
1:E:288:VAL:HA	1:E:292:MSE:SE	2.29	0.83
1:H:259:ARG:HH12	1:H:295:PRO:HD2	1.43	0.83
1:E:344:ALA:O	6:E:680:HOH:O	1.96	0.83
1:D:121:ASP:O	1:D:123:THR:N	2.12	0.83
1:A:263:GLU:HG2	6:A:655:HOH:O	1.77	0.83
1:E:100:TYR:OH	2:E:401:MES:H51	1.79	0.83
1:H:16:ARG:HG3	6:H:680:HOH:O	1.78	0.83
1:B:101:ALA:O	6:B:680:HOH:O	1.97	0.83
1:G:288:VAL:HG13	1:G:292:MSE:SE	2.28	0.83
1:A:4:MSE:CB	1:A:8:THR:HB	2.09	0.83
1:C:88:ARG:NH1	6:C:501:HOH:O	2.12	0.83
1:D:335:ALA:HA	1:D:339:HIS:HB2	1.61	0.82
1:B:97:ASP:O	6:B:624:HOH:O	1.96	0.82
1:G:16:ARG:HG3	1:G:56:GLU:HG2	1.61	0.82
1:C:3:GLY:N	6:C:666:HOH:O	2.11	0.82
1:B:104:ASP:OD2	1:B:119:TYR:OH	1.97	0.82
1:E:147:ASN:HD21	1:E:358:ARG:HH11	1.25	0.82
1:A:347:ARG:NE	6:A:671:HOH:O	2.04	0.82
1:D:264:ARG:HD2	6:D:662:HOH:O	1.78	0.82
1:F:225:ARG:HG2	1:F:231:VAL:HG12	1.59	0.82
1:F:364:GLU:HB3	1:G:8:THR:HG22	1.61	0.82
1:H:16:ARG:O	6:H:668:HOH:O	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:GLU:OE1	6:H:683:HOH:O	1.98	0.82
1:G:21:THR:OG1	6:G:592:HOH:O	1.98	0.82
1:F:132:LEU:O	1:F:165:ARG:NE	2.13	0.82
1:G:336:LEU:HB2	1:G:337:MSE:HE2	1.62	0.82
1:C:126:GLU:N	6:C:679:HOH:O	2.12	0.82
1:E:124:THR:HB	1:E:126:GLU:HG2	1.59	0.81
1:A:266:ARG:NH1	1:A:281:GLU:OE2	2.14	0.81
1:F:365:ASP:H	1:G:8:THR:HG22	1.46	0.81
1:E:292:MSE:SE	6:E:573:HOH:O	2.49	0.81
1:C:367:GLN:OE1	6:C:594:HOH:O	1.99	0.81
1:G:253:ARG:HH11	3:G:403:GOL:H32	1.44	0.81
1:A:39:GLN:HE22	1:A:44:TYR:H	1.26	0.81
1:F:225:ARG:HG2	1:F:231:VAL:HG12	1.63	0.81
1:D:116:ARG:NH1	1:D:135:PRO:O	2.14	0.81
1:F:216:ASP:HB3	6:F:656:HOH:O	1.79	0.81
1:E:367:GLN:HG2	6:E:671:HOH:O	1.81	0.81
1:G:333:CYS:N	1:G:337:MSE:SE	2.63	0.81
1:C:92:CYS:SG	1:C:116:ARG:NH2	2.54	0.81
1:H:266:ARG:NH1	6:H:568:HOH:O	2.13	0.81
1:A:236:ASP:OD2	6:A:602:HOH:O	1.99	0.81
1:C:375:ARG:NH2	6:C:684:HOH:O	2.13	0.81
1:D:43:ARG:NE	6:D:653:HOH:O	2.12	0.81
4:F:408:CL:CL	6:F:661:HOH:O	2.35	0.81
1:C:65:GLU:OE1	6:C:555:HOH:O	1.98	0.81
1:H:252:HIS:HD2	6:H:647:HOH:O	1.61	0.81
1:B:9:ARG:NH1	6:B:633:HOH:O	2.12	0.81
1:H:168:ARG:NE	3:H:404:CL:CL	2.51	0.81
1:H:97:ASP:OD1	1:H:98:ASP:N	2.14	0.81
1:F:213:ARG:NH1	3:F:406:GOL:O2	2.13	0.81
1:H:147:ASN:HD21	1:H:358:ARG:HH11	1.29	0.81
1:F:263:GLU:OE2	6:F:585:HOH:O	1.99	0.80
1:D:347:ARG:NE	6:D:672:HOH:O	2.14	0.80
1:C:147:ASN:OD1	6:C:691:HOH:O	1.99	0.80
1:C:102:GLY:HA2	3:D:403:GOL:H31	1.63	0.80
1:H:96:THR:OG1	1:H:98:ASP:OD1	1.99	0.80
1:A:165:ARG:HH21	1:A:165:ARG:HB3	1.46	0.80
6:B:680:HOH:O	1:D:39:GLN:HA	1.79	0.80
1:B:253:ARG:HD3	3:C:403:GOL:H11	1.62	0.80
1:C:16:ARG:HG3	6:C:688:HOH:O	1.80	0.80
1:F:34:TYR:CD2	1:H:23:ASP:HA	2.15	0.80
1:G:36:ARG:HE	1:H:321:GLY:HA2	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:ASP:O	6:E:576:HOH:O	1.99	0.80
1:C:289:LYS:NZ	6:C:636:HOH:O	2.13	0.80
1:H:251:VAL:HA	1:H:254:GLN:HE21	1.44	0.80
1:A:134:GLU:O	1:A:165:ARG:NH1	2.15	0.80
1:C:198:SER:HB2	6:C:656:HOH:O	1.81	0.80
1:D:36:ARG:HA	1:D:39:GLN:HE21	1.47	0.80
1:F:9:ARG:NH2	1:F:63:GLY:O	2.14	0.80
1:E:16:ARG:NH2	1:E:59:GLU:OE1	2.15	0.80
1:F:347:ARG:HB3	1:F:352:ILE:HB	1.63	0.80
1:G:97:ASP:N	1:G:97:ASP:OD1	2.12	0.80
1:E:96:THR:O	1:E:98:ASP:N	2.15	0.80
1:C:371:GLU:OE1	6:C:638:HOH:O	1.98	0.80
1:D:116:ARG:NH1	1:D:135:PRO:O	2.14	0.80
1:A:16:ARG:HB2	1:A:56:GLU:HG2	1.62	0.80
1:C:149:LEU:O	6:C:662:HOH:O	1.99	0.80
1:B:134:GLU:O	1:B:165:ARG:NH1	2.14	0.80
1:E:213:ARG:HH11	3:E:402:GOL:H2	1.45	0.80
1:E:236:ASP:OD2	6:E:659:HOH:O	1.99	0.80
1:B:344:ALA:O	1:B:348:ALA:N	2.15	0.80
1:D:342:LEU:O	1:D:347:ARG:NH1	2.15	0.80
1:B:332:GLU:HB2	1:B:337:MSE:SE	2.31	0.80
1:D:292:MSE:HE1	1:D:295:PRO:HA	1.64	0.80
1:C:189:ASP:OD1	6:C:654:HOH:O	2.00	0.79
1:A:88:ARG:NH2	6:A:603:HOH:O	2.13	0.79
1:E:254:GLN:NE2	6:E:567:HOH:O	2.15	0.79
1:C:264:ARG:NH2	1:C:374:SER:OG	2.15	0.79
1:A:104:ASP:OD1	1:A:119:TYR:OH	2.01	0.79
1:G:213:ARG:NH2	3:G:402:GOL:O2	2.12	0.79
1:E:4:MSE:HE2	6:E:652:HOH:O	1.81	0.79
1:G:4:MSE:HG3	1:G:9:ARG:HG2	1.63	0.79
1:D:336:LEU:HD22	1:D:337:MSE:SE	2.31	0.79
1:A:88:ARG:NH1	6:A:618:HOH:O	2.14	0.79
1:E:116:ARG:NH2	1:E:136:ASP:OD2	2.16	0.79
1:G:197:LLP:HE3	1:G:323:SER:HB2	1.64	0.79
1:A:322:VAL:HG13	1:A:337:MSE:SE	2.31	0.79
1:G:312:LEU:HD11	1:G:337:MSE:HE1	1.62	0.79
1:A:152:VAL:O	1:A:284:GLN:NE2	2.16	0.79
1:E:15:ARG:O	6:E:655:HOH:O	2.00	0.79
1:A:36:ARG:HH11	1:B:337:MSE:HG3	1.47	0.79
1:F:214:ASP:OD1	6:F:661:HOH:O	2.00	0.79
1:C:310:ARG:NH1	1:C:313:ASP:OD2	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:GLN:HB3	1:F:113:GLN:HG2	1.63	0.79
1:G:4:MSE:O	1:G:9:ARG:NH2	2.16	0.79
1:G:65:GLU:OE1	6:G:550:HOH:O	2.00	0.79
1:E:350:ARG:NH2	6:E:658:HOH:O	2.15	0.79
1:G:9:ARG:HH12	1:G:66:ARG:NE	1.81	0.79
1:B:36:ARG:HH11	1:B:45:PHE:HD1	1.31	0.79
1:C:214:ASP:OD2	6:C:659:HOH:O	2.00	0.78
1:H:39:GLN:HE22	1:H:44:TYR:HB2	1.48	0.78
1:B:152:VAL:HG11	1:B:292:MSE:HE1	1.66	0.78
1:B:66:ARG:NH2	6:B:683:HOH:O	2.16	0.78
1:C:113:GLN:HE21	1:D:113:GLN:HG2	1.48	0.78
1:D:343:SER:OG	1:D:344:ALA:N	2.15	0.78
1:E:259:ARG:NH1	6:E:646:HOH:O	2.15	0.78
1:F:355:SER:OG	6:F:652:HOH:O	2.00	0.78
1:H:16:ARG:HH11	1:H:16:ARG:HA	1.48	0.78
1:F:340:ARG:H	1:F:341:PRO:HD2	1.48	0.78
1:H:332:GLU:HB2	1:H:337:MSE:SE	2.33	0.78
1:C:263:GLU:OE1	1:C:266:ARG:NH1	2.17	0.78
1:E:4:MSE:SE	6:E:662:HOH:O	2.50	0.78
1:G:104:ASP:OD1	1:G:119:TYR:OH	2.01	0.78
1:B:18:SER:N	6:B:668:HOH:O	2.16	0.78
1:G:332:GLU:OE2	1:G:358:ARG:NH2	2.16	0.78
1:C:150:LEU:O	1:C:282:HIS:NE2	2.12	0.78
1:D:292:MSE:CE	1:D:295:PRO:HA	2.13	0.78
1:C:320:CYS:SG	1:C:337:MSE:HE1	2.23	0.78
1:D:350:ARG:O	1:D:352:ILE:N	2.14	0.78
1:E:312:LEU:O	1:F:37:ARG:NH2	2.17	0.78
1:H:100:TYR:HE1	2:H:401:MES:H81	1.49	0.78
1:C:93:VAL:HG22	1:C:139:LEU:HB3	1.66	0.78
1:F:323:SER:O	6:F:531:HOH:O	2.01	0.78
1:E:16:ARG:NE	1:E:59:GLU:OE1	2.17	0.78
1:A:136:ASP:OD1	6:A:652:HOH:O	2.00	0.78
1:D:168:ARG:NH2	3:D:404:GOL:O3	2.17	0.78
1:B:94:VAL:HG11	1:B:131:ALA:HB1	1.66	0.78
1:G:40:ASP:HB2	6:G:667:HOH:O	1.84	0.78
1:H:213:ARG:NH1	3:H:402:GOL:O2	2.16	0.78
1:B:116:ARG:NH2	1:B:135:PRO:O	2.16	0.78
1:A:292:MSE:SE	1:A:294:ALA:O	2.52	0.78
1:B:132:LEU:O	1:B:165:ARG:NE	2.17	0.77
1:B:104:ASP:OD2	6:B:590:HOH:O	2.01	0.77
1:E:236:ASP:OD1	6:E:579:HOH:O	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:MSE:SE	6:E:642:HOH:O	2.52	0.77
1:G:340:ARG:HA	1:G:347:ARG:HH21	1.49	0.77
1:D:17:PRO:HG2	6:D:678:HOH:O	1.84	0.77
1:B:126:GLU:OE2	6:B:501:HOH:O	2.00	0.77
1:H:152:VAL:O	1:H:284:GLN:NE2	2.17	0.77
1:B:263:GLU:OE2	6:B:601:HOH:O	2.02	0.77
1:C:9:ARG:HH22	1:C:66:ARG:HH21	1.30	0.77
1:E:88:ARG:HG2	1:E:88:ARG:HH21	1.49	0.77
1:A:4:MSE:HB3	1:A:8:THR:CB	2.11	0.77
1:G:147:ASN:HD21	1:G:358:ARG:HD2	1.49	0.77
1:D:134:GLU:O	1:D:165:ARG:NH1	2.17	0.77
1:F:97:ASP:HA	1:F:119:TYR:HD2	1.48	0.77
1:D:252:HIS:ND1	6:D:660:HOH:O	2.18	0.77
1:E:281:GLU:OE2	6:E:501:HOH:O	2.02	0.77
1:H:337:MSE:HE3	3:H:404:GOL:H31	1.66	0.77
1:G:59:GLU:OE2	6:G:647:HOH:O	2.03	0.77
1:F:319:THR:HB	1:F:330:LEU:HD23	1.67	0.77
1:D:338:THR:HG22	1:D:339:HIS:CD2	2.20	0.77
1:G:347:ARG:O	1:G:352:ILE:N	2.17	0.77
1:D:333:CYS:O	1:D:337:MSE:HB2	1.85	0.77
1:C:199:ILE:HG23	1:C:244:LEU:HD21	1.65	0.77
1:B:342:LEU:O	1:B:347:ARG:NH1	2.18	0.77
1:F:314:ARG:NH1	6:F:651:HOH:O	2.18	0.77
1:H:337:MSE:O	4:H:406:CL:CL	2.40	0.77
1:E:96:THR:OG1	1:E:98:ASP:OD2	2.01	0.77
1:D:18:SER:O	1:D:20:GLY:N	2.18	0.77
1:E:285:HIS:ND1	6:E:582:HOH:O	2.17	0.77
1:H:112:ARG:NE	6:H:694:HOH:O	2.18	0.77
1:E:334:PRO:HB3	1:E:339:HIS:ND1	2.00	0.77
1:H:147:ASN:HD21	1:H:358:ARG:HH11	1.33	0.77
1:G:132:LEU:HB3	1:G:165:ARG:HG3	1.67	0.77
1:E:42:PRO:HD2	6:E:661:HOH:O	1.83	0.77
6:C:696:HOH:O	1:D:37:ARG:HD3	1.84	0.77
1:A:198:SER:HB2	6:A:660:HOH:O	1.85	0.77
1:D:124:THR:OG1	1:D:126:GLU:OE1	2.02	0.77
1:G:19:ALA:HB1	6:G:670:HOH:O	1.84	0.77
1:A:54:ARG:NH1	6:A:673:HOH:O	2.16	0.77
1:B:20:GLY:O	6:B:612:HOH:O	2.03	0.76
1:H:108:ASP:OD1	6:H:673:HOH:O	2.02	0.76
1:G:180:LEU:HD22	1:G:294:ALA:HB3	1.66	0.76
1:B:98:ASP:N	1:B:98:ASP:OD2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:379:GLY:O	6:F:611:HOH:O	2.02	0.76
1:A:4:MSE:N	6:A:608:HOH:O	2.17	0.76
1:A:5:ARG:N	1:D:368:ASP:OD1	2.19	0.76
1:A:367:GLN:HG3	6:A:658:HOH:O	1.83	0.76
1:E:98:ASP:HA	1:E:350:ARG:HH22	1.50	0.76
1:D:313:ASP:OD2	6:D:570:HOH:O	2.03	0.76
1:B:121:ASP:OD2	1:B:124:THR:OG1	2.03	0.76
1:G:355:SER:OG	6:G:1336:HOH:O	2.03	0.76
1:H:340:ARG:O	6:H:659:HOH:O	2.03	0.76
1:F:41:GLU:N	6:F:672:HOH:O	2.17	0.76
1:A:9:ARG:NH2	1:A:63:GLY:O	2.16	0.76
1:E:335:ALA:O	6:E:659:HOH:O	2.03	0.76
1:G:323:SER:HA	2:G:401:MES:O1S	1.84	0.76
1:A:157:GLU:OE2	1:A:161:ARG:NH2	2.19	0.76
1:C:131:ALA:O	1:C:133:ALA:N	2.14	0.76
1:D:332:GLU:OE2	1:D:338:THR:OG1	2.04	0.76
1:B:116:ARG:NH2	1:B:134:GLU:OE2	2.17	0.76
1:D:97:ASP:HB3	6:D:682:HOH:O	1.86	0.76
1:E:259:ARG:NH1	6:E:671:HOH:O	2.18	0.76
1:F:65:GLU:OE1	6:F:529:HOH:O	2.02	0.76
1:C:327:VAL:HG13	1:C:363:ILE:HG12	1.66	0.76
1:F:288:VAL:HA	1:F:292:MSE:HE3	1.67	0.76
1:D:309:GLU:OE2	6:D:501:HOH:O	2.02	0.76
1:C:4:MSE:SE	1:C:12:HIS:HB2	2.35	0.76
1:C:88:ARG:HD2	6:C:670:HOH:O	1.86	0.76
1:E:160:ARG:NH2	6:E:653:HOH:O	2.19	0.76
1:E:131:ALA:O	1:E:133:ALA:N	2.18	0.76
1:C:199:ILE:HG23	1:C:244:LEU:HD13	1.68	0.76
1:A:135:PRO:HG3	1:E:112:ARG:HH21	1.51	0.76
1:H:11:VAL:HA	1:H:245:HIS:HD2	1.50	0.76
1:B:180:LEU:HD22	1:B:294:ALA:HB3	1.66	0.76
1:D:316:THR:OG1	1:D:375:ARG:NH1	2.18	0.76
1:A:118:ARG:NH1	1:A:130:ALA:O	2.19	0.76
1:H:259:ARG:NE	6:H:665:HOH:O	2.18	0.76
1:F:130:ALA:HB2	6:F:650:HOH:O	1.84	0.76
1:D:132:LEU:O	1:D:165:ARG:NE	2.18	0.76
1:E:112:ARG:NH1	6:E:630:HOH:O	2.19	0.75
1:F:310:ARG:O	1:F:314:ARG:NH1	2.19	0.75
1:B:97:ASP:O	1:B:350:ARG:NH1	2.19	0.75
1:H:4:MSE:O	1:H:9:ARG:NE	2.19	0.75
1:B:236:ASP:OD1	6:B:663:HOH:O	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:ARG:NH1	6:D:575:HOH:O	2.17	0.75
1:G:9:ARG:HH22	1:G:66:ARG:NE	1.82	0.75
1:E:252:HIS:CD2	6:E:665:HOH:O	2.39	0.75
3:E:403:GOL:H11	6:E:674:HOH:O	1.85	0.75
1:E:160:ARG:HD2	6:E:664:HOH:O	1.85	0.75
1:C:35:GLU:OE1	6:C:683:HOH:O	2.03	0.75
1:D:252:HIS:HB3	6:D:667:HOH:O	1.85	0.75
1:A:124:THR:OG1	1:A:126:GLU:OE1	2.03	0.75
1:B:380:GLY:O	6:B:650:HOH:O	2.04	0.75
1:H:283:PRO:O	6:H:649:HOH:O	2.03	0.75
2:D:401:MES:O1S	6:D:558:HOH:O	2.04	0.75
1:C:36:ARG:NH2	1:D:320:CYS:SG	2.59	0.75
1:C:9:ARG:HG2	6:C:667:HOH:O	1.85	0.75
1:A:4:MSE:HG2	6:A:655:HOH:O	1.86	0.75
1:D:288:VAL:HG13	1:D:292:MSE:HE2	1.68	0.75
1:C:157:GLU:OE1	1:C:160:ARG:NH1	2.19	0.75
1:D:339:HIS:O	1:D:347:ARG:NH1	2.19	0.75
1:H:109:LEU:HD23	6:H:662:HOH:O	1.87	0.75
1:G:132:LEU:O	1:G:165:ARG:NH1	2.17	0.75
1:C:320:CYS:HB3	6:C:629:HOH:O	1.84	0.75
1:C:229:GLY:O	1:D:74:SER:OG	2.05	0.75
1:E:4:MSE:SE	1:E:9:ARG:HG2	2.37	0.75
1:F:264:ARG:HG2	6:F:675:HOH:O	1.86	0.75
1:A:346:ALA:HA	1:A:349:ARG:HG3	1.68	0.75
1:B:259:ARG:HH12	1:B:295:PRO:HG2	1.52	0.75
1:E:20:GLY:HA2	6:G:667:HOH:O	1.86	0.75
1:G:143:GLU:HG3	1:G:172:ASP:HB3	1.69	0.75
1:C:39:GLN:HE22	1:C:44:TYR:H	1.33	0.75
1:C:253:ARG:HH11	1:C:253:ARG:HG3	1.51	0.75
6:A:686:HOH:O	1:D:367:GLN:HG3	1.87	0.75
1:A:194:SER:O	6:A:541:HOH:O	2.05	0.75
1:A:333:CYS:O	1:A:335:ALA:N	2.19	0.75
1:C:180:LEU:O	1:C:293:SER:N	2.18	0.75
1:H:214:ASP:HB3	1:H:217:LEU:HB3	1.69	0.75
1:D:160:ARG:O	6:D:665:HOH:O	2.05	0.75
1:D:314:ARG:HD3	1:D:379:GLY:HA3	1.69	0.75
1:G:168:ARG:NE	4:G:407:CL:CL	2.56	0.75
1:H:332:GLU:OE1	1:H:358:ARG:NH2	2.20	0.74
1:E:320:CYS:HB3	6:E:694:HOH:O	1.85	0.74
1:E:33:THR:OG1	6:E:609:HOH:O	2.03	0.74
1:G:332:GLU:HA	1:G:337:MSE:SE	2.37	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:TYR:OH	6:C:585:HOH:O	2.05	0.74
1:G:17:PRO:HA	6:G:659:HOH:O	1.85	0.74
1:A:338:THR:HA	4:A:406:CL:CL	2.24	0.74
1:F:338:THR:HG23	1:F:339:HIS:HD2	1.52	0.74
1:G:345:GLU:O	1:G:349:ARG:N	2.20	0.74
1:F:168:ARG:HH22	3:F:403:GOL:H2	1.51	0.74
1:C:112:ARG:NH2	6:C:588:HOH:O	2.21	0.74
1:B:283:PRO:HB2	1:B:284:GLN:HE21	1.53	0.74
1:D:264:ARG:HH21	1:D:370:ALA:HB1	1.51	0.74
1:E:175:PHE:CE2	1:E:298:ILE:HG13	2.23	0.74
1:H:65:GLU:OE1	6:H:568:HOH:O	2.05	0.74
1:B:367:GLN:OE1	6:B:671:HOH:O	2.06	0.74
1:H:168:ARG:HH22	3:H:404:GOL:H32	1.52	0.74
1:G:4:MSE:SE	1:G:4:MSE:N	2.69	0.74
1:B:339:HIS:NE2	6:B:582:HOH:O	2.20	0.74
1:F:118:ARG:NH2	1:F:134:GLU:OE2	2.20	0.74
1:C:36:ARG:NH2	6:C:587:HOH:O	2.20	0.74
1:F:147:ASN:ND2	1:F:358:ARG:HH11	1.86	0.74
1:A:45:PHE:N	1:A:50:GLU:OE1	2.20	0.74
1:G:204:ASP:O	6:G:612:HOH:O	2.06	0.74
1:E:4:MSE:HB2	1:E:9:ARG:HG2	1.70	0.74
1:G:216:ASP:OD1	6:G:679:HOH:O	2.04	0.74
1:C:154:ASP:OD2	6:C:565:HOH:O	2.04	0.74
1:F:134:GLU:O	1:F:165:ARG:NH1	2.21	0.74
1:B:118:ARG:HG2	1:B:134:GLU:HG3	1.69	0.74
1:E:285:HIS:HB3	6:E:649:HOH:O	1.88	0.74
1:G:332:GLU:N	1:G:358:ARG:O	2.20	0.74
1:A:214:ASP:OD1	6:A:677:HOH:O	2.05	0.74
1:D:168:ARG:HH12	3:D:403:GOL:H31	1.53	0.74
1:F:343:SER:O	1:F:345:GLU:N	2.20	0.74
1:A:4:MSE:HE1	6:D:668:HOH:O	1.87	0.74
1:C:16:ARG:NH1	6:C:588:HOH:O	2.20	0.74
1:H:350:ARG:NH2	6:H:615:HOH:O	2.21	0.74
1:C:33:THR:C	1:C:34:TYR:HD2	1.92	0.74
1:C:95:SER:HB2	1:C:141:TRP:HB3	1.70	0.74
1:D:42:PRO:HB3	1:D:45:PHE:HZ	1.52	0.74
1:G:116:ARG:NH1	1:G:134:GLU:OE1	2.20	0.74
1:D:95:SER:HB2	1:D:141:TRP:HB3	1.70	0.74
1:D:334:PRO:HG2	1:D:356:LEU:HD23	1.69	0.74
1:D:116:ARG:NH2	1:D:135:PRO:O	2.18	0.73
1:C:93:VAL:HG22	1:C:139:LEU:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:404:GOL:H31	1:H:337:MSE:HE3	1.69	0.73
1:C:176:ALA:HB1	1:C:180:LEU:HD12	1.68	0.73
1:E:345:GLU:O	1:E:347:ARG:N	2.20	0.73
1:E:16:ARG:NH2	1:E:59:GLU:OE2	2.19	0.73
1:H:68:PRO:HD2	1:H:213:ARG:HG2	1.69	0.73
1:B:147:ASN:ND2	6:B:626:HOH:O	2.21	0.73
1:D:197:LLP:HD3	1:D:324:LEU:HD23	1.70	0.73
1:E:339:HIS:O	1:E:347:ARG:NH1	2.20	0.73
1:B:89:PRO:HD3	6:B:694:HOH:O	1.88	0.73
1:E:292:MSE:SE	1:E:295:PRO:HA	2.38	0.73
1:E:367:GLN:NE2	6:E:672:HOH:O	2.21	0.73
1:H:91:GLN:HB3	1:H:138:ALA:HB2	1.69	0.73
1:H:11:VAL:HA	1:H:245:HIS:HD2	1.53	0.73
1:A:214:ASP:OD2	6:A:648:HOH:O	2.06	0.73
1:B:213:ARG:HH11	3:B:403:GOL:H2	1.53	0.73
1:C:288:VAL:HG13	1:C:292:MSE:HE3	1.69	0.73
1:C:23:ASP:OD2	6:C:544:HOH:O	2.06	0.73
1:D:88:ARG:NH2	4:D:405:CL:CL	2.58	0.73
1:F:9:ARG:NH2	1:F:63:GLY:O	2.21	0.73
1:G:46:TYR:CD2	2:H:401:MES:H61	2.22	0.73
1:H:4:MSE:O	1:H:9:ARG:NE	2.20	0.73
1:F:68:PRO:HD2	1:F:213:ARG:HG2	1.69	0.73
1:B:288:VAL:HA	1:B:292:MSE:HE3	1.70	0.73
1:C:143:GLU:OE1	6:C:544:HOH:O	2.07	0.73
1:B:27:PRO:HD2	3:B:404:GOL:H31	1.70	0.73
1:F:368:ASP:OD2	1:G:5:ARG:N	2.21	0.73
1:G:19:ALA:O	1:G:21:THR:N	2.20	0.73
1:H:86:LEU:HD13	3:H:404:GOL:H2	1.71	0.73
1:F:353:GLY:O	6:F:641:HOH:O	2.06	0.73
1:D:116:ARG:NH1	1:D:134:GLU:OE1	2.18	0.73
1:F:4:MSE:HE3	6:F:638:HOH:O	1.88	0.73
1:C:381:THR:O	6:C:501:HOH:O	2.05	0.73
1:B:29:HIS:ND1	1:D:23:ASP:OD2	2.20	0.73
1:B:181:GLN:HB2	1:B:292:MSE:HE3	1.71	0.73
1:E:285:HIS:ND1	6:E:643:HOH:O	2.22	0.73
1:D:346:ALA:O	1:D:348:ALA:N	2.22	0.73
1:B:149:LEU:HD11	1:B:351:GLY:HA3	1.71	0.73
1:B:197:LLP:O3	6:B:658:HOH:O	2.07	0.73
2:E:401:MES:H52	6:E:606:HOH:O	1.89	0.73
1:A:36:ARG:HG2	1:B:320:CYS:SG	2.29	0.73
1:A:37:ARG:NH2	1:B:315:PHE:O	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ASP:OD1	6:C:554:HOH:O	2.07	0.73
2:C:401:MES:H61	1:D:46:TYR:CD2	2.24	0.73
1:G:56:GLU:OE1	6:G:569:HOH:O	2.05	0.73
1:C:236:ASP:OD1	6:C:542:HOH:O	2.06	0.73
1:H:343:SER:H	1:H:346:ALA:HB3	1.54	0.73
1:H:6:PHE:CE2	1:H:179:VAL:HA	2.24	0.73
1:B:259:ARG:HH11	1:B:259:ARG:HG2	1.54	0.73
1:D:6:PHE:N	6:D:679:HOH:O	2.21	0.73
1:D:6:PHE:N	6:D:680:HOH:O	2.21	0.73
1:E:90:GLY:N	1:E:114:GLY:O	2.16	0.73
1:A:112:ARG:CZ	1:E:135:PRO:HG3	2.18	0.73
1:B:5:ARG:HG2	6:B:693:HOH:O	1.89	0.73
1:E:42:PRO:O	6:E:636:HOH:O	2.06	0.73
1:B:41:GLU:OE2	6:B:502:HOH:O	2.07	0.72
1:H:39:GLN:HG3	1:H:42:PRO:HA	1.71	0.72
1:B:16:ARG:HB2	1:B:56:GLU:HG2	1.71	0.72
1:C:380:GLY:N	6:C:676:HOH:O	2.22	0.72
1:C:180:LEU:HD22	1:C:294:ALA:HB3	1.71	0.72
1:F:236:ASP:OD1	6:F:591:HOH:O	2.07	0.72
1:A:335:ALA:O	6:A:630:HOH:O	2.07	0.72
1:D:323:SER:HB3	1:D:330:LEU:HD13	1.71	0.72
1:D:95:SER:HB2	1:D:141:TRP:HB3	1.71	0.72
1:C:199:ILE:HG23	1:C:244:LEU:HD13	1.71	0.72
1:C:88:ARG:HH12	1:D:112:ARG:HG3	1.54	0.72
1:C:327:VAL:HG23	1:C:363:ILE:HG12	1.70	0.72
1:H:322:VAL:HB	2:H:401:MES:H72	1.72	0.72
1:B:337:MSE:N	1:B:340:ARG:HB2	2.04	0.72
1:H:340:ARG:O	6:H:647:HOH:O	2.06	0.72
1:H:9:ARG:NH2	1:H:63:GLY:O	2.21	0.72
1:D:342:LEU:O	1:D:347:ARG:NH1	2.22	0.72
1:F:37:ARG:NH1	6:F:572:HOH:O	2.23	0.72
1:H:109:LEU:O	6:H:662:HOH:O	2.07	0.72
1:F:338:THR:HG21	6:F:652:HOH:O	1.89	0.72
1:A:302:ASP:OD1	6:A:577:HOH:O	2.07	0.72
1:C:253:ARG:NH1	1:C:257:THR:OG1	2.15	0.72
1:D:344:ALA:HB1	6:D:682:HOH:O	1.88	0.72
1:D:254:GLN:NE2	6:D:577:HOH:O	2.22	0.72
1:E:104:ASP:OD1	1:E:119:TYR:OH	2.03	0.72
1:G:189:ASP:HB3	4:G:408:CL:CL	2.26	0.72
1:D:98:ASP:N	1:D:98:ASP:OD1	2.21	0.72
1:G:333:CYS:O	1:G:337:MSE:HB2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:SER:OG	6:A:622:HOH:O	2.08	0.72
1:D:9:ARG:NE	6:D:663:HOH:O	2.22	0.72
1:D:95:SER:OG	1:D:96:THR:N	2.17	0.72
1:E:98:ASP:N	1:E:98:ASP:OD2	2.20	0.72
1:G:339:HIS:O	1:G:347:ARG:NH1	2.22	0.72
1:E:332:GLU:HG3	1:E:334:PRO:HD3	1.72	0.72
1:A:36:ARG:NH2	6:A:609:HOH:O	2.18	0.72
1:B:116:ARG:HH21	1:B:134:GLU:HB3	1.54	0.72
1:B:98:ASP:OD1	1:B:98:ASP:N	2.23	0.72
1:D:343:SER:O	1:D:347:ARG:HB2	1.89	0.72
1:E:282:HIS:HB3	1:E:285:HIS:HB2	1.71	0.72
1:F:316:THR:OG1	1:F:375:ARG:NH1	2.21	0.72
1:H:343:SER:O	1:H:347:ARG:N	2.23	0.72
1:F:368:ASP:OD2	1:G:5:ARG:N	2.20	0.72
1:D:55:GLU:OE1	6:D:564:HOH:O	2.07	0.72
1:A:344:ALA:HA	1:A:347:ARG:HG3	1.72	0.72
1:C:263:GLU:OE1	1:C:266:ARG:NH1	2.23	0.72
1:F:337:MSE:O	6:F:590:HOH:O	2.07	0.72
1:B:292:MSE:SE	1:B:292:MSE:N	2.73	0.72
1:E:337:MSE:SE	1:E:337:MSE:N	2.73	0.72
1:G:302:ASP:OD1	6:G:1483:HOH:O	2.06	0.72
1:F:143:GLU:HG3	1:F:172:ASP:HB3	1.72	0.72
1:H:34:TYR:OH	6:H:613:HOH:O	2.07	0.72
1:B:292:MSE:SE	6:B:641:HOH:O	2.58	0.72
1:B:371:GLU:OE1	6:B:603:HOH:O	2.07	0.72
1:D:345:GLU:O	1:D:349:ARG:N	2.22	0.71
1:A:127:GLY:O	1:A:130:ALA:N	2.23	0.71
1:E:340:ARG:HA	1:E:347:ARG:HH12	1.55	0.71
1:C:100:TYR:CE1	2:C:401:MES:H82	2.25	0.71
1:F:332:GLU:HG2	1:F:358:ARG:HB3	1.69	0.71
1:C:263:GLU:OE1	1:C:266:ARG:NH1	2.23	0.71
1:H:264:ARG:HD2	1:H:370:ALA:HB1	1.70	0.71
1:G:4:MSE:HG2	6:G:649:HOH:O	1.88	0.71
1:G:323:SER:HB3	1:H:46:TYR:HE1	1.53	0.71
1:H:264:ARG:HE	1:H:370:ALA:HB1	1.55	0.71
1:E:259:ARG:NH1	6:E:597:HOH:O	2.20	0.71
1:C:350:ARG:NH2	6:C:622:HOH:O	2.24	0.71
1:C:56:GLU:OE1	6:C:561:HOH:O	2.07	0.71
1:D:17:PRO:HG2	6:D:639:HOH:O	1.88	0.71
1:F:379:GLY:O	6:F:592:HOH:O	2.07	0.71
1:E:120:ALA:O	6:E:669:HOH:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:ALA:O	1:G:133:ALA:N	2.23	0.71
1:C:181:GLN:HG3	1:C:292:MSE:HG2	1.72	0.71
1:H:4:MSE:HE2	6:H:666:HOH:O	1.89	0.71
1:B:112:ARG:NH2	6:B:625:HOH:O	2.22	0.71
1:G:303:TYR:OH	6:G:670:HOH:O	2.08	0.71
1:H:252:HIS:ND1	6:H:692:HOH:O	2.23	0.71
1:C:263:GLU:OE2	1:C:266:ARG:NH1	2.23	0.71
1:E:328:HIS:ND1	6:E:515:HOH:O	2.22	0.71
1:G:56:GLU:OE1	6:G:582:HOH:O	2.08	0.71
1:C:338:THR:O	1:C:339:HIS:ND1	2.23	0.71
1:A:8:THR:HG23	1:D:364:GLU:HG2	1.72	0.71
1:C:113:GLN:HG3	6:C:681:HOH:O	1.90	0.71
1:H:213:ARG:NH1	3:H:402:GOL:O2	2.19	0.71
1:D:338:THR:O	1:D:339:HIS:ND1	2.24	0.71
1:B:54:ARG:NH1	6:B:633:HOH:O	2.22	0.71
1:H:11:VAL:HA	1:H:245:HIS:HD2	1.55	0.71
1:B:109:LEU:HB3	6:B:671:HOH:O	1.89	0.71
1:E:338:THR:HG22	2:E:401:MES:H32	1.73	0.71
1:B:344:ALA:HA	1:B:347:ARG:HB2	1.73	0.71
1:D:252:HIS:HB3	6:D:652:HOH:O	1.89	0.71
1:C:160:ARG:HE	1:C:161:ARG:HH21	1.38	0.71
1:H:285:HIS:CD2	6:H:661:HOH:O	2.43	0.71
1:G:347:ARG:O	1:G:352:ILE:N	2.23	0.71
1:B:118:ARG:NH2	1:B:119:TYR:O	2.23	0.71
1:C:92:CYS:SG	1:C:116:ARG:NH1	2.64	0.71
1:A:100:TYR:HB2	6:A:696:HOH:O	1.90	0.71
1:D:40:ASP:O	6:D:618:HOH:O	2.07	0.71
1:H:197:LLP:O3	6:H:534:HOH:O	2.08	0.71
1:A:343:SER:H	1:A:346:ALA:HB3	1.54	0.71
1:G:97:ASP:HB3	1:G:119:TYR:HB3	1.71	0.71
1:B:321:GLY:O	6:B:556:HOH:O	2.07	0.71
1:E:154:ASP:OD2	6:E:563:HOH:O	2.07	0.71
1:A:338:THR:O	6:A:592:HOH:O	2.08	0.71
1:C:263:GLU:HG3	6:C:688:HOH:O	1.90	0.71
1:A:252:HIS:O	6:A:553:HOH:O	2.07	0.71
1:F:339:HIS:HB3	1:F:342:LEU:HG	1.72	0.71
1:H:4:MSE:O	1:H:9:ARG:NH2	2.24	0.71
1:E:213:ARG:NH2	6:E:589:HOH:O	2.23	0.71
1:A:39:GLN:HE22	1:A:44:TYR:H	1.39	0.71
1:B:120:ALA:O	6:B:681:HOH:O	2.08	0.71
1:E:204:ASP:OD2	1:H:242:ARG:NE	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:THR:OG1	1:E:375:ARG:NH1	2.23	0.71
1:D:347:ARG:O	1:D:352:ILE:N	2.23	0.71
1:H:17:PRO:O	6:H:645:HOH:O	2.09	0.71
1:A:161:ARG:NH1	6:A:605:HOH:O	2.24	0.71
1:C:374:SER:OG	6:C:501:HOH:O	2.09	0.71
1:C:56:GLU:OE2	6:C:603:HOH:O	2.08	0.71
1:F:97:ASP:O	1:F:350:ARG:NH2	2.23	0.70
1:F:5:ARG:N	1:G:368:ASP:OD2	2.24	0.70
1:H:88:ARG:N	1:H:91:GLN:OE1	2.23	0.70
1:F:332:GLU:OE2	1:F:338:THR:OG1	2.09	0.70
1:H:134:GLU:O	1:H:165:ARG:NH1	2.23	0.70
1:H:285:HIS:CE1	6:H:668:HOH:O	2.44	0.70
2:C:401:MES:H61	1:D:46:TYR:CD2	2.25	0.70
1:H:104:ASP:O	1:H:108:ASP:N	2.22	0.70
1:C:282:HIS:HB3	1:C:285:HIS:HB3	1.72	0.70
1:D:320:CYS:SG	1:D:337:MSE:HE1	2.31	0.70
1:H:168:ARG:HH22	3:H:404:GOL:H32	1.55	0.70
1:B:124:THR:OG1	1:B:127:GLY:N	2.24	0.70
1:D:332:GLU:OE1	1:D:338:THR:OG1	2.08	0.70
1:E:313:ASP:HA	1:F:37:ARG:HH21	1.56	0.70
1:A:319:THR:OG1	6:A:607:HOH:O	2.08	0.70
1:B:160:ARG:NH1	6:B:582:HOH:O	2.21	0.70
1:A:16:ARG:HB2	1:A:56:GLU:HG2	1.71	0.70
1:H:147:ASN:HD21	1:H:358:ARG:HH11	1.39	0.70
1:H:43:ARG:NH2	1:H:44:TYR:OH	2.23	0.70
1:D:143:GLU:HG3	1:D:172:ASP:HB3	1.73	0.70
1:F:113:GLN:O	6:F:603:HOH:O	2.09	0.70
1:H:253:ARG:NH1	1:H:253:ARG:O	2.23	0.70
1:F:367:GLN:HE21	1:F:367:GLN:HA	1.55	0.70
1:C:248:SER:OG	6:C:663:HOH:O	2.08	0.70
1:B:36:ARG:NH2	6:B:509:HOH:O	2.23	0.70
1:D:264:ARG:HH22	1:D:367:GLN:HE22	1.39	0.70
1:B:54:ARG:HH12	1:B:231:VAL:HB	1.55	0.70
1:H:152:VAL:H	1:H:284:GLN:NE2	1.89	0.70
1:H:360:SER:OG	6:H:554:HOH:O	2.08	0.70
1:E:298:ILE:HD11	1:E:324:LEU:HD13	1.72	0.70
1:C:112:ARG:NH2	6:C:501:HOH:O	2.18	0.70
1:H:343:SER:O	1:H:347:ARG:HB2	1.91	0.70
1:E:18:SER:OG	6:E:586:HOH:O	2.08	0.70
1:A:97:ASP:N	1:A:97:ASP:OD2	2.23	0.70
1:D:96:THR:O	1:D:99:VAL:HB	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:ASP:OD1	1:F:119:TYR:OH	2.08	0.70
1:G:113:GLN:OE1	1:H:88:ARG:NH2	2.25	0.70
1:H:281:GLU:OE2	6:H:501:HOH:O	2.09	0.70
1:H:259:ARG:NH1	6:H:625:HOH:O	2.24	0.70
1:A:161:ARG:NH1	6:A:678:HOH:O	2.24	0.70
1:A:4:MSE:HE1	6:D:660:HOH:O	1.92	0.70
1:F:84:LEU:O	6:F:559:HOH:O	2.08	0.70
1:F:253:ARG:HD2	3:F:404:GOL:H11	1.74	0.70
1:E:375:ARG:NH2	6:E:617:HOH:O	2.14	0.70
1:E:116:ARG:HH22	1:E:136:ASP:HB2	1.57	0.70
1:C:303:TYR:O	1:C:355:SER:OG	2.10	0.70
1:D:259:ARG:NH2	6:D:628:HOH:O	2.25	0.70
1:F:147:ASN:HD21	1:F:358:ARG:HH11	1.37	0.70
1:F:31:SER:HB3	1:F:34:TYR:HE2	1.56	0.70
1:E:347:ARG:O	1:E:351:GLY:N	2.21	0.70
1:A:316:THR:OG1	1:A:375:ARG:NH1	2.24	0.70
1:F:365:ASP:N	1:G:7:GLY:O	2.25	0.70
1:G:112:ARG:O	1:H:88:ARG:NH2	2.22	0.70
1:A:337:MSE:HG2	1:B:36:ARG:NH1	2.06	0.70
1:B:214:ASP:HB3	1:B:217:LEU:HB3	1.73	0.70
1:C:213:ARG:NH2	3:C:403:GOL:O2	2.24	0.70
3:A:402:GOL:O3	3:A:402:GOL:O1	2.09	0.70
1:C:39:GLN:HE22	1:C:44:TYR:H	1.39	0.70
1:D:35:GLU:HG3	1:D:38:ALA:H	1.56	0.70
1:H:236:ASP:OD2	6:H:681:HOH:O	2.10	0.70
1:C:297:ALA:HB3	6:C:609:HOH:O	1.92	0.70
1:A:284:GLN:NE2	6:A:671:HOH:O	2.25	0.70
1:A:336:LEU:C	1:A:340:ARG:HD3	2.13	0.70
1:B:6:PHE:HA	1:B:9:ARG:HE	1.57	0.70
1:G:43:ARG:HD2	6:G:1462:HOH:O	1.92	0.70
1:B:227:THR:HG1	3:B:404:GOL:HO3	1.38	0.70
1:C:343:SER:OG	1:C:344:ALA:N	2.23	0.70
1:H:100:TYR:CE1	2:H:401:MES:H81	2.26	0.70
1:B:98:ASP:OD1	1:B:98:ASP:N	2.22	0.70
1:F:160:ARG:HD2	1:F:161:ARG:HH22	1.57	0.69
1:A:37:ARG:NH1	1:B:312:LEU:O	2.24	0.69
1:A:180:LEU:HD22	1:A:294:ALA:HB3	1.74	0.69
1:D:150:LEU:HD22	1:D:175:PHE:HE2	1.55	0.69
1:H:305:GLY:O	6:H:502:HOH:O	2.10	0.69
1:C:56:GLU:OE2	6:C:535:HOH:O	2.09	0.69
1:C:197:LLP:O3	6:C:554:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:THR:OG1	6:C:633:HOH:O	2.10	0.69
1:C:39:GLN:OE1	1:C:43:ARG:N	2.18	0.69
1:B:350:ARG:NH1	6:B:627:HOH:O	2.25	0.69
1:C:350:ARG:HG3	6:C:672:HOH:O	1.92	0.69
1:D:98:ASP:OD2	1:D:98:ASP:N	2.25	0.69
1:A:116:ARG:NH2	1:A:136:ASP:OD2	2.25	0.69
1:A:36:ARG:HH21	1:A:36:ARG:HB2	1.56	0.69
1:E:292:MSE:HE3	6:E:651:HOH:O	1.91	0.69
1:H:97:ASP:OD2	6:H:656:HOH:O	2.10	0.69
1:E:39:GLN:NE2	1:E:43:ARG:H	1.89	0.69
1:A:336:LEU:O	1:A:340:ARG:NH2	2.26	0.69
1:H:4:MSE:SE	6:H:616:HOH:O	2.59	0.69
1:B:322:VAL:HG12	1:B:332:GLU:OE2	1.92	0.69
1:A:368:ASP:OD1	1:D:5:ARG:NH1	2.25	0.69
1:B:55:GLU:OE1	6:B:607:HOH:O	2.08	0.69
1:D:281:GLU:OE1	6:D:501:HOH:O	2.10	0.69
1:G:231:VAL:HG22	1:G:232:PRO:HD2	1.73	0.69
1:A:34:TYR:OH	6:A:571:HOH:O	2.07	0.69
1:H:132:LEU:O	1:H:165:ARG:NE	2.25	0.69
1:G:168:ARG:NH2	4:G:406:CL:CL	2.61	0.69
1:E:332:GLU:HG2	1:E:358:ARG:HB3	1.74	0.69
1:B:4:MSE:O	1:B:6:PHE:N	2.24	0.69
1:G:184:LEU:HB3	1:G:213:ARG:HH22	1.57	0.69
1:H:332:GLU:OE2	1:H:358:ARG:NH2	2.25	0.69
1:F:150:LEU:HD22	1:F:175:PHE:HZ	1.58	0.69
2:C:401:MES:H61	1:D:46:TYR:CD2	2.27	0.69
1:H:168:ARG:HH22	3:H:404:GOL:H32	1.58	0.69
1:E:280:PRO:HA	1:E:285:HIS:HD2	1.56	0.69
1:E:347:ARG:HB3	1:E:352:ILE:HB	1.74	0.69
1:G:46:TYR:CD2	2:H:401:MES:H61	2.28	0.69
1:D:43:ARG:HB3	1:D:44:TYR:CD2	2.26	0.69
1:F:116:ARG:NH1	1:F:134:GLU:OE1	2.25	0.69
1:H:347:ARG:HG2	1:H:352:ILE:HB	1.75	0.69
1:B:365:ASP:OD2	3:B:402:GOL:O3	2.09	0.69
1:F:320:CYS:SG	1:F:337:MSE:HE1	2.33	0.69
1:C:134:GLU:O	1:C:165:ARG:NH1	2.26	0.69
1:C:310:ARG:NH1	1:C:313:ASP:OD2	2.23	0.69
1:H:323:SER:O	6:H:515:HOH:O	2.10	0.69
1:H:236:ASP:OD2	6:H:616:HOH:O	2.11	0.69
1:C:225:ARG:HG2	1:C:231:VAL:HG12	1.74	0.69
1:B:172:ASP:OD2	6:B:521:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:GLY:O	1:C:22:GLY:N	2.26	0.69
1:G:100:TYR:HE1	2:G:401:MES:H81	1.57	0.69
1:D:6:PHE:O	6:D:663:HOH:O	2.11	0.69
1:C:342:LEU:HD13	6:C:673:HOH:O	1.92	0.69
1:E:124:THR:HB	1:E:126:GLU:HG2	1.74	0.69
1:A:371:GLU:OE1	6:A:617:HOH:O	2.11	0.69
1:A:124:THR:HG23	1:A:127:GLY:H	1.58	0.69
4:A:407:CL:CL	1:B:36:ARG:NH1	2.62	0.69
1:C:236:ASP:OD2	6:C:573:HOH:O	2.09	0.69
1:E:98:ASP:N	1:E:98:ASP:OD2	2.23	0.69
1:E:37:ARG:NH1	1:F:312:LEU:O	2.24	0.69
1:B:288:VAL:O	1:B:292:MSE:SE	2.60	0.69
1:D:108:ASP:OD2	6:D:656:HOH:O	2.10	0.69
1:A:4:MSE:HA	1:A:9:ARG:HG3	1.74	0.69
1:G:36:ARG:HH11	1:G:36:ARG:HG3	1.58	0.69
1:E:74:SER:OG	1:F:229:GLY:O	2.11	0.69
1:A:9:ARG:HG2	6:A:668:HOH:O	1.91	0.69
1:H:65:GLU:OE1	6:H:553:HOH:O	2.11	0.69
1:G:285:HIS:CE1	6:G:659:HOH:O	2.45	0.68
1:F:253:ARG:NH1	3:F:405:GOL:O1	2.26	0.68
1:H:52:PRO:O	1:H:56:GLU:HG3	1.93	0.68
1:D:148:PRO:HD3	1:D:339:HIS:HE1	1.58	0.68
1:A:35:GLU:OE2	1:A:37:ARG:NE	2.22	0.68
1:E:161:ARG:HD2	6:E:689:HOH:O	1.93	0.68
1:E:39:GLN:HE22	1:E:44:TYR:N	1.92	0.68
1:C:124:THR:HG23	1:C:127:GLY:H	1.58	0.68
1:C:342:LEU:HD22	1:C:342:LEU:H	1.59	0.68
1:F:225:ARG:HG2	1:F:231:VAL:HG12	1.76	0.68
1:E:38:ALA:O	6:E:661:HOH:O	2.10	0.68
1:F:214:ASP:OD2	6:F:665:HOH:O	2.10	0.68
1:F:332:GLU:HG2	1:F:333:CYS:N	2.08	0.68
1:E:143:GLU:HG3	1:E:172:ASP:HB3	1.76	0.68
1:D:254:GLN:NE2	6:D:654:HOH:O	2.26	0.68
1:A:236:ASP:OD1	6:A:644:HOH:O	2.11	0.68
1:C:181:GLN:HE22	1:C:183:PRO:HG3	1.59	0.68
1:C:292:MSE:HG3	6:C:656:HOH:O	1.94	0.68
1:H:213:ARG:NE	3:H:402:GOL:O2	2.24	0.68
1:F:58:GLU:OE1	6:F:541:HOH:O	2.09	0.68
1:H:113:GLN:OE1	6:H:603:HOH:O	2.11	0.68
1:A:97:ASP:OD1	1:A:97:ASP:N	2.24	0.68
1:C:39:GLN:HE22	1:C:44:TYR:H	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:259:ARG:NH2	6:H:501:HOH:O	2.27	0.68
1:C:50:GLU:OE2	6:C:610:HOH:O	2.12	0.68
1:B:96:THR:HG22	6:B:687:HOH:O	1.93	0.68
1:C:160:ARG:NH1	6:C:694:HOH:O	2.25	0.68
1:C:38:ALA:O	1:C:40:ASP:N	2.26	0.68
1:C:4:MSE:HE3	1:C:9:ARG:HG2	1.74	0.68
1:F:332:GLU:OE1	1:F:358:ARG:NH2	2.26	0.68
1:G:152:VAL:HB	1:G:284:GLN:HG3	1.75	0.68
1:D:39:GLN:O	6:D:599:HOH:O	2.10	0.68
1:G:18:SER:N	6:G:657:HOH:O	2.18	0.68
1:F:168:ARG:NH2	4:F:408:CL:CL	2.53	0.68
1:A:36:ARG:NH2	1:A:36:ARG:HB2	2.07	0.68
1:C:160:ARG:HB3	1:C:161:ARG:HH21	1.57	0.68
1:D:9:ARG:NH2	1:D:63:GLY:O	2.26	0.68
1:G:58:GLU:OE1	6:G:606:HOH:O	2.10	0.68
1:B:132:LEU:HB3	1:B:165:ARG:HD3	1.76	0.68
1:E:336:LEU:HB3	1:E:337:MSE:SE	2.44	0.68
1:H:147:ASN:ND2	1:H:358:ARG:HH11	1.90	0.68
1:A:9:ARG:HH12	1:A:66:ARG:HE	1.41	0.68
1:D:94:VAL:HG11	1:D:131:ALA:HB1	1.73	0.68
1:C:112:ARG:NH1	6:C:502:HOH:O	2.27	0.68
1:H:6:PHE:HE2	1:H:179:VAL:HG22	1.58	0.68
1:H:105:GLY:O	6:H:673:HOH:O	2.09	0.68
1:C:147:ASN:ND2	1:C:175:PHE:HE2	1.92	0.68
1:A:97:ASP:HB2	1:A:350:ARG:HH11	1.58	0.68
1:B:241:ARG:HA	1:B:244:LEU:HD12	1.76	0.68
1:F:125:PRO:HA	1:F:128:ILE:HD12	1.74	0.68
1:B:96:THR:HG23	1:B:99:VAL:HG13	1.76	0.68
1:D:213:ARG:CZ	6:D:653:HOH:O	2.41	0.68
1:D:98:ASP:OD2	1:D:98:ASP:N	2.25	0.68
1:G:336:LEU:O	1:G:337:MSE:HG3	1.93	0.68
1:E:104:ASP:HB3	6:E:674:HOH:O	1.94	0.68
1:C:380:GLY:HA3	6:C:667:HOH:O	1.92	0.68
1:E:336:LEU:HG	6:E:693:HOH:O	1.93	0.68
1:H:65:GLU:HG3	1:H:211:VAL:HG11	1.76	0.68
1:C:132:LEU:HD12	1:C:161:ARG:HB3	1.75	0.68
1:D:4:MSE:O	1:D:9:ARG:NH2	2.27	0.68
1:G:233:GLY:HA3	6:H:681:HOH:O	1.93	0.68
1:A:160:ARG:HE	1:A:161:ARG:HH11	1.42	0.68
1:G:316:THR:OG1	1:G:375:ARG:NH1	2.26	0.68
1:B:371:GLU:OE2	1:C:5:ARG:NH1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:LEU:HB3	6:F:639:HOH:O	1.93	0.68
1:A:4:MSE:HE3	1:A:4:MSE:N	2.09	0.68
1:E:39:GLN:NE2	1:E:44:TYR:HB2	2.09	0.68
1:E:100:TYR:HE1	2:E:401:MES:H82	1.58	0.68
1:C:35:GLU:OE2	1:C:37:ARG:NE	2.25	0.68
1:A:199:ILE:HG23	1:A:244:LEU:HD13	1.75	0.68
1:E:160:ARG:HB3	1:E:161:ARG:NH1	2.08	0.68
1:A:37:ARG:HD2	6:B:509:HOH:O	1.93	0.68
1:D:9:ARG:NE	6:D:567:HOH:O	2.26	0.68
1:G:213:ARG:HH21	3:G:402:GOL:HO2	1.41	0.68
1:G:346:ALA:O	1:G:350:ARG:N	2.25	0.67
1:D:337:MSE:O	1:D:340:ARG:N	2.27	0.67
1:D:68:PRO:O	6:D:569:HOH:O	2.11	0.67
1:F:339:HIS:O	1:F:347:ARG:NH1	2.27	0.67
1:E:8:THR:HG23	1:H:364:GLU:HG2	1.76	0.67
1:F:109:LEU:HD23	1:F:112:ARG:HH22	1.58	0.67
1:C:89:PRO:HB3	1:C:114:GLY:HA3	1.76	0.67
1:B:19:ALA:HA	6:B:680:HOH:O	1.93	0.67
1:D:104:ASP:HA	1:D:107:PHE:HB2	1.75	0.67
1:G:332:GLU:HB3	1:G:358:ARG:HB3	1.75	0.67
1:E:55:GLU:OE1	6:E:572:HOH:O	2.11	0.67
1:C:18:SER:OG	6:C:564:HOH:O	2.12	0.67
1:E:5:ARG:N	1:H:368:ASP:OD2	2.20	0.67
1:F:16:ARG:HB2	1:F:56:GLU:OE2	1.94	0.67
1:A:91:GLN:HB3	1:A:138:ALA:HB2	1.76	0.67
1:C:351:GLY:O	6:C:563:HOH:O	2.13	0.67
1:E:39:GLN:NE2	1:E:41:GLU:O	2.27	0.67
1:C:112:ARG:HB3	1:D:88:ARG:HH12	1.59	0.67
1:B:9:ARG:HD2	1:B:64:LEU:HA	1.76	0.67
1:E:367:GLN:HG3	6:H:691:HOH:O	1.92	0.67
1:C:47:GLY:O	1:C:54:ARG:NH1	2.28	0.67
1:H:152:VAL:O	1:H:284:GLN:NE2	2.26	0.67
1:E:154:ASP:OD2	6:E:643:HOH:O	2.13	0.67
1:E:102:GLY:HA2	3:F:405:GOL:H31	1.77	0.67
1:H:16:ARG:HA	1:H:16:ARG:HH11	1.58	0.67
1:B:338:THR:HG22	2:B:401:MES:H71	1.77	0.67
1:D:160:ARG:O	6:D:675:HOH:O	2.13	0.67
1:E:16:ARG:CZ	6:E:666:HOH:O	2.41	0.67
1:D:132:LEU:O	1:D:165:ARG:NE	2.28	0.67
1:H:275:HIS:HE1	6:H:666:HOH:O	1.77	0.67
1:A:332:GLU:OE2	1:A:338:THR:OG1	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:LEU:O	1:F:113:GLN:NE2	2.25	0.67
1:A:36:ARG:NE	6:A:534:HOH:O	2.26	0.67
1:H:292:MSE:HE2	1:H:294:ALA:O	1.94	0.67
1:A:44:TYR:OH	1:A:55:GLU:OE2	2.10	0.67
1:D:336:LEU:HD13	1:D:337:MSE:SE	2.44	0.67
1:D:35:GLU:OE2	1:D:37:ARG:HB2	1.95	0.67
1:E:98:ASP:O	6:E:682:HOH:O	2.12	0.67
1:D:346:ALA:O	1:D:348:ALA:N	2.28	0.67
1:E:288:VAL:HG13	1:E:292:MSE:SE	2.45	0.67
1:G:101:ALA:HA	1:G:104:ASP:HB3	1.76	0.67
1:B:236:ASP:OD2	6:B:659:HOH:O	2.13	0.67
1:B:292:MSE:H	1:B:292:MSE:SE	2.26	0.67
1:B:338:THR:O	1:B:341:PRO:HD2	1.93	0.67
1:C:180:LEU:HD22	1:C:294:ALA:HB3	1.77	0.67
1:C:213:ARG:NH1	6:C:574:HOH:O	2.21	0.67
1:E:39:GLN:NE2	6:E:599:HOH:O	2.27	0.67
1:E:319:THR:HG23	1:F:35:GLU:OE1	1.94	0.67
1:A:40:ASP:OD1	6:A:686:HOH:O	2.12	0.67
1:F:306:GLY:HA3	1:F:310:ARG:HH11	1.60	0.67
1:G:217:LEU:HD22	4:G:408:CL:CL	2.32	0.67
1:E:355:SER:HB3	6:E:651:HOH:O	1.93	0.67
1:F:328:HIS:O	6:F:547:HOH:O	2.11	0.67
1:B:126:GLU:O	1:B:130:ALA:N	2.27	0.67
1:G:292:MSE:HE3	6:G:605:HOH:O	1.95	0.67
1:D:168:ARG:HH22	3:D:404:GOL:H32	1.58	0.67
1:H:11:VAL:HA	1:H:245:HIS:HD2	1.59	0.67
1:D:358:ARG:HH11	1:D:358:ARG:HB3	1.58	0.67
1:F:355:SER:HB2	6:F:646:HOH:O	1.95	0.67
1:F:44:TYR:OH	1:F:55:GLU:OE1	2.12	0.67
1:E:253:ARG:HD2	6:E:653:HOH:O	1.95	0.67
1:B:348:ALA:O	1:B:351:GLY:N	2.28	0.67
1:G:259:ARG:NH2	1:G:295:PRO:HD2	2.10	0.67
1:D:17:PRO:HA	6:D:651:HOH:O	1.94	0.67
1:A:309:GLU:CD	1:A:309:GLU:H	1.98	0.67
1:A:65:GLU:OE1	6:A:535:HOH:O	2.12	0.67
1:H:291:GLN:HG3	1:H:292:MSE:HG3	1.77	0.67
1:B:43:ARG:NH2	1:B:55:GLU:OE2	2.27	0.67
1:F:96:THR:HA	1:F:120:ALA:H	1.60	0.67
1:F:204:ASP:OD2	6:F:588:HOH:O	2.13	0.67
1:G:108:ASP:OD1	6:G:581:HOH:O	2.12	0.67
1:H:3:GLY:O	1:H:8:THR:HB	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:PRO:O	6:C:561:HOH:O	2.12	0.67
1:F:253:ARG:HH11	3:F:404:GOL:H31	1.60	0.67
1:C:4:MSE:O	6:C:672:HOH:O	2.11	0.67
1:F:314:ARG:CZ	1:F:379:GLY:HA2	2.25	0.67
1:A:252:HIS:O	6:A:574:HOH:O	2.10	0.67
1:B:342:LEU:HB2	1:B:347:ARG:HD3	1.77	0.66
1:D:94:VAL:N	1:D:139:LEU:O	2.28	0.66
1:E:66:ARG:NH1	6:E:616:HOH:O	2.27	0.66
1:C:288:VAL:HG13	1:C:292:MSE:HE2	1.75	0.66
1:C:98:ASP:HA	1:C:350:ARG:CZ	2.25	0.66
1:E:263:GLU:OE1	6:E:501:HOH:O	2.12	0.66
1:D:323:SER:HA	6:D:675:HOH:O	1.95	0.66
1:E:34:TYR:OH	6:E:616:HOH:O	2.13	0.66
1:E:39:GLN:NE2	1:G:21:THR:O	2.27	0.66
1:D:157:GLU:OE1	1:D:160:ARG:NH1	2.27	0.66
1:B:90:GLY:N	1:B:114:GLY:O	2.21	0.66
1:E:98:ASP:HB2	6:E:682:HOH:O	1.95	0.66
1:H:37:ARG:O	1:H:39:GLN:N	2.27	0.66
1:C:125:PRO:HG2	6:C:648:HOH:O	1.96	0.66
1:F:65:GLU:OE1	6:F:537:HOH:O	2.13	0.66
1:H:147:ASN:HD21	1:H:358:ARG:HH11	1.43	0.66
1:D:100:TYR:HB2	6:D:645:HOH:O	1.95	0.66
1:F:259:ARG:NH2	6:F:666:HOH:O	2.06	0.66
1:B:334:PRO:HA	1:B:338:THR:OG1	1.95	0.66
1:H:9:ARG:HG2	6:H:662:HOH:O	1.95	0.66
1:G:365:ASP:OD2	6:G:1396:HOH:O	2.13	0.66
1:E:146:THR:HG1	1:E:151:THR:HG1	1.39	0.66
1:G:43:ARG:HD2	6:G:659:HOH:O	1.94	0.66
1:A:18:SER:N	6:A:647:HOH:O	2.28	0.66
1:F:259:ARG:NH2	6:F:619:HOH:O	2.28	0.66
1:C:45:PHE:N	1:C:50:GLU:OE1	2.22	0.66
1:C:93:VAL:HG13	1:C:139:LEU:HB3	1.78	0.66
1:A:375:ARG:NH2	6:A:556:HOH:O	2.24	0.66
1:B:98:ASP:OD1	1:B:98:ASP:N	2.28	0.66
1:A:33:THR:HG23	1:C:24:VAL:HB	1.76	0.66
1:E:322:VAL:O	1:F:33:THR:HG21	1.95	0.66
1:H:355:SER:OG	6:H:556:HOH:O	2.12	0.66
1:G:354:GLU:O	6:G:1379:HOH:O	2.14	0.66
1:A:338:THR:OG1	1:A:339:HIS:N	2.29	0.66
1:C:263:GLU:OE2	6:C:501:HOH:O	2.12	0.66
1:C:112:ARG:O	1:D:88:ARG:NH1	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:ASP:OD1	6:E:612:HOH:O	2.13	0.66
1:B:180:LEU:HD22	1:B:294:ALA:HB3	1.78	0.66
1:D:339:HIS:HA	1:D:342:LEU:HB3	1.78	0.66
1:E:109:LEU:HD12	6:E:619:HOH:O	1.96	0.66
1:H:291:GLN:HG2	1:H:292:MSE:SE	2.46	0.66
1:C:214:ASP:HB2	4:C:406:CL:CL	2.31	0.66
1:E:345:GLU:O	1:E:347:ARG:N	2.29	0.66
1:G:64:LEU:HD11	1:G:244:LEU:HD21	1.77	0.66
1:B:339:HIS:HD2	1:B:342:LEU:HD12	1.61	0.66
1:B:97:ASP:HB2	6:B:680:HOH:O	1.94	0.66
1:F:9:ARG:NH2	1:F:66:ARG:HG3	2.09	0.66
1:H:168:ARG:NE	4:H:406:CL:CL	2.61	0.66
1:H:4:MSE:HE2	6:H:667:HOH:O	1.94	0.66
1:B:157:GLU:OE2	6:B:594:HOH:O	2.12	0.66
1:C:319:THR:HB	1:C:330:LEU:HD23	1.78	0.66
1:F:150:LEU:HD22	1:F:175:PHE:HE2	1.60	0.66
1:H:116:ARG:NH2	1:H:135:PRO:O	2.22	0.66
1:H:11:VAL:HA	1:H:245:HIS:CD2	2.30	0.66
1:E:36:ARG:O	1:E:38:ALA:N	2.29	0.66
1:G:322:VAL:O	1:H:33:THR:HG21	1.96	0.66
1:G:213:ARG:NH2	3:G:402:GOL:O2	2.20	0.66
1:B:100:TYR:HE1	2:B:401:MES:H82	1.60	0.66
1:E:15:ARG:C	1:E:16:ARG:HD2	2.15	0.66
1:H:11:VAL:HA	1:H:245:HIS:HD2	1.60	0.66
1:C:54:ARG:HD3	6:C:687:HOH:O	1.94	0.66
1:C:149:LEU:O	6:C:597:HOH:O	2.14	0.66
1:H:56:GLU:OE1	6:H:554:HOH:O	2.14	0.66
1:C:303:TYR:OH	1:C:314:ARG:NH2	2.29	0.66
1:G:379:GLY:O	6:G:630:HOH:O	2.13	0.66
1:H:197:LLP:O3	6:H:537:HOH:O	2.12	0.66
1:C:213:ARG:HE	3:C:402:GOL:H11	1.59	0.66
1:E:337:MSE:O	6:E:591:HOH:O	2.13	0.66
1:E:56:GLU:OE2	6:E:531:HOH:O	2.12	0.66
1:B:346:ALA:O	1:B:350:ARG:N	2.29	0.66
1:D:309:GLU:OE1	6:D:501:HOH:O	2.14	0.66
1:H:161:ARG:NH2	1:H:164:GLU:OE2	2.29	0.66
1:B:351:GLY:O	6:B:598:HOH:O	2.14	0.66
1:C:98:ASP:HB2	1:C:146:THR:HB	1.78	0.66
1:F:117:VAL:HG23	6:F:673:HOH:O	1.96	0.66
1:H:157:GLU:HA	1:H:160:ARG:NH1	2.11	0.66
1:B:4:MSE:SE	1:C:368:ASP:HB3	2.46	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ILE:HG23	1:C:244:LEU:HD13	1.77	0.66
1:F:113:GLN:O	6:F:553:HOH:O	2.12	0.66
1:A:368:ASP:OD1	1:D:5:ARG:NH1	2.25	0.66
1:E:39:GLN:HE22	1:E:44:TYR:H	1.44	0.66
1:G:214:ASP:HB2	6:G:680:HOH:O	1.96	0.66
1:C:16:ARG:HA	6:C:668:HOH:O	1.95	0.66
1:C:65:GLU:OE1	6:C:569:HOH:O	2.13	0.66
1:E:104:ASP:OD2	1:E:119:TYR:OH	2.12	0.66
1:E:181:GLN:CD	1:E:292:MSE:SE	2.84	0.66
1:B:12:HIS:CE1	1:B:15:ARG:HH12	2.14	0.65
1:E:95:SER:O	1:E:120:ALA:N	2.27	0.65
1:H:97:ASP:HA	1:H:119:TYR:HD2	1.61	0.65
1:G:347:ARG:NE	6:G:618:HOH:O	2.14	0.65
1:H:96:THR:HG22	1:H:120:ALA:O	1.94	0.65
1:A:5:ARG:O	1:A:9:ARG:HG3	1.96	0.65
1:A:40:ASP:OD1	6:A:677:HOH:O	2.14	0.65
1:G:189:ASP:OD1	6:G:1413:HOH:O	2.12	0.65
1:E:124:THR:OG1	1:E:127:GLY:N	2.18	0.65
1:A:4:MSE:HG3	1:A:9:ARG:HG2	1.78	0.65
1:A:168:ARG:NH1	3:A:402:GOL:O1	2.27	0.65
1:E:124:THR:HB	1:E:126:GLU:HG2	1.78	0.65
1:A:236:ASP:OD1	6:A:669:HOH:O	2.14	0.65
1:G:337:MSE:O	1:G:339:HIS:N	2.29	0.65
1:C:43:ARG:HB3	1:C:44:TYR:CD1	2.30	0.65
1:F:3:GLY:N	6:F:639:HOH:O	2.29	0.65
1:H:343:SER:OG	1:H:344:ALA:N	2.28	0.65
1:B:116:ARG:NH2	1:B:135:PRO:O	2.25	0.65
1:G:285:HIS:ND1	6:G:659:HOH:O	2.29	0.65
1:H:334:PRO:HG2	1:H:356:LEU:HD23	1.76	0.65
1:D:253:ARG:HH12	1:D:366:PRO:HD3	1.61	0.65
1:C:338:THR:OG1	1:C:338:THR:O	2.10	0.65
1:F:118:ARG:HE	1:F:120:ALA:HB2	1.61	0.65
1:C:23:ASP:OD2	6:C:547:HOH:O	2.12	0.65
1:F:98:ASP:N	1:F:98:ASP:OD1	2.26	0.65
1:H:337:MSE:SE	3:H:404:GOL:O3	2.64	0.65
1:H:132:LEU:O	1:H:165:ARG:NE	2.27	0.65
1:D:122:LEU:HA	1:D:128:ILE:HG12	1.77	0.65
1:F:134:GLU:O	1:F:165:ARG:NH1	2.27	0.65
1:B:365:ASP:HA	3:B:402:GOL:H32	1.77	0.65
1:C:319:THR:HG23	1:D:35:GLU:OE1	1.97	0.65
1:H:339:HIS:O	1:H:347:ARG:HD2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:HIS:NE2	6:C:639:HOH:O	2.30	0.65
1:A:46:TYR:CD2	2:B:401:MES:H61	2.31	0.65
1:D:37:ARG:HG3	6:D:654:HOH:O	1.95	0.65
1:C:92:CYS:SG	1:C:134:GLU:HG2	2.36	0.65
1:D:292:MSE:O	6:D:596:HOH:O	2.14	0.65
1:C:180:LEU:HD22	1:C:294:ALA:HB3	1.77	0.65
1:E:321:GLY:HA2	1:E:337:MSE:SE	2.46	0.65
1:H:11:VAL:HA	1:H:245:HIS:CD2	2.31	0.65
1:C:292:MSE:CE	1:C:295:PRO:HA	2.26	0.65
1:B:19:ALA:O	1:B:21:THR:N	2.25	0.65
1:C:199:ILE:HG23	1:C:244:LEU:HD13	1.77	0.65
1:A:86:LEU:HB3	3:A:402:GOL:H11	1.77	0.65
1:G:147:ASN:HD21	1:G:358:ARG:HH11	1.45	0.65
1:C:199:ILE:HG23	1:C:244:LEU:HD13	1.78	0.65
1:E:18:SER:OG	6:E:571:HOH:O	2.14	0.65
1:A:17:PRO:HG2	6:A:650:HOH:O	1.97	0.65
1:B:12:HIS:HE1	1:B:15:ARG:HH12	1.44	0.65
1:G:114:GLY:O	6:G:502:HOH:O	2.14	0.65
1:H:161:ARG:NH2	1:H:164:GLU:OE2	2.29	0.65
1:A:118:ARG:HG3	1:A:134:GLU:HG3	1.78	0.65
1:D:350:ARG:HD3	1:D:352:ILE:HD12	1.79	0.65
1:A:227:THR:HA	4:A:405:GOL:H31	1.79	0.65
1:E:367:GLN:HG3	6:E:649:HOH:O	1.96	0.65
1:H:18:SER:HB3	1:H:23:ASP:H	1.60	0.65
1:E:37:ARG:HD2	1:F:313:ASP:HA	1.77	0.65
1:A:350:ARG:HB3	1:A:352:ILE:HD13	1.78	0.65
1:C:213:ARG:NH2	3:C:402:GOL:O2	2.28	0.65
1:H:4:MSE:N	6:H:657:HOH:O	2.24	0.65
1:F:342:LEU:HB3	6:F:669:HOH:O	1.97	0.65
1:B:337:MSE:SE	6:B:660:HOH:O	2.64	0.65
1:D:292:MSE:SE	1:D:294:ALA:C	2.85	0.65
1:H:147:ASN:ND2	1:H:358:ARG:HH11	1.95	0.65
1:H:96:THR:OG1	1:H:98:ASP:OD1	2.14	0.65
1:B:96:THR:HG23	1:B:122:LEU:HD12	1.78	0.65
1:B:109:LEU:HB3	6:B:677:HOH:O	1.95	0.65
1:H:35:GLU:HG3	1:H:37:ARG:O	1.95	0.65
1:C:16:ARG:NH2	1:C:59:GLU:OE1	2.30	0.65
1:D:334:PRO:HA	1:D:338:THR:HB	1.78	0.65
1:E:113:GLN:HE21	1:E:113:GLN:HA	1.62	0.65
1:E:343:SER:OG	1:E:345:GLU:O	2.11	0.65
1:G:316:THR:OG1	1:G:375:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ALA:N	6:B:680:HOH:O	2.30	0.65
1:F:4:MSE:HE2	1:F:4:MSE:HA	1.78	0.65
1:H:87:VAL:O	6:H:590:HOH:O	2.13	0.65
1:A:177:SER:OG	1:A:179:VAL:HG22	1.97	0.65
1:E:23:ASP:OD2	1:G:29:HIS:ND1	2.30	0.65
1:H:264:ARG:HG2	6:H:665:HOH:O	1.96	0.65
1:F:134:GLU:O	1:F:165:ARG:NH1	2.30	0.65
1:A:342:LEU:HD22	1:A:343:SER:H	1.60	0.65
1:G:379:GLY:O	6:G:655:HOH:O	2.13	0.65
1:A:35:GLU:OE2	1:A:37:ARG:HD3	1.97	0.65
1:D:332:GLU:CD	1:D:358:ARG:HH12	1.99	0.65
1:A:236:ASP:OD1	6:A:588:HOH:O	2.13	0.65
1:G:367:GLN:O	1:G:371:GLU:HG2	1.97	0.65
1:A:112:ARG:HE	1:E:135:PRO:HG2	1.60	0.65
1:C:124:THR:OG1	1:C:127:GLY:N	2.26	0.65
1:D:337:MSE:O	1:D:340:ARG:HB3	1.97	0.65
1:A:222:ARG:O	1:A:226:THR:OG1	2.15	0.65
1:A:41:GLU:O	1:A:43:ARG:HG3	1.96	0.64
1:H:124:THR:OG1	1:H:126:GLU:OE1	2.09	0.64
1:B:100:TYR:HE1	2:B:401:MES:C8	2.10	0.64
1:B:180:LEU:HD22	1:B:294:ALA:HB3	1.78	0.64
1:H:34:TYR:OH	6:H:567:HOH:O	2.09	0.64
1:B:332:GLU:OE1	1:B:338:THR:OG1	2.09	0.64
1:F:168:ARG:NH1	3:F:402:GOL:O1	2.30	0.64
1:F:338:THR:HG23	1:F:339:HIS:ND1	2.13	0.64
1:C:102:GLY:HA2	3:C:402:GOL:H32	1.79	0.64
1:E:41:GLU:O	1:E:43:ARG:N	2.30	0.64
1:F:214:ASP:HB3	1:F:217:LEU:HB3	1.80	0.64
1:D:347:ARG:NE	1:D:354:GLU:OE2	2.31	0.64
1:E:111:ALA:HA	1:E:115:VAL:H	1.62	0.64
1:E:4:MSE:SE	1:E:9:ARG:HA	2.47	0.64
1:C:338:THR:OG1	1:C:339:HIS:ND1	2.30	0.64
1:A:113:GLN:OE1	6:A:575:HOH:O	2.14	0.64
1:C:92:CYS:SG	1:C:134:GLU:HG2	2.36	0.64
1:F:35:GLU:OE2	1:F:37:ARG:NH1	2.30	0.64
1:B:65:GLU:OE1	6:B:639:HOH:O	2.15	0.64
1:C:302:ASP:OD1	6:C:533:HOH:O	2.13	0.64
1:A:5:ARG:NH1	1:D:368:ASP:OD2	2.29	0.64
1:F:368:ASP:OD1	1:G:5:ARG:NH1	2.31	0.64
1:A:177:SER:OG	1:A:179:VAL:HG22	1.98	0.64
1:D:197:LLP:O3	6:D:559:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:365:ASP:OD2	6:F:573:HOH:O	2.15	0.64
1:G:112:ARG:O	1:H:88:ARG:NH2	2.21	0.64
1:G:36:ARG:HH12	1:H:337:MSE:HG2	1.62	0.64
1:D:379:GLY:HA3	6:D:671:HOH:O	1.97	0.64
1:E:98:ASP:HA	1:E:350:ARG:NH2	2.11	0.64
1:A:179:VAL:HG23	1:A:180:LEU:HG	1.79	0.64
1:G:123:THR:OG1	6:G:685:HOH:O	2.13	0.64
1:H:112:ARG:HB3	6:H:679:HOH:O	1.97	0.64
1:D:281:GLU:OE1	6:D:501:HOH:O	2.14	0.64
2:C:401:MES:H61	1:D:46:TYR:CD2	2.32	0.64
1:A:134:GLU:O	6:A:655:HOH:O	2.15	0.64
1:C:39:GLN:O	1:C:41:GLU:N	2.31	0.64
1:G:97:ASP:OD2	1:G:97:ASP:N	2.25	0.64
1:D:9:ARG:HD2	6:D:670:HOH:O	1.95	0.64
1:G:113:GLN:NE2	1:H:113:GLN:OE1	2.31	0.64
1:C:39:GLN:NE2	1:C:43:ARG:H	1.95	0.64
1:A:152:VAL:O	1:A:284:GLN:NE2	2.31	0.64
1:F:4:MSE:O	6:F:658:HOH:O	2.15	0.64
1:D:149:LEU:HD11	1:D:351:GLY:HA3	1.80	0.64
1:B:29:HIS:ND1	1:D:23:ASP:OD2	2.28	0.64
1:B:143:GLU:OE2	6:B:575:HOH:O	2.15	0.64
1:E:309:GLU:OE1	6:E:501:HOH:O	2.15	0.64
1:H:336:LEU:HB2	1:H:337:MSE:SE	2.47	0.64
1:D:289:LYS:O	6:D:596:HOH:O	2.15	0.64
1:E:5:ARG:O	1:E:9:ARG:HG3	1.97	0.64
1:G:4:MSE:HG2	1:G:8:THR:HG22	1.80	0.64
1:A:188:ALA:O	1:A:213:ARG:NH1	2.27	0.64
1:F:34:TYR:HD1	1:F:44:TYR:HB3	1.63	0.64
1:G:160:ARG:HB3	1:G:161:ARG:HE	1.63	0.64
1:D:36:ARG:O	1:D:38:ALA:N	2.31	0.64
1:E:164:GLU:OE2	6:E:649:HOH:O	2.15	0.64
1:B:300:SER:HB3	1:B:356:LEU:HD11	1.80	0.64
1:F:292:MSE:HE2	1:F:295:PRO:HA	1.80	0.64
1:H:341:PRO:HG2	6:H:687:HOH:O	1.97	0.64
1:D:92:CYS:HB2	1:D:116:ARG:CZ	2.28	0.64
1:D:56:GLU:OE1	6:D:539:HOH:O	2.15	0.64
1:C:132:LEU:O	1:C:165:ARG:NE	2.24	0.64
1:D:43:ARG:HH11	1:D:43:ARG:HG3	1.62	0.64
1:E:291:GLN:HG3	1:E:292:MSE:CE	2.28	0.64
1:A:224:TYR:OH	6:A:579:HOH:O	2.14	0.64
1:D:60:CYS:SG	1:D:244:LEU:HD13	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ALA:N	6:C:606:HOH:O	2.30	0.64
1:F:59:GLU:O	6:F:566:HOH:O	2.15	0.64
1:D:338:THR:O	1:D:340:ARG:N	2.31	0.64
1:A:37:ARG:HD2	6:A:672:HOH:O	1.96	0.64
1:B:121:ASP:OD1	6:B:612:HOH:O	2.15	0.64
1:F:314:ARG:NH2	1:F:376:ALA:O	2.31	0.64
3:B:402:GOL:O3	3:B:402:GOL:O1	2.12	0.64
1:A:337:MSE:HE3	6:A:658:HOH:O	1.97	0.64
1:G:147:ASN:HD21	1:G:358:ARG:HH11	1.46	0.64
1:D:168:ARG:HH22	3:D:404:GOL:HO3	1.44	0.64
3:G:404:GOL:O1	3:G:404:GOL:O3	2.13	0.64
1:E:236:ASP:OD2	6:E:617:HOH:O	2.15	0.64
1:H:281:GLU:HB2	6:H:648:HOH:O	1.98	0.64
1:B:59:GLU:O	6:B:579:HOH:O	2.15	0.64
1:C:354:GLU:OE2	6:C:652:HOH:O	2.15	0.64
1:D:108:ASP:O	1:D:112:ARG:N	2.28	0.64
1:G:313:ASP:HA	1:H:37:ARG:HD2	1.79	0.64
1:H:17:PRO:HA	6:H:646:HOH:O	1.98	0.64
1:H:346:ALA:O	1:H:348:ALA:N	2.31	0.64
1:E:334:PRO:HB3	1:E:339:HIS:ND1	2.12	0.64
1:D:332:GLU:HG2	1:D:358:ARG:HH12	1.63	0.64
1:D:347:ARG:HA	1:D:350:ARG:HD2	1.79	0.64
1:C:340:ARG:HA	6:C:658:HOH:O	1.97	0.64
1:H:112:ARG:HB2	6:H:662:HOH:O	1.98	0.64
1:B:90:GLY:N	1:B:114:GLY:O	2.23	0.64
1:B:89:PRO:HG2	1:E:90:GLY:HA3	1.80	0.64
1:D:36:ARG:O	1:D:39:GLN:N	2.31	0.64
1:F:44:TYR:OH	1:F:55:GLU:OE1	2.05	0.64
1:G:343:SER:O	1:G:347:ARG:NE	2.23	0.64
1:D:4:MSE:O	1:D:9:ARG:NH1	2.31	0.64
1:B:292:MSE:CE	1:B:295:PRO:HA	2.28	0.63
1:C:68:PRO:HG2	1:C:213:ARG:HA	1.80	0.63
1:G:34:TYR:OH	6:G:521:HOH:O	2.14	0.63
1:A:189:ASP:HA	1:A:213:ARG:HH22	1.62	0.63
1:D:332:GLU:CG	1:D:358:ARG:HH12	2.10	0.63
1:A:37:ARG:NH2	1:B:320:CYS:H	1.93	0.63
1:A:16:ARG:HD2	1:A:17:PRO:HD2	1.80	0.63
1:D:168:ARG:NH2	3:D:403:GOL:O3	2.31	0.63
1:D:16:ARG:O	1:D:18:SER:N	2.32	0.63
1:G:36:ARG:NH2	4:H:407:CL:CL	2.68	0.63
1:G:354:GLU:O	6:G:656:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:333:CYS:O	1:H:337:MSE:SE	2.66	0.63
1:E:157:GLU:O	1:E:161:ARG:HG2	1.97	0.63
1:C:149:LEU:O	6:C:621:HOH:O	2.15	0.63
1:E:3:GLY:O	6:E:568:HOH:O	2.15	0.63
1:G:125:PRO:HA	1:G:128:ILE:HD12	1.80	0.63
1:A:21:THR:OG1	1:A:23:ASP:OD1	2.12	0.63
1:E:109:LEU:HD12	6:E:644:HOH:O	1.98	0.63
1:B:43:ARG:NH1	6:B:639:HOH:O	2.30	0.63
1:C:94:VAL:HG11	1:C:131:ALA:HB1	1.80	0.63
1:F:365:ASP:N	1:G:8:THR:HG22	2.13	0.63
1:B:343:SER:C	1:B:345:GLU:H	1.99	0.63
1:G:330:LEU:HB2	1:G:360:SER:HB3	1.80	0.63
1:C:292:MSE:HE3	1:C:295:PRO:HA	1.80	0.63
1:E:33:THR:HG23	1:G:24:VAL:HB	1.79	0.63
1:F:310:ARG:HG2	6:F:504:HOH:O	1.98	0.63
1:G:328:HIS:O	6:G:575:HOH:O	2.15	0.63
1:C:309:GLU:HG3	1:C:310:ARG:NH2	2.13	0.63
1:G:60:CYS:SG	1:G:244:LEU:HD13	2.38	0.63
1:A:14:GLY:O	1:A:16:ARG:N	2.32	0.63
1:C:109:LEU:HD13	6:C:562:HOH:O	1.98	0.63
1:A:111:ALA:O	1:E:116:ARG:HD3	1.99	0.63
1:A:136:ASP:OD1	1:F:88:ARG:NE	2.30	0.63
1:H:108:ASP:O	1:H:112:ARG:N	2.23	0.63
1:F:118:ARG:HE	1:F:131:ALA:HA	1.62	0.63
1:G:259:ARG:NH2	6:G:666:HOH:O	2.31	0.63
1:C:102:GLY:HA2	3:D:403:GOL:H31	1.79	0.63
1:F:236:ASP:OD2	6:F:629:HOH:O	2.15	0.63
1:F:259:ARG:NH1	1:F:295:PRO:HD2	2.14	0.63
1:G:36:ARG:NH1	4:H:407:CL:CL	2.68	0.63
1:E:282:HIS:HB3	1:E:285:HIS:HB2	1.81	0.63
1:E:264:ARG:NH2	1:E:374:SER:OG	2.31	0.63
1:H:97:ASP:N	1:H:97:ASP:OD1	2.28	0.63
1:G:36:ARG:HH21	1:H:322:VAL:HG13	1.63	0.63
1:B:132:LEU:O	1:B:165:ARG:NE	2.32	0.63
1:C:372:ASP:HA	1:C:375:ARG:NH2	2.12	0.63
1:D:4:MSE:N	6:D:676:HOH:O	2.31	0.63
1:D:264:ARG:HD3	6:D:659:HOH:O	1.96	0.63
1:C:113:GLN:NE2	1:D:113:GLN:OE1	2.32	0.63
1:C:316:THR:OG1	1:C:375:ARG:NH1	2.31	0.63
1:B:42:PRO:HB3	1:B:45:PHE:HZ	1.62	0.63
1:F:343:SER:O	1:F:345:GLU:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:HG2	1:B:56:GLU:HG2	1.80	0.63
5:G:405:GOL:O3	5:G:405:GOL:O1	2.17	0.63
1:B:84:LEU:O	6:B:593:HOH:O	2.15	0.63
1:D:323:SER:N	2:D:401:MES:O3S	2.32	0.63
1:H:96:THR:HA	1:H:120:ALA:O	1.98	0.63
1:C:263:GLU:OE2	6:C:618:HOH:O	2.15	0.63
1:D:378:ALA:O	6:D:501:HOH:O	2.15	0.63
1:A:37:ARG:NH2	1:B:315:PHE:O	2.30	0.63
1:A:177:SER:OG	1:A:179:VAL:HG12	1.98	0.63
1:A:74:SER:OG	1:B:231:VAL:O	2.17	0.63
1:C:199:ILE:HG23	1:C:244:LEU:HD13	1.81	0.63
1:A:4:MSE:O	1:A:9:ARG:NE	2.31	0.63
1:H:105:GLY:HA2	1:H:108:ASP:HB2	1.80	0.63
1:H:96:THR:O	1:H:99:VAL:N	2.32	0.63
1:B:97:ASP:N	1:B:97:ASP:OD1	2.18	0.63
1:G:248:SER:HB2	6:G:542:HOH:O	1.99	0.63
3:G:403:GOL:H31	1:H:102:GLY:HA2	1.79	0.63
1:D:197:LLP:NZ	2:D:401:MES:O1S	2.31	0.63
1:H:36:ARG:NH2	6:H:650:HOH:O	2.30	0.63
1:F:340:ARG:O	6:F:597:HOH:O	2.15	0.63
1:F:96:THR:O	1:F:98:ASP:N	2.31	0.63
1:D:276:TYR:CZ	1:D:295:PRO:HB2	2.34	0.63
1:E:111:ALA:HA	1:E:115:VAL:O	1.99	0.63
1:F:9:ARG:NE	1:F:63:GLY:O	2.31	0.63
1:D:30:VAL:O	6:D:580:HOH:O	2.14	0.63
1:F:288:VAL:O	1:F:292:MSE:HG3	1.98	0.63
1:F:343:SER:HA	6:F:656:HOH:O	1.99	0.63
1:H:350:ARG:NH1	6:H:683:HOH:O	2.12	0.63
1:A:259:ARG:HE	1:A:295:PRO:HG3	1.64	0.63
1:F:154:ASP:OD1	6:F:551:HOH:O	2.16	0.63
1:D:97:ASP:HA	1:D:119:TYR:HB2	1.78	0.63
1:A:137:LEU:H	1:A:165:ARG:HH11	1.45	0.63
1:C:16:ARG:NH1	6:C:568:HOH:O	2.31	0.63
1:H:173:ASN:OD1	1:H:181:GLN:NE2	2.31	0.63
1:B:66:ARG:HH21	1:B:66:ARG:HG2	1.63	0.63
1:B:96:THR:O	1:B:98:ASP:N	2.32	0.62
1:D:36:ARG:HA	1:D:39:GLN:NE2	2.14	0.62
1:E:292:MSE:HG2	6:E:667:HOH:O	1.98	0.62
1:E:346:ALA:HA	1:E:349:ARG:CZ	2.29	0.62
1:A:353:GLY:HA3	6:A:678:HOH:O	1.99	0.62
1:D:305:GLY:O	1:D:310:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:ASP:O	1:E:99:VAL:N	2.31	0.62
1:H:105:GLY:O	1:H:109:LEU:N	2.32	0.62
1:B:276:TYR:CZ	1:B:295:PRO:HB2	2.34	0.62
1:C:116:ARG:NH2	1:C:116:ARG:HB2	2.13	0.62
1:B:29:HIS:ND1	1:D:23:ASP:OD2	2.32	0.62
1:H:251:VAL:HA	1:H:254:GLN:HE21	1.65	0.62
1:A:21:THR:OG1	6:A:632:HOH:O	2.15	0.62
1:D:345:GLU:HA	1:D:348:ALA:HB3	1.81	0.62
1:A:116:ARG:HB3	1:A:116:ARG:HH11	1.64	0.62
1:D:213:ARG:HD2	6:D:675:HOH:O	1.99	0.62
1:A:339:HIS:O	1:A:347:ARG:NH1	2.31	0.62
1:C:32:THR:HG1	1:C:33:THR:HG1	1.45	0.62
1:B:181:GLN:HB2	1:B:292:MSE:CE	2.29	0.62
1:B:152:VAL:H	1:B:284:GLN:NE2	1.97	0.62
6:A:690:HOH:O	1:B:322:VAL:HG22	1.98	0.62
1:E:298:ILE:HD11	1:E:324:LEU:HD13	1.82	0.62
1:G:347:ARG:O	1:G:351:GLY:N	2.32	0.62
1:A:132:LEU:O	1:A:165:ARG:NH1	2.33	0.62
1:F:345:GLU:HA	1:F:348:ALA:HB3	1.81	0.62
1:G:323:SER:HB3	1:H:46:TYR:CE1	2.32	0.62
1:F:332:GLU:HB2	1:F:337:MSE:CE	2.25	0.62
1:B:15:ARG:HG3	6:B:623:HOH:O	1.98	0.62
1:B:338:THR:O	1:B:341:PRO:HD2	1.99	0.62
1:F:332:GLU:HG2	1:F:358:ARG:HB3	1.80	0.62
1:E:332:GLU:HB2	1:E:337:MSE:SE	2.49	0.62
1:C:343:SER:OG	1:C:344:ALA:N	2.32	0.62
1:E:39:GLN:HE22	1:E:44:TYR:HB2	1.64	0.62
1:D:248:SER:O	1:D:252:HIS:HD2	1.82	0.62
1:F:222:ARG:O	1:F:226:THR:HG23	1.99	0.62
1:A:264:ARG:NH2	1:A:374:SER:OG	2.32	0.62
1:D:39:GLN:HE22	1:D:44:TYR:H	1.48	0.62
3:A:402:GOL:HO3	3:A:402:GOL:HO1	1.47	0.62
1:D:132:LEU:HA	1:D:137:LEU:HD22	1.81	0.62
1:H:44:TYR:OH	1:H:55:GLU:OE2	2.16	0.62
1:D:152:VAL:HG22	1:D:284:GLN:HB2	1.80	0.62
1:A:88:ARG:HG2	6:A:670:HOH:O	1.99	0.62
1:B:368:ASP:OD2	1:C:5:ARG:N	2.23	0.62
1:A:342:LEU:O	1:A:347:ARG:NH1	2.33	0.62
1:B:340:ARG:O	1:B:342:LEU:N	2.29	0.62
1:B:371:GLU:OE2	1:C:5:ARG:NH1	2.32	0.62
1:E:154:ASP:OD2	6:E:679:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:375:ARG:HD3	6:H:636:HOH:O	1.98	0.62
1:B:332:GLU:OE2	1:B:338:THR:HG23	1.99	0.62
1:A:168:ARG:HH12	3:A:402:GOL:HO1	1.47	0.62
1:F:18:SER:HB3	6:F:587:HOH:O	2.00	0.62
1:F:39:GLN:HE22	1:F:44:TYR:HB2	1.64	0.62
1:F:168:ARG:NH1	6:F:653:HOH:O	2.21	0.62
1:D:346:ALA:HA	1:D:349:ARG:CZ	2.30	0.62
1:A:135:PRO:HG3	1:E:112:ARG:NH2	2.14	0.62
1:H:96:THR:O	1:H:99:VAL:N	2.33	0.62
1:A:279:LEU:HB3	1:A:281:GLU:HG3	1.82	0.62
1:F:322:VAL:HG12	1:F:337:MSE:HE3	1.80	0.62
1:D:184:LEU:HB3	1:D:213:ARG:HH22	1.65	0.62
1:E:346:ALA:HA	1:E:349:ARG:NE	2.15	0.62
1:F:116:ARG:NH1	1:F:134:GLU:OE2	2.32	0.62
1:F:320:CYS:HB3	6:F:636:HOH:O	1.99	0.62
1:C:39:GLN:O	1:C:41:GLU:N	2.32	0.62
1:G:4:MSE:SE	1:G:4:MSE:H	2.32	0.62
1:A:100:TYR:OH	2:A:401:MES:H51	1.99	0.62
1:C:124:THR:HB	6:C:660:HOH:O	1.99	0.62
1:B:133:ALA:HA	1:B:165:ARG:HH11	1.65	0.62
1:F:338:THR:CG2	1:F:339:HIS:HD2	2.12	0.62
1:G:347:ARG:O	1:G:352:ILE:N	2.31	0.62
1:H:6:PHE:HE2	1:H:179:VAL:HA	1.65	0.62
1:B:55:GLU:O	1:B:59:GLU:HG3	1.99	0.62
1:D:4:MSE:N	6:D:670:HOH:O	2.32	0.62
1:E:4:MSE:N	6:E:619:HOH:O	2.11	0.62
1:G:112:ARG:O	1:H:88:ARG:NH2	2.32	0.62
1:E:319:THR:HG23	1:F:35:GLU:OE1	1.99	0.62
1:D:264:ARG:NE	1:D:374:SER:OG	2.33	0.62
1:G:101:ALA:O	1:G:105:GLY:N	2.33	0.62
1:E:367:GLN:OE1	6:E:671:HOH:O	2.16	0.62
1:H:152:VAL:H	1:H:284:GLN:HE22	1.45	0.62
1:H:333:CYS:N	1:H:337:MSE:SE	2.70	0.62
1:C:143:GLU:OE1	6:C:530:HOH:O	2.16	0.62
1:B:29:HIS:ND1	1:D:23:ASP:OD2	2.31	0.62
1:C:375:ARG:HG3	6:C:657:HOH:O	2.00	0.62
1:E:39:GLN:HE22	1:E:44:TYR:HB2	1.62	0.62
1:E:337:MSE:SE	6:E:607:HOH:O	2.68	0.62
1:G:259:ARG:HH21	1:G:295:PRO:HD2	1.63	0.62
1:A:180:LEU:HD22	1:A:294:ALA:HB3	1.81	0.62
1:C:43:ARG:NH1	6:C:595:HOH:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:GLN:HG3	1:E:292:MSE:HE1	1.81	0.62
1:F:168:ARG:HH22	3:F:402:GOL:H11	1.65	0.62
1:F:337:MSE:O	1:F:340:ARG:HB2	1.99	0.62
1:A:334:PRO:HB3	1:A:339:HIS:CD2	2.35	0.62
1:F:157:GLU:OE1	1:F:160:ARG:NH1	2.20	0.62
1:G:90:GLY:N	1:G:114:GLY:O	2.30	0.62
1:G:312:LEU:HD11	1:G:337:MSE:HE1	1.82	0.62
1:F:35:GLU:OE2	1:F:37:ARG:HD3	1.99	0.62
1:A:4:MSE:HE1	6:A:688:HOH:O	2.00	0.62
1:C:36:ARG:HB3	1:D:320:CYS:SG	2.39	0.62
1:H:316:THR:OG1	1:H:375:ARG:NH1	2.31	0.62
1:H:16:ARG:HA	1:H:16:ARG:NH1	2.13	0.62
1:C:16:ARG:NH2	1:C:59:GLU:OE2	2.27	0.61
1:B:15:ARG:HG3	1:B:16:ARG:N	2.13	0.61
1:F:152:VAL:HG21	1:F:288:VAL:HG22	1.82	0.61
1:F:339:HIS:HB3	1:F:342:LEU:HD12	1.81	0.61
1:A:39:GLN:HB3	1:C:20:GLY:O	2.00	0.61
1:G:36:ARG:HH11	1:G:36:ARG:HG2	1.64	0.61
1:C:16:ARG:HD2	1:C:56:GLU:CG	2.30	0.61
1:H:16:ARG:NE	1:H:59:GLU:OE1	2.30	0.61
1:C:42:PRO:HB3	6:C:667:HOH:O	1.99	0.61
1:A:189:ASP:HB3	4:A:406:CL:CL	2.37	0.61
1:H:109:LEU:HA	1:H:112:ARG:HD2	1.83	0.61
1:B:9:ARG:HD2	1:B:64:LEU:HD23	1.82	0.61
1:D:351:GLY:HA2	6:D:677:HOH:O	2.00	0.61
1:D:88:ARG:H	1:D:91:GLN:NE2	1.99	0.61
1:G:292:MSE:SE	1:G:294:ALA:H	2.33	0.61
1:C:332:GLU:OE2	1:C:338:THR:OG1	2.17	0.61
1:H:42:PRO:HB3	1:H:45:PHE:CZ	2.35	0.61
1:D:347:ARG:O	1:D:350:ARG:N	2.24	0.61
1:B:100:TYR:HE1	2:B:401:MES:H82	1.65	0.61
1:E:313:ASP:OD1	6:E:626:HOH:O	2.16	0.61
1:D:291:GLN:HE21	1:D:292:MSE:SE	2.33	0.61
1:E:319:THR:HG23	1:F:35:GLU:HB2	1.82	0.61
1:G:337:MSE:C	1:G:339:HIS:H	2.03	0.61
1:A:160:ARG:HE	1:A:161:ARG:HH11	1.46	0.61
1:A:42:PRO:HG3	6:A:653:HOH:O	2.00	0.61
1:A:189:ASP:HA	1:A:213:ARG:HH22	1.66	0.61
1:B:182:GLN:OE1	6:B:562:HOH:O	2.16	0.61
1:D:41:GLU:O	1:D:43:ARG:N	2.34	0.61
1:F:367:GLN:OE1	6:F:654:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ARG:HD3	1:B:313:ASP:HA	1.81	0.61
1:D:124:THR:OG1	1:D:126:GLU:OE1	2.19	0.61
1:H:137:LEU:HG	1:H:167:ALA:HB2	1.82	0.61
1:E:213:ARG:NE	3:E:402:GOL:O3	2.33	0.61
1:A:36:ARG:HH22	1:B:337:MSE:HG2	1.65	0.61
1:C:88:ARG:NH2	6:C:670:HOH:O	2.02	0.61
1:F:343:SER:HB3	1:F:345:GLU:H	1.66	0.61
1:B:109:LEU:O	1:B:113:GLN:HG2	2.00	0.61
1:C:4:MSE:HG2	6:C:657:HOH:O	1.98	0.61
1:A:189:ASP:OD1	4:A:406:CL:CL	2.56	0.61
1:B:9:ARG:CZ	1:B:66:ARG:HE	2.13	0.61
1:C:16:ARG:NE	1:C:59:GLU:OE1	2.33	0.61
1:H:87:VAL:O	6:H:662:HOH:O	2.16	0.61
1:E:100:TYR:HB2	6:E:618:HOH:O	2.01	0.61
1:E:322:VAL:HG21	1:F:46:TYR:HB2	1.83	0.61
1:H:126:GLU:OE2	1:H:126:GLU:N	2.33	0.61
1:C:224:TYR:OH	6:C:584:HOH:O	2.16	0.61
1:C:292:MSE:SE	6:C:644:HOH:O	2.69	0.61
1:C:33:THR:O	1:C:34:TYR:HD2	1.84	0.61
1:A:199:ILE:HG23	1:A:244:LEU:HD21	1.82	0.61
1:B:345:GLU:HA	1:B:348:ALA:HB3	1.82	0.61
1:E:146:THR:HG22	6:E:656:HOH:O	2.00	0.61
1:B:288:VAL:HA	1:B:292:MSE:SE	2.51	0.61
1:H:168:ARG:HH12	3:H:405:GOL:H32	1.64	0.61
1:A:199:ILE:HG23	1:A:244:LEU:HD13	1.82	0.61
1:A:347:ARG:NH2	1:A:354:GLU:OE1	2.34	0.61
1:H:109:LEU:HA	1:H:112:ARG:HB2	1.82	0.61
1:B:339:HIS:CD2	1:B:342:LEU:HD12	2.35	0.61
1:B:259:ARG:NH1	6:B:694:HOH:O	2.34	0.61
1:E:98:ASP:HB2	6:E:684:HOH:O	2.00	0.61
1:G:312:LEU:CD1	1:G:337:MSE:HE1	2.31	0.61
1:A:4:MSE:SE	1:A:9:ARG:HG3	2.50	0.61
1:D:173:ASN:OD1	1:D:181:GLN:NE2	2.34	0.61
1:A:309:GLU:H	1:A:309:GLU:CD	2.03	0.61
1:B:88:ARG:NH2	6:B:608:HOH:O	2.33	0.61
1:E:37:ARG:NH2	1:F:315:PHE:O	2.30	0.61
1:A:113:GLN:OE1	6:A:596:HOH:O	2.16	0.61
1:A:132:LEU:HD23	1:A:161:ARG:HB3	1.83	0.61
1:B:342:LEU:O	1:B:347:ARG:NH1	2.34	0.61
1:F:347:ARG:HB3	1:F:352:ILE:HB	1.80	0.61
1:H:267:ALA:O	6:H:501:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:GLU:OE2	1:F:37:ARG:NH1	2.33	0.61
1:C:146:THR:OG1	1:C:151:THR:OG1	2.09	0.61
1:D:88:ARG:HB2	1:D:91:GLN:HG3	1.82	0.61
1:F:343:SER:O	1:F:347:ARG:N	2.34	0.61
1:H:16:ARG:HB2	1:H:56:GLU:OE2	2.00	0.61
1:B:152:VAL:H	1:B:284:GLN:HE22	1.49	0.61
1:A:252:HIS:O	6:A:565:HOH:O	2.16	0.61
1:B:282:HIS:CE1	1:B:284:GLN:HG3	2.36	0.61
1:E:291:GLN:HG3	1:E:292:MSE:HG2	1.81	0.61
1:F:104:ASP:HA	1:F:107:PHE:HB2	1.82	0.61
1:G:43:ARG:NH2	1:G:55:GLU:OE1	2.33	0.61
1:C:222:ARG:NH2	6:C:550:HOH:O	2.32	0.61
1:G:20:GLY:O	6:G:654:HOH:O	2.16	0.61
1:H:157:GLU:HA	1:H:160:ARG:NH1	2.15	0.61
1:F:91:GLN:HA	1:F:136:ASP:HB2	1.83	0.61
1:F:100:TYR:OH	2:F:401:MES:H62	2.00	0.61
1:F:97:ASP:O	1:F:350:ARG:NH1	2.34	0.61
1:A:179:VAL:HG23	1:A:180:LEU:HG	1.81	0.61
1:H:334:PRO:HB3	1:H:339:HIS:HD2	1.66	0.61
1:F:130:ALA:HB2	6:F:650:HOH:O	2.00	0.61
1:G:58:GLU:OE1	6:G:664:HOH:O	2.16	0.61
1:H:132:LEU:HD22	1:H:137:LEU:HD21	1.83	0.61
1:A:36:ARG:HH11	1:B:337:MSE:CG	2.14	0.61
1:E:336:LEU:O	1:E:337:MSE:SE	2.68	0.61
1:C:309:GLU:HG3	1:C:310:ARG:HH22	1.65	0.61
1:E:116:ARG:NH2	1:E:135:PRO:O	2.32	0.61
1:E:168:ARG:HH22	3:E:403:GOL:H11	1.66	0.61
1:C:242:ARG:NH1	6:C:531:HOH:O	2.34	0.61
1:A:342:LEU:O	1:A:347:ARG:NH1	2.34	0.61
1:F:165:ARG:NH2	6:F:660:HOH:O	2.34	0.61
1:G:19:ALA:N	6:G:667:HOH:O	2.14	0.61
1:G:347:ARG:NH2	6:G:651:HOH:O	1.98	0.61
1:H:60:CYS:SG	1:H:244:LEU:HD13	2.41	0.61
1:H:11:VAL:HA	1:H:245:HIS:HD2	1.64	0.61
1:E:116:ARG:NH2	1:E:136:ASP:HB2	2.15	0.61
1:E:181:GLN:OE1	1:E:292:MSE:SE	2.69	0.61
1:C:134:GLU:O	1:C:165:ARG:NH1	2.33	0.60
1:E:213:ARG:NE	3:E:402:GOL:O3	2.32	0.60
1:E:35:GLU:OE2	1:E:37:ARG:N	2.31	0.60
1:G:309:GLU:HG3	6:G:675:HOH:O	2.00	0.60
1:A:337:MSE:SE	1:A:337:MSE:N	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:NH2	1:B:134:GLU:OE2	2.20	0.60
1:F:6:PHE:O	1:F:9:ARG:HG2	2.01	0.60
1:D:320:CYS:HB2	6:D:648:HOH:O	1.99	0.60
1:G:231:VAL:HG12	1:G:232:PRO:HD2	1.81	0.60
1:F:343:SER:O	1:F:346:ALA:N	2.32	0.60
1:G:284:GLN:HB3	1:G:287:VAL:HB	1.82	0.60
1:C:33:THR:HG23	6:C:670:HOH:O	2.01	0.60
1:E:336:LEU:O	1:E:340:ARG:HB2	2.01	0.60
1:E:297:ALA:HB3	6:E:608:HOH:O	2.01	0.60
1:H:236:ASP:OD2	6:H:650:HOH:O	2.15	0.60
1:B:18:SER:N	6:B:560:HOH:O	2.34	0.60
1:B:333:CYS:O	1:B:337:MSE:HB2	2.00	0.60
1:E:312:LEU:O	1:F:37:ARG:NH2	2.34	0.60
1:H:92:CYS:HB2	1:H:137:LEU:HA	1.83	0.60
1:D:264:ARG:HD2	1:D:374:SER:OG	2.01	0.60
1:B:197:LLP:NZ	2:B:401:MES:O1S	2.34	0.60
1:D:259:ARG:NH1	6:D:642:HOH:O	2.34	0.60
1:B:29:HIS:ND1	1:D:23:ASP:OD2	2.33	0.60
1:D:180:LEU:HD22	1:D:294:ALA:HB3	1.83	0.60
1:D:168:ARG:HH22	3:D:403:GOL:H31	1.65	0.60
3:E:403:GOL:O3	3:E:403:GOL:O1	2.17	0.60
1:A:337:MSE:HG3	1:A:338:THR:N	2.16	0.60
1:A:213:ARG:NH2	6:A:555:HOH:O	2.27	0.60
1:E:47:GLY:O	1:E:54:ARG:NH2	2.35	0.60
1:G:101:ALA:HA	1:G:104:ASP:HB2	1.84	0.60
1:B:156:ALA:O	1:B:160:ARG:HG3	2.01	0.60
1:C:338:THR:HG23	1:C:339:HIS:ND1	2.16	0.60
1:B:16:ARG:NH1	6:B:665:HOH:O	2.33	0.60
1:A:177:SER:OG	1:A:179:VAL:HG22	2.00	0.60
1:C:310:ARG:HB3	1:C:314:ARG:HH12	1.66	0.60
1:G:96:THR:O	1:G:99:VAL:N	2.34	0.60
1:A:322:VAL:O	1:A:323:SER:HB3	2.02	0.60
1:C:11:VAL:HA	1:C:245:HIS:ND1	2.17	0.60
1:A:116:ARG:NH2	1:A:136:ASP:HB2	2.16	0.60
1:F:225:ARG:CG	1:F:231:VAL:HG12	2.32	0.60
1:G:94:VAL:HG11	1:G:131:ALA:HB1	1.83	0.60
1:B:100:TYR:OH	2:B:401:MES:H62	2.01	0.60
1:H:259:ARG:CZ	6:H:665:HOH:O	2.49	0.60
1:B:249:LEU:HD21	1:C:253:ARG:HD2	1.83	0.60
1:E:96:THR:OG1	1:E:98:ASP:OD2	2.18	0.60
1:F:43:ARG:O	1:F:50:GLU:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:GLY:H	1:D:115:VAL:HA	1.67	0.60
1:A:27:PRO:HB2	1:C:27:PRO:HB2	1.83	0.60
1:A:35:GLU:OE1	1:A:37:ARG:NH1	2.35	0.60
1:D:55:GLU:O	1:D:59:GLU:HG3	2.02	0.60
1:D:322:VAL:HG12	1:D:332:GLU:OE2	2.00	0.60
2:E:401:MES:H61	1:F:46:TYR:CD2	2.36	0.60
1:B:44:TYR:CE2	1:D:21:THR:HG22	2.37	0.60
1:E:335:ALA:HA	1:E:347:ARG:NH1	2.16	0.60
1:G:180:LEU:HD22	1:G:294:ALA:HB3	1.82	0.60
1:B:100:TYR:OH	2:B:401:MES:H62	2.01	0.60
1:D:334:PRO:O	1:D:339:HIS:N	2.27	0.60
1:C:169:VAL:N	1:C:189:ASP:OD2	2.29	0.60
1:F:332:GLU:CB	1:F:337:MSE:HE2	2.26	0.60
1:B:16:ARG:O	3:B:405:GOL:O3	2.18	0.60
1:C:173:ASN:OD1	1:C:181:GLN:NE2	2.35	0.60
1:D:168:ARG:NH2	4:D:405:CL:CL	2.71	0.60
1:E:88:ARG:HG2	1:E:88:ARG:NH2	2.14	0.60
1:D:132:LEU:HB3	1:D:165:ARG:HG3	1.83	0.60
1:E:371:GLU:OE2	6:E:639:HOH:O	2.16	0.60
1:G:6:PHE:HA	1:G:9:ARG:HD2	1.81	0.60
1:G:320:CYS:SG	1:G:337:MSE:HE1	2.41	0.60
1:D:319:THR:HB	1:D:330:LEU:HD23	1.84	0.60
1:H:84:LEU:HD12	1:H:106:LEU:HB3	1.83	0.60
1:D:88:ARG:H	1:D:91:GLN:HE21	1.47	0.60
1:E:147:ASN:ND2	1:E:358:ARG:HH11	1.98	0.60
1:F:123:THR:HG23	1:F:124:THR:HG23	1.84	0.60
1:C:23:ASP:O	6:C:564:HOH:O	2.16	0.60
1:E:288:VAL:HA	1:E:292:MSE:HE2	1.82	0.60
1:B:325:GLY:O	6:B:526:HOH:O	2.17	0.60
1:E:19:ALA:O	1:E:21:THR:N	2.33	0.60
1:B:6:PHE:O	1:B:9:ARG:HB2	2.02	0.60
1:F:54:ARG:HG3	1:F:237:CYS:SG	2.42	0.60
1:D:95:SER:OG	1:D:96:THR:N	2.35	0.60
1:E:121:ASP:OD1	1:E:123:THR:OG1	2.13	0.60
1:E:347:ARG:HA	1:E:350:ARG:HB2	1.84	0.60
1:F:9:ARG:HH21	1:F:64:LEU:HA	1.67	0.60
1:E:101:ALA:O	1:E:105:GLY:N	2.34	0.60
1:A:137:LEU:H	1:A:165:ARG:NH1	1.99	0.60
1:E:160:ARG:HD2	1:E:161:ARG:NH1	2.17	0.60
1:A:165:ARG:HB3	1:A:165:ARG:HH21	1.66	0.60
1:C:338:THR:HB	2:C:401:MES:H71	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:SER:N	6:D:660:HOH:O	2.35	0.60
1:H:116:ARG:NH2	1:H:135:PRO:O	2.35	0.60
6:F:607:HOH:O	1:G:3:GLY:HA3	2.02	0.60
1:E:214:ASP:OD1	6:E:644:HOH:O	2.16	0.60
1:F:5:ARG:O	1:F:9:ARG:HG2	2.01	0.60
1:H:180:LEU:HD22	1:H:294:ALA:HB3	1.82	0.60
1:G:89:PRO:HB3	1:G:113:GLN:O	2.01	0.60
1:A:33:THR:HA	6:A:690:HOH:O	2.02	0.60
1:C:371:GLU:OE1	6:C:631:HOH:O	2.16	0.60
1:D:88:ARG:H	1:D:91:GLN:NE2	2.00	0.60
1:D:280:PRO:HA	1:D:285:HIS:CD2	2.37	0.60
1:A:36:ARG:HB2	1:A:36:ARG:CZ	2.32	0.60
1:B:351:GLY:O	6:B:623:HOH:O	2.16	0.60
1:F:21:THR:OG1	1:F:23:ASP:OD1	2.16	0.60
1:C:347:ARG:HB3	1:C:352:ILE:HB	1.84	0.60
1:A:214:ASP:OD2	1:A:216:ASP:N	2.34	0.60
1:B:236:ASP:OD1	6:B:599:HOH:O	2.16	0.60
1:E:16:ARG:HH11	1:E:16:ARG:HB3	1.66	0.60
1:A:213:ARG:HB3	3:A:404:GOL:H32	1.84	0.60
1:E:343:SER:O	1:E:347:ARG:NH1	2.35	0.60
1:A:259:ARG:NH1	6:A:586:HOH:O	2.06	0.60
1:D:344:ALA:HA	1:D:347:ARG:HG3	1.83	0.60
1:B:5:ARG:NH1	1:C:368:ASP:OD1	2.35	0.60
1:G:156:ALA:O	1:G:160:ARG:HG3	2.02	0.60
1:G:39:GLN:HA	6:G:678:HOH:O	2.02	0.60
1:H:320:CYS:SG	1:H:337:MSE:HE1	2.41	0.60
1:H:340:ARG:O	1:H:342:LEU:N	2.35	0.60
1:F:36:ARG:O	1:F:38:ALA:N	2.34	0.59
1:H:116:ARG:NH2	1:H:134:GLU:OE1	2.30	0.59
1:F:134:GLU:O	1:F:165:ARG:NH1	2.31	0.59
1:E:160:ARG:NH2	6:E:675:HOH:O	2.10	0.59
2:G:401:MES:H52	1:H:46:TYR:CD2	2.37	0.59
1:H:100:TYR:CE1	2:H:401:MES:H71	2.36	0.59
1:C:283:PRO:HB2	1:C:284:GLN:NE2	2.16	0.59
1:H:134:GLU:O	1:H:165:ARG:NH1	2.34	0.59
1:E:354:GLU:O	1:E:355:SER:OG	2.20	0.59
1:E:16:ARG:CZ	6:E:667:HOH:O	2.50	0.59
1:F:42:PRO:O	6:F:618:HOH:O	2.16	0.59
1:G:152:VAL:HG11	1:G:288:VAL:HG23	1.85	0.59
1:H:147:ASN:ND2	1:H:358:ARG:HH11	2.01	0.59
1:B:264:ARG:NH1	6:B:618:HOH:O	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:TYR:HE1	2:C:401:MES:H82	1.68	0.59
1:H:137:LEU:H	1:H:165:ARG:HH11	1.48	0.59
1:G:197:LLP:O3	6:G:541:HOH:O	2.16	0.59
1:A:17:PRO:O	3:A:403:GOL:O1	2.20	0.59
1:G:319:THR:HB	1:G:330:LEU:HD23	1.84	0.59
1:A:213:ARG:NH1	3:A:404:GOL:O2	2.36	0.59
1:G:16:ARG:O	1:G:18:SER:N	2.35	0.59
1:D:88:ARG:H	1:D:91:GLN:NE2	2.00	0.59
1:D:92:CYS:HB2	1:D:116:ARG:NE	2.17	0.59
1:E:309:GLU:H	1:E:309:GLU:CD	2.06	0.59
1:C:381:THR:OG1	6:C:637:HOH:O	2.15	0.59
1:E:40:ASP:O	1:E:42:PRO:HD3	2.02	0.59
1:E:332:GLU:OE2	1:E:358:ARG:NH2	2.35	0.59
1:C:31:SER:HB3	1:C:34:TYR:CE2	2.38	0.59
1:B:277:PRO:HA	1:B:282:HIS:CD2	2.37	0.59
1:B:326:GLY:HA3	6:B:666:HOH:O	2.02	0.59
1:D:124:THR:HG23	1:D:127:GLY:H	1.67	0.59
1:A:347:ARG:HG2	1:A:352:ILE:HB	1.84	0.59
1:A:132:LEU:HD12	1:A:137:LEU:HD21	1.83	0.59
1:G:313:ASP:HA	1:H:37:ARG:NH1	2.17	0.59
1:A:282:HIS:CG	1:A:283:PRO:HD2	2.38	0.59
1:D:112:ARG:HD2	6:D:670:HOH:O	2.01	0.59
1:G:14:GLY:HA2	1:G:59:GLU:OE1	2.02	0.59
1:B:4:MSE:O	1:B:5:ARG:HG3	2.02	0.59
1:C:19:ALA:O	1:C:21:THR:N	2.34	0.59
1:B:216:ASP:O	6:B:573:HOH:O	2.17	0.59
1:B:4:MSE:HB3	1:B:8:THR:HB	1.83	0.59
1:C:58:GLU:OE1	6:C:613:HOH:O	2.17	0.59
1:G:225:ARG:HG2	1:G:231:VAL:HG12	1.82	0.59
1:A:214:ASP:OD1	6:A:622:HOH:O	2.17	0.59
1:D:180:LEU:HD22	1:D:294:ALA:HB3	1.84	0.59
1:H:289:LYS:NZ	6:H:676:HOH:O	2.21	0.59
1:B:241:ARG:HA	1:B:244:LEU:HD12	1.84	0.59
3:G:403:GOL:H11	1:H:102:GLY:HA2	1.82	0.59
1:H:3:GLY:C	1:H:4:MSE:SE	2.90	0.59
1:B:15:ARG:HH21	1:B:15:ARG:HB2	1.67	0.59
1:B:283:PRO:HB2	1:B:284:GLN:OE1	2.03	0.59
1:C:116:ARG:NH1	1:C:134:GLU:HG2	2.17	0.59
1:E:39:GLN:NE2	1:G:21:THR:O	2.28	0.59
1:B:238:PHE:HA	6:B:604:HOH:O	2.03	0.59
1:F:60:CYS:SG	1:F:244:LEU:HD13	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ARG:HH12	1:A:66:ARG:NE	2.00	0.59
1:B:292:MSE:HE2	6:B:584:HOH:O	2.02	0.59
1:C:18:SER:OG	6:C:593:HOH:O	2.17	0.59
1:H:93:VAL:HG22	1:H:139:LEU:HB3	1.84	0.59
1:E:147:ASN:OD1	1:E:148:PRO:HA	2.02	0.59
1:H:253:ARG:NH1	6:H:664:HOH:O	2.34	0.59
1:H:36:ARG:NH2	6:H:677:HOH:O	2.35	0.59
1:E:8:THR:HG23	1:H:364:GLU:CG	2.33	0.59
1:H:259:ARG:HH12	1:H:295:PRO:CD	2.14	0.59
1:F:100:TYR:HE1	2:F:401:MES:H31	1.67	0.59
1:A:18:SER:N	6:A:578:HOH:O	2.21	0.59
1:A:32:THR:OG1	6:A:527:HOH:O	2.16	0.59
1:F:150:LEU:HD22	1:F:175:PHE:HE2	1.66	0.59
1:F:46:TYR:N	1:F:50:GLU:OE1	2.36	0.59
1:A:337:MSE:HG2	1:B:36:ARG:HH11	1.67	0.59
1:A:98:ASP:HA	1:A:350:ARG:HH21	1.68	0.59
1:E:16:ARG:HG2	6:E:668:HOH:O	2.01	0.59
1:E:333:CYS:O	1:E:336:LEU:N	2.27	0.59
1:G:354:GLU:HG2	6:G:666:HOH:O	2.01	0.59
1:B:322:VAL:HG23	1:B:323:SER:N	2.18	0.59
1:D:282:HIS:HB3	1:D:285:HIS:HB2	1.85	0.59
1:H:303:TYR:O	1:H:355:SER:OG	2.20	0.59
1:E:84:LEU:HD11	1:E:107:PHE:HD1	1.67	0.59
1:H:84:LEU:HD12	1:H:106:LEU:HB3	1.84	0.59
1:A:29:HIS:NE2	3:A:403:GOL:H2	2.17	0.59
1:C:112:ARG:HG3	1:C:112:ARG:HH21	1.68	0.59
1:E:84:LEU:HD11	1:E:107:PHE:HD1	1.66	0.59
1:C:33:THR:HA	6:C:670:HOH:O	2.02	0.59
1:D:319:THR:HB	1:D:330:LEU:HD23	1.83	0.59
1:E:89:PRO:HB3	1:E:114:GLY:HA3	1.85	0.59
1:H:9:ARG:HH11	1:H:66:ARG:HD3	1.68	0.59
1:B:364:GLU:HB3	1:C:8:THR:HG23	1.84	0.59
1:B:365:ASP:OD2	1:B:366:PRO:HD2	2.03	0.59
1:G:160:ARG:HG3	1:G:161:ARG:HE	1.67	0.59
1:G:340:ARG:O	1:G:342:LEU:N	2.31	0.59
1:B:66:ARG:HH21	1:B:66:ARG:CG	2.16	0.59
1:D:39:GLN:HB3	1:D:42:PRO:HB3	1.84	0.59
1:C:95:SER:O	1:C:120:ALA:N	2.35	0.59
1:B:92:CYS:HB3	1:B:137:LEU:HA	1.85	0.59
1:C:43:ARG:NH1	6:C:672:HOH:O	2.36	0.59
1:B:6:PHE:HB2	1:B:9:ARG:NH1	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:LEU:HD13	1:H:235:LEU:HD13	1.84	0.59
1:F:340:ARG:NH1	6:F:684:HOH:O	2.36	0.59
1:H:180:LEU:HD22	1:H:294:ALA:HB3	1.85	0.59
1:A:92:CYS:HA	1:A:116:ARG:HB2	1.84	0.59
1:F:123:THR:O	1:F:123:THR:OG1	2.16	0.59
1:G:233:GLY:HA3	6:H:667:HOH:O	2.03	0.59
1:F:292:MSE:HE2	6:F:598:HOH:O	2.01	0.59
1:B:225:ARG:HG2	1:B:231:VAL:HG22	1.85	0.59
1:D:98:ASP:OD1	1:D:98:ASP:N	2.35	0.59
1:E:345:GLU:O	1:E:348:ALA:N	2.36	0.59
1:B:131:ALA:O	1:B:133:ALA:N	2.35	0.59
1:D:107:PHE:O	1:D:111:ALA:N	2.33	0.59
1:G:259:ARG:HD3	6:G:668:HOH:O	2.01	0.59
1:F:279:LEU:HD22	6:F:504:HOH:O	2.03	0.59
1:H:97:ASP:HB3	1:H:119:TYR:HB3	1.84	0.59
1:A:189:ASP:HA	1:A:213:ARG:HH22	1.68	0.59
1:F:340:ARG:HA	1:F:347:ARG:HH12	1.68	0.59
1:F:340:ARG:HA	1:F:347:ARG:NH1	2.18	0.59
1:F:316:THR:OG1	1:F:375:ARG:NH1	2.36	0.59
1:G:157:GLU:OE2	1:G:160:ARG:NH1	2.34	0.59
1:D:94:VAL:HA	1:D:118:ARG:O	2.02	0.58
1:A:174:THR:HB	1:A:197:LLP:H2'2	1.85	0.58
1:C:17:PRO:HD2	6:C:658:HOH:O	2.03	0.58
1:E:96:THR:HB	1:E:98:ASP:OD2	2.03	0.58
1:H:285:HIS:CE1	6:H:659:HOH:O	2.56	0.58
1:F:197:LLP:HB2	1:F:324:LEU:HD12	1.85	0.58
1:H:100:TYR:OH	2:H:401:MES:H62	2.03	0.58
1:C:96:THR:O	1:C:99:VAL:HG13	2.03	0.58
1:E:314:ARG:NE	1:E:376:ALA:O	2.26	0.58
1:B:213:ARG:NH2	6:B:572:HOH:O	2.35	0.58
1:E:160:ARG:NH2	6:E:610:HOH:O	2.36	0.58
1:B:174:THR:O	6:B:530:HOH:O	2.17	0.58
1:F:90:GLY:N	1:F:114:GLY:O	2.29	0.58
1:G:4:MSE:CE	6:G:684:HOH:O	2.50	0.58
1:C:181:GLN:HG3	1:C:292:MSE:CG	2.33	0.58
1:D:35:GLU:OE2	1:D:37:ARG:NH2	2.34	0.58
1:E:332:GLU:OE1	1:E:358:ARG:NH2	2.36	0.58
1:G:147:ASN:HD21	1:G:358:ARG:NH1	2.01	0.58
1:C:233:GLY:O	1:C:236:ASP:HB3	2.02	0.58
1:E:116:ARG:NE	6:E:613:HOH:O	2.36	0.58
1:B:19:ALA:O	1:B:21:THR:N	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:ARG:NE	1:D:370:ALA:HB1	2.18	0.58
1:F:121:ASP:O	1:F:122:LEU:HG	2.02	0.58
1:A:213:ARG:NH1	3:A:404:GOL:O2	2.34	0.58
1:E:90:GLY:C	1:E:116:ARG:HE	2.06	0.58
1:F:300:SER:HB2	1:F:356:LEU:HD11	1.85	0.58
1:G:116:ARG:HD3	6:G:501:HOH:O	2.04	0.58
1:A:122:LEU:HA	1:A:128:ILE:HG13	1.84	0.58
1:A:322:VAL:HG13	1:B:36:ARG:HH22	1.69	0.58
1:E:367:GLN:NE2	6:E:613:HOH:O	2.35	0.58
1:E:315:PHE:HB2	1:F:37:ARG:HH12	1.68	0.58
1:C:96:THR:HA	1:C:120:ALA:O	2.02	0.58
1:B:36:ARG:HB2	1:B:36:ARG:HH21	1.67	0.58
1:E:92:CYS:SG	1:E:134:GLU:HG2	2.43	0.58
1:B:6:PHE:HA	1:B:9:ARG:NE	2.06	0.58
1:H:266:ARG:NE	6:H:504:HOH:O	2.33	0.58
1:G:214:ASP:HB3	1:G:217:LEU:HB3	1.84	0.58
1:E:347:ARG:HB2	1:E:352:ILE:HB	1.84	0.58
1:H:3:GLY:O	1:H:4:MSE:SE	2.72	0.58
1:B:91:GLN:HA	1:B:136:ASP:HB3	1.85	0.58
1:F:189:ASP:HB3	5:F:407:CL:CL	2.41	0.58
1:F:84:LEU:HD13	1:F:110:ALA:HB2	1.85	0.58
1:G:213:ARG:HE	3:G:402:GOL:H11	1.68	0.58
1:H:213:ARG:NE	3:H:402:GOL:O2	2.31	0.58
1:F:291:GLN:HE21	1:F:292:MSE:HE2	1.68	0.58
1:H:43:ARG:NH1	1:H:44:TYR:OH	2.36	0.58
1:A:124:THR:OG1	1:A:126:GLU:OE1	2.20	0.58
1:F:173:ASN:HB3	1:F:193:TYR:CE1	2.38	0.58
1:F:54:ARG:NH1	6:F:652:HOH:O	2.17	0.58
1:G:354:GLU:HG2	6:G:618:HOH:O	2.04	0.58
1:C:88:ARG:NH2	6:C:503:HOH:O	2.35	0.58
1:F:259:ARG:HH21	1:F:295:PRO:HD3	1.68	0.58
1:G:254:GLN:NE2	1:G:325:GLY:O	2.32	0.58
1:C:350:ARG:NH1	6:C:646:HOH:O	2.28	0.58
1:E:143:GLU:HG3	1:E:172:ASP:HB3	1.86	0.58
1:E:96:THR:O	1:E:99:VAL:HG13	2.04	0.58
1:G:6:PHE:HA	1:G:9:ARG:HG3	1.84	0.58
1:A:128:ILE:O	1:A:131:ALA:HB3	2.04	0.58
1:F:364:GLU:HB3	1:G:8:THR:HG23	1.86	0.58
1:F:40:ASP:N	6:F:672:HOH:O	2.36	0.58
1:B:160:ARG:HG3	6:B:691:HOH:O	2.03	0.58
1:D:88:ARG:H	1:D:91:GLN:NE2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:ARG:NH1	1:G:59:GLU:OE1	2.37	0.58
1:F:94:VAL:HG22	1:F:118:ARG:HB3	1.85	0.58
1:E:338:THR:O	1:E:341:PRO:HD2	2.03	0.58
1:C:380:GLY:HA2	6:C:506:HOH:O	2.02	0.58
1:D:88:ARG:H	1:D:91:GLN:HE21	1.50	0.58
1:C:16:ARG:HB2	1:C:17:PRO:CD	2.34	0.58
1:G:113:GLN:HE21	1:H:113:GLN:CD	2.06	0.58
1:H:109:LEU:O	1:H:113:GLN:N	2.35	0.58
1:H:180:LEU:HD22	1:H:294:ALA:HB3	1.85	0.58
1:G:336:LEU:CB	1:G:337:MSE:HE2	2.32	0.58
1:F:282:HIS:O	1:F:285:HIS:HB2	2.04	0.58
1:G:96:THR:OG1	6:G:1434:HOH:O	2.17	0.58
1:D:291:GLN:HG3	1:D:292:MSE:CG	2.33	0.58
1:E:282:HIS:HB3	1:E:285:HIS:HB2	1.84	0.58
1:F:94:VAL:HG11	1:F:131:ALA:HB1	1.85	0.58
1:E:119:TYR:OH	6:E:621:HOH:O	2.13	0.58
1:E:65:GLU:HG3	1:E:211:VAL:HG11	1.85	0.58
1:A:116:ARG:HE	1:E:112:ARG:HA	1.68	0.58
1:A:43:ARG:NH1	6:A:680:HOH:O	2.36	0.58
1:A:337:MSE:HG2	6:A:577:HOH:O	2.03	0.58
1:B:152:VAL:H	1:B:284:GLN:NE2	2.02	0.58
1:F:23:ASP:OD2	1:H:29:HIS:ND1	2.35	0.58
1:A:347:ARG:O	1:A:351:GLY:N	2.37	0.58
1:D:6:PHE:HA	1:D:9:ARG:HG2	1.86	0.58
1:B:9:ARG:HD3	6:B:683:HOH:O	2.04	0.58
1:E:347:ARG:NH2	6:E:648:HOH:O	2.03	0.58
1:C:213:ARG:HH21	3:C:403:GOL:H31	1.69	0.58
1:D:104:ASP:HA	1:D:107:PHE:HB2	1.85	0.58
1:F:134:GLU:O	1:F:165:ARG:NH1	2.34	0.58
1:A:332:GLU:HG2	1:A:358:ARG:HB3	1.86	0.58
1:E:177:SER:HB2	1:E:178:PRO:HD2	1.85	0.58
1:H:180:LEU:HB3	1:H:292:MSE:CE	2.34	0.58
1:D:35:GLU:HG2	1:D:37:ARG:H	1.69	0.58
1:A:91:GLN:HA	1:A:136:ASP:HB3	1.86	0.58
1:F:340:ARG:O	6:F:611:HOH:O	2.17	0.58
1:A:214:ASP:OD1	6:A:621:HOH:O	2.17	0.58
1:D:213:ARG:HG2	6:D:653:HOH:O	2.02	0.58
1:G:322:VAL:O	1:H:33:THR:HG21	2.03	0.58
1:H:137:LEU:HB3	1:H:165:ARG:HE	1.67	0.58
1:A:253:ARG:HD3	6:A:670:HOH:O	2.03	0.58
1:B:368:ASP:OD2	1:C:5:ARG:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:HG21	1:A:235:LEU:HD23	1.86	0.58
1:C:372:ASP:HA	1:C:375:ARG:HH22	1.68	0.58
1:F:332:GLU:HB2	1:F:337:MSE:SE	2.53	0.58
1:B:334:PRO:HA	1:B:338:THR:OG1	2.03	0.58
1:E:104:ASP:OD2	6:E:605:HOH:O	2.17	0.58
1:E:35:GLU:OE2	1:E:38:ALA:N	2.36	0.58
1:H:100:TYR:CE1	2:H:401:MES:H82	2.38	0.58
1:D:43:ARG:O	1:D:50:GLU:HG2	2.03	0.58
1:C:148:PRO:HD3	1:C:339:HIS:CE1	2.39	0.58
1:E:16:ARG:NE	6:E:666:HOH:O	2.36	0.58
1:H:133:ALA:C	1:H:165:ARG:HH11	2.07	0.58
1:E:100:TYR:HE1	2:E:401:MES:H31	1.69	0.57
1:H:89:PRO:HB3	1:H:114:GLY:HA3	1.86	0.57
1:A:116:ARG:NH2	1:A:136:ASP:OD2	2.37	0.57
1:C:16:ARG:HD3	1:C:56:GLU:HG2	1.84	0.57
1:D:333:CYS:HB3	1:D:336:LEU:HB2	1.86	0.57
1:E:96:THR:HG21	1:E:143:GLU:H	1.68	0.57
1:E:288:VAL:HG13	1:E:292:MSE:HE1	1.86	0.57
1:A:131:ALA:C	1:A:133:ALA:H	2.07	0.57
1:A:259:ARG:NH2	6:A:649:HOH:O	2.37	0.57
1:D:371:GLU:O	1:D:375:ARG:HB2	2.04	0.57
1:G:333:CYS:HB3	1:G:337:MSE:CE	2.34	0.57
1:D:41:GLU:N	6:D:654:HOH:O	2.31	0.57
1:F:340:ARG:O	6:F:585:HOH:O	2.17	0.57
2:C:401:MES:H61	1:D:46:TYR:CG	2.38	0.57
1:E:131:ALA:O	1:E:134:GLU:HG2	2.04	0.57
1:E:180:LEU:HD22	1:E:294:ALA:HB3	1.86	0.57
1:E:46:TYR:CD2	2:F:401:MES:H61	2.39	0.57
1:D:371:GLU:O	1:D:375:ARG:HD3	2.04	0.57
1:F:188:ALA:O	1:F:213:ARG:NH1	2.34	0.57
1:F:18:SER:OG	6:F:566:HOH:O	2.17	0.57
1:A:54:ARG:NH1	6:A:662:HOH:O	2.28	0.57
1:D:250:ARG:C	1:D:254:GLN:HE21	2.06	0.57
1:F:35:GLU:OE2	1:F:37:ARG:NH2	2.37	0.57
1:B:350:ARG:NH1	6:B:680:HOH:O	2.36	0.57
1:A:4:MSE:HG3	6:A:566:HOH:O	2.04	0.57
1:B:5:ARG:HB2	1:C:365:ASP:CG	2.24	0.57
1:A:112:ARG:NH2	1:E:135:PRO:HG3	2.19	0.57
1:F:180:LEU:HD22	1:F:294:ALA:HB3	1.86	0.57
1:A:292:MSE:HE2	1:A:295:PRO:HA	1.87	0.57
1:F:54:ARG:NH1	1:F:232:PRO:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:401:MES:H61	1:H:46:TYR:CD2	2.40	0.57
1:A:168:ARG:NE	4:A:405:CL:CL	2.59	0.57
1:E:46:TYR:CD2	2:F:401:MES:H61	2.38	0.57
1:A:59:GLU:O	6:A:664:HOH:O	2.17	0.57
1:H:174:THR:HB	1:H:197:LLP:H2'2	1.85	0.57
1:B:95:SER:OG	1:B:96:THR:N	2.37	0.57
1:C:94:VAL:HG21	1:C:131:ALA:HB1	1.85	0.57
1:G:320:CYS:SG	1:H:36:ARG:NH2	2.78	0.57
1:E:368:ASP:OD1	1:H:5:ARG:NH1	2.38	0.57
1:G:333:CYS:O	1:G:337:MSE:HE3	2.05	0.57
1:B:152:VAL:H	1:B:284:GLN:HE21	1.52	0.57
1:B:288:VAL:HA	1:B:292:MSE:HE1	1.86	0.57
1:B:95:SER:OG	1:B:96:THR:N	2.36	0.57
1:G:197:LLP:CE	1:G:323:SER:HB2	2.34	0.57
1:A:266:ARG:NH2	1:A:281:GLU:OE1	2.37	0.57
1:G:152:VAL:HG13	1:G:284:GLN:HB2	1.87	0.57
1:C:198:SER:HB3	6:C:542:HOH:O	2.03	0.57
1:C:32:THR:HG22	1:D:206:LEU:HD23	1.85	0.57
1:H:59:GLU:HG3	6:H:684:HOH:O	2.03	0.57
1:A:74:SER:OG	1:B:231:VAL:O	2.22	0.57
1:F:137:LEU:HB3	1:F:165:ARG:NH1	2.19	0.57
1:C:288:VAL:O	1:C:292:MSE:HB3	2.03	0.57
1:A:199:ILE:CG2	1:A:244:LEU:HD21	2.35	0.57
1:C:94:VAL:HG11	1:C:131:ALA:HB1	1.86	0.57
1:E:321:GLY:N	1:E:337:MSE:HE1	2.19	0.57
1:B:16:ARG:NH1	1:B:56:GLU:HG3	2.19	0.57
1:A:9:ARG:HD3	6:A:679:HOH:O	2.03	0.57
1:C:147:ASN:HD21	1:C:358:ARG:NH1	1.93	0.57
1:A:44:TYR:CD2	1:C:21:THR:HA	2.39	0.57
1:D:264:ARG:NH1	6:D:614:HOH:O	2.17	0.57
1:C:302:ASP:OD2	6:C:529:HOH:O	2.17	0.57
1:H:42:PRO:HB2	1:H:45:PHE:CZ	2.39	0.57
1:E:314:ARG:NH1	1:E:378:ALA:HB3	2.20	0.57
1:A:36:ARG:NH2	1:B:337:MSE:HG2	2.18	0.57
1:B:134:GLU:O	1:B:165:ARG:NH1	2.37	0.57
1:B:334:PRO:HA	1:B:338:THR:HG1	1.68	0.57
1:B:339:HIS:HA	1:B:341:PRO:HD2	1.87	0.57
2:C:401:MES:H51	2:C:401:MES:O2S	2.04	0.57
1:E:128:ILE:O	1:E:132:LEU:HB2	2.05	0.57
1:F:95:SER:OG	1:F:96:THR:N	2.37	0.57
1:F:4:MSE:SE	6:F:648:HOH:O	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:THR:HB	1:B:330:LEU:HD23	1.85	0.57
1:D:279:LEU:C	1:D:281:GLU:H	2.07	0.57
1:D:149:LEU:HD21	1:D:351:GLY:HA3	1.85	0.57
1:F:277:PRO:CB	1:F:292:MSE:HE1	2.33	0.57
1:G:19:ALA:O	1:G:21:THR:N	2.37	0.57
1:F:39:GLN:NE2	1:F:44:TYR:O	2.35	0.57
1:H:147:ASN:ND2	1:H:358:ARG:HH11	2.01	0.57
1:B:4:MSE:HB3	6:B:654:HOH:O	2.05	0.57
1:C:18:SER:OG	6:C:580:HOH:O	2.18	0.57
1:B:336:LEU:O	1:B:340:ARG:HD2	2.04	0.57
1:B:317:LEU:HD11	1:B:364:GLU:HG2	1.86	0.57
1:A:16:ARG:NH2	1:A:59:GLU:OE1	2.35	0.57
1:A:83:LEU:HD13	1:A:210:LEU:HD13	1.85	0.57
1:H:108:ASP:OD2	6:H:622:HOH:O	2.17	0.57
1:E:322:VAL:HB	2:E:401:MES:H72	1.87	0.57
1:B:14:GLY:O	1:B:16:ARG:N	2.37	0.57
1:F:11:VAL:HA	1:F:245:HIS:ND1	2.19	0.57
1:F:338:THR:HG23	1:F:339:HIS:CD2	2.36	0.57
1:G:292:MSE:SE	1:G:294:ALA:C	2.93	0.57
1:F:6:PHE:HE2	1:F:179:VAL:HG22	1.70	0.57
1:D:112:ARG:NH2	6:D:588:HOH:O	2.36	0.57
1:F:104:ASP:HA	1:F:107:PHE:HB2	1.85	0.57
1:A:180:LEU:HD22	1:A:294:ALA:HB3	1.87	0.57
1:D:313:ASP:OD1	6:D:501:HOH:O	2.16	0.57
1:F:249:LEU:HD23	3:F:404:GOL:H2	1.86	0.57
1:G:342:LEU:HD11	6:G:1460:HOH:O	2.03	0.57
1:B:332:GLU:OE2	1:B:338:THR:OG1	2.21	0.57
1:E:321:GLY:O	1:E:337:MSE:HE1	2.05	0.57
1:D:4:MSE:SE	1:D:5:ARG:HG3	2.55	0.57
1:C:116:ARG:HH11	1:C:134:GLU:HG2	1.69	0.57
1:C:180:LEU:HD22	1:C:294:ALA:HB3	1.87	0.57
1:F:143:GLU:HG3	1:F:172:ASP:HB3	1.87	0.57
1:A:337:MSE:HE1	1:B:36:ARG:CZ	2.32	0.57
1:D:96:THR:HA	1:D:120:ALA:H	1.70	0.57
1:F:180:LEU:HD22	1:F:294:ALA:HB3	1.86	0.57
3:F:403:GOL:H11	1:G:253:ARG:HD3	1.87	0.57
1:H:100:TYR:HE1	2:H:401:MES:H71	1.70	0.57
1:B:225:ARG:HG2	1:B:231:VAL:HG12	1.85	0.57
1:E:336:LEU:HB2	1:E:337:MSE:SE	2.55	0.57
1:G:262:VAL:HG11	1:G:279:LEU:HD21	1.86	0.57
1:G:367:GLN:O	1:G:371:GLU:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:GLU:OE2	1:H:37:ARG:NH2	2.37	0.57
1:F:339:HIS:HB2	1:F:347:ARG:HD3	1.87	0.57
1:G:375:ARG:HG3	6:G:686:HOH:O	2.04	0.57
1:B:259:ARG:NH1	6:B:654:HOH:O	2.37	0.57
1:G:233:GLY:HA3	6:H:653:HOH:O	2.03	0.57
1:H:118:ARG:NH1	1:H:134:GLU:OE2	2.34	0.57
1:H:197:LLP:HD2	1:H:324:LEU:HG	1.87	0.57
1:A:205:VAL:HG23	1:A:236:ASP:HB3	1.87	0.57
1:B:66:ARG:NH2	6:B:648:HOH:O	2.27	0.57
1:B:95:SER:HB2	1:B:141:TRP:HB3	1.87	0.57
1:A:242:ARG:NE	1:D:204:ASP:OD2	2.25	0.57
1:E:111:ALA:HA	1:E:115:VAL:O	2.05	0.57
1:E:104:ASP:OD1	1:E:119:TYR:OH	2.22	0.57
1:A:157:GLU:OE2	1:A:161:ARG:HD3	2.05	0.57
1:B:26:PRO:HB3	3:B:404:GOL:H2	1.87	0.57
1:C:16:ARG:NH1	1:C:59:GLU:OE1	2.38	0.57
1:G:16:ARG:HA	1:G:16:ARG:HE	1.70	0.57
1:C:277:PRO:O	1:C:288:VAL:HG11	2.05	0.57
1:F:236:ASP:OD2	6:F:589:HOH:O	2.17	0.57
1:H:134:GLU:O	1:H:165:ARG:NH1	2.37	0.57
1:H:320:CYS:SG	1:H:337:MSE:HE1	2.44	0.57
1:H:346:ALA:HA	1:H:349:ARG:HB2	1.86	0.57
1:C:182:GLN:OE1	6:C:621:HOH:O	2.18	0.56
1:D:338:THR:OG1	1:D:338:THR:O	2.22	0.56
1:E:86:LEU:HD13	3:E:403:GOL:H11	1.86	0.56
1:A:95:SER:OG	1:A:96:THR:N	2.38	0.56
1:D:132:LEU:HB2	1:D:165:ARG:HG3	1.87	0.56
1:G:36:ARG:NH2	4:H:406:CL:CL	2.72	0.56
1:E:340:ARG:HG3	6:E:650:HOH:O	2.05	0.56
1:B:95:SER:HB2	1:B:141:TRP:HB3	1.86	0.56
1:F:253:ARG:NH1	3:F:405:GOL:O1	2.37	0.56
1:G:134:GLU:O	1:G:165:ARG:NH2	2.36	0.56
1:C:160:ARG:O	6:C:564:HOH:O	2.17	0.56
1:A:35:GLU:OE1	1:B:319:THR:HG23	2.05	0.56
1:E:280:PRO:HA	1:E:285:HIS:CE1	2.40	0.56
1:G:40:ASP:N	6:G:667:HOH:O	2.38	0.56
1:B:9:ARG:NE	6:B:670:HOH:O	2.38	0.56
1:C:160:ARG:O	6:C:548:HOH:O	2.16	0.56
1:E:345:GLU:OE2	1:E:349:ARG:NH1	2.38	0.56
1:E:254:GLN:OE1	6:E:566:HOH:O	2.18	0.56
1:B:16:ARG:NH1	3:B:405:GOL:H12	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:ASP:OD2	1:G:146:THR:HB	2.05	0.56
1:G:322:VAL:HG21	1:H:46:TYR:HB2	1.87	0.56
1:D:335:ALA:HA	1:D:347:ARG:HD3	1.87	0.56
1:A:337:MSE:HE3	1:B:36:ARG:CZ	2.35	0.56
1:A:333:CYS:HB3	1:A:336:LEU:HD12	1.87	0.56
1:G:323:SER:OG	1:G:324:LEU:N	2.38	0.56
1:H:180:LEU:HD22	1:H:294:ALA:HB3	1.87	0.56
1:B:345:GLU:HA	1:B:348:ALA:HB3	1.87	0.56
1:D:175:PHE:CZ	1:D:298:ILE:HB	2.41	0.56
1:G:4:MSE:HB2	1:G:8:THR:HB	1.86	0.56
1:A:44:TYR:OH	1:A:55:GLU:OE2	2.19	0.56
1:E:27:PRO:HB2	1:G:27:PRO:HB2	1.88	0.56
1:A:37:ARG:NH2	1:B:315:PHE:O	2.36	0.56
1:G:125:PRO:HA	1:G:128:ILE:HD12	1.87	0.56
1:G:195:THR:HA	1:G:199:ILE:HB	1.87	0.56
1:E:27:PRO:HB2	1:G:27:PRO:HB2	1.86	0.56
1:G:98:ASP:N	1:G:98:ASP:OD1	2.32	0.56
1:H:96:THR:C	1:H:119:TYR:HD2	2.09	0.56
1:B:11:VAL:HG13	1:C:327:VAL:HG13	1.87	0.56
1:C:39:GLN:HB2	1:C:42:PRO:HA	1.87	0.56
1:H:253:ARG:HD3	6:H:542:HOH:O	2.04	0.56
1:B:116:ARG:HH21	1:B:134:GLU:HB3	1.69	0.56
1:F:35:GLU:OE2	1:F:37:ARG:HD3	2.05	0.56
1:C:107:PHE:HB3	1:C:117:VAL:HG21	1.87	0.56
1:E:96:THR:O	1:E:96:THR:OG1	2.23	0.56
1:H:84:LEU:HG	1:H:141:TRP:CZ3	2.40	0.56
1:F:39:GLN:OE1	1:F:44:TYR:N	2.32	0.56
1:G:15:ARG:O	1:G:17:PRO:HD2	2.06	0.56
1:C:253:ARG:NH1	6:C:595:HOH:O	2.38	0.56
1:F:92:CYS:HB2	1:F:116:ARG:NH1	2.20	0.56
1:A:206:LEU:HD11	1:B:48:ARG:HB2	1.87	0.56
1:E:339:HIS:HB3	1:E:342:LEU:HB2	1.87	0.56
1:F:16:ARG:HD3	1:F:56:GLU:HG2	1.88	0.56
1:C:333:CYS:H	1:C:337:MSE:SE	2.37	0.56
1:G:11:VAL:HA	1:G:245:HIS:ND1	2.21	0.56
1:A:100:TYR:N	1:A:143:GLU:OE1	2.38	0.56
1:A:322:VAL:HB	2:A:401:MES:H71	1.85	0.56
3:G:404:GOL:O1	3:G:404:GOL:O3	2.16	0.56
1:D:36:ARG:NH2	6:D:622:HOH:O	2.39	0.56
1:E:116:ARG:NH2	1:E:136:ASP:HB2	2.20	0.56
1:B:6:PHE:CE2	1:B:179:VAL:HG22	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:MSE:HB2	6:C:570:HOH:O	2.05	0.56
1:H:35:GLU:OE2	1:H:37:ARG:HB2	2.06	0.56
1:F:277:PRO:HA	1:F:282:HIS:CD2	2.40	0.56
1:C:277:PRO:HA	1:C:282:HIS:CD2	2.41	0.56
1:D:18:SER:HB2	6:D:604:HOH:O	2.04	0.56
1:G:197:LLP:O3	6:G:539:HOH:O	2.18	0.56
1:D:367:GLN:O	1:D:371:GLU:HG3	2.06	0.56
1:D:40:ASP:O	6:D:642:HOH:O	2.18	0.56
1:E:199:ILE:HG23	1:E:244:LEU:HD21	1.87	0.56
1:F:321:GLY:O	1:F:337:MSE:HE1	2.05	0.56
1:E:116:ARG:NH2	1:E:136:ASP:OD2	2.38	0.56
1:H:18:SER:HB2	1:H:23:ASP:HB2	1.87	0.56
1:H:323:SER:OG	1:H:324:LEU:N	2.38	0.56
1:B:107:PHE:HB3	1:B:117:VAL:HG11	1.86	0.56
1:D:97:ASP:HB2	6:D:606:HOH:O	2.06	0.56
1:C:143:GLU:OE2	6:C:579:HOH:O	2.18	0.56
1:C:330:LEU:HB2	1:C:360:SER:HB3	1.87	0.56
1:F:4:MSE:CE	1:F:4:MSE:HA	2.29	0.56
1:A:23:ASP:O	6:A:578:HOH:O	2.18	0.56
1:B:36:ARG:O	1:B:39:GLN:HG2	2.05	0.56
1:A:56:GLU:OE2	3:A:403:GOL:O3	2.24	0.56
1:H:34:TYR:OH	6:H:594:HOH:O	2.16	0.56
1:A:328:HIS:O	1:A:330:LEU:HD12	2.06	0.56
1:A:368:ASP:OD1	1:D:4:MSE:SE	2.74	0.56
1:A:116:ARG:HH22	1:A:135:PRO:HG2	1.71	0.56
1:A:97:ASP:O	1:A:99:VAL:N	2.39	0.56
6:G:647:HOH:O	1:H:33:THR:HG23	2.06	0.56
1:D:131:ALA:O	1:D:134:GLU:HG2	2.06	0.56
1:C:116:ARG:NH2	6:C:501:HOH:O	2.38	0.56
1:C:358:ARG:NH1	2:C:401:MES:O3S	2.39	0.56
1:F:74:SER:HA	1:F:232:PRO:HB3	1.88	0.56
1:G:371:GLU:HB3	1:G:375:ARG:NH2	2.21	0.56
1:F:121:ASP:O	1:F:122:LEU:HD23	2.04	0.56
1:D:9:ARG:NH2	1:D:66:ARG:HG3	2.21	0.56
1:A:342:LEU:HD22	1:A:343:SER:N	2.20	0.56
1:C:147:ASN:ND2	1:C:358:ARG:HH11	1.95	0.56
1:E:242:ARG:NH1	6:E:519:HOH:O	2.30	0.56
1:E:249:LEU:HG	6:E:680:HOH:O	2.06	0.56
1:B:254:GLN:OE1	6:B:641:HOH:O	2.18	0.56
1:D:291:GLN:O	6:D:512:HOH:O	2.18	0.56
1:E:348:ALA:CB	6:E:694:HOH:O	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:GLY:O	1:H:4:MSE:SE	2.74	0.56
1:H:6:PHE:CD1	1:H:9:ARG:NH1	2.74	0.56
1:A:24:VAL:HB	1:C:33:THR:HG23	1.86	0.56
1:C:34:TYR:HD2	1:C:45:PHE:O	1.89	0.56
1:B:288:VAL:HG22	1:B:292:MSE:CE	2.36	0.56
1:D:322:VAL:HG11	1:D:338:THR:HG23	1.87	0.56
1:D:97:ASP:HA	1:D:119:TYR:HB3	1.87	0.56
1:D:104:ASP:OD1	1:D:119:TYR:OH	2.15	0.56
1:H:101:ALA:O	1:H:105:GLY:N	2.38	0.56
1:A:116:ARG:HH21	1:A:136:ASP:HB2	1.70	0.56
1:A:213:ARG:NH2	6:A:567:HOH:O	2.26	0.56
1:B:339:HIS:N	6:B:668:HOH:O	2.21	0.56
1:C:334:PRO:HA	1:C:338:THR:HG23	1.87	0.56
1:C:342:LEU:O	1:C:347:ARG:NH1	2.38	0.56
1:D:134:GLU:O	1:D:165:ARG:NH1	2.38	0.56
1:B:252:HIS:O	1:B:253:ARG:HB3	2.06	0.56
1:B:151:THR:HB	1:B:284:GLN:HE22	1.70	0.56
1:D:375:ARG:HD2	6:D:646:HOH:O	2.06	0.56
1:D:44:TYR:OH	1:D:55:GLU:OE2	2.17	0.56
1:F:302:ASP:OD2	6:F:524:HOH:O	2.17	0.56
1:H:264:ARG:HG2	6:H:590:HOH:O	2.05	0.56
1:A:126:GLU:O	1:A:130:ALA:N	2.39	0.56
1:A:4:MSE:O	1:A:8:THR:HB	2.06	0.56
1:B:346:ALA:HB1	1:B:350:ARG:HE	1.71	0.56
1:C:14:GLY:HA2	1:C:59:GLU:OE1	2.06	0.56
1:E:26:PRO:HB2	6:E:671:HOH:O	2.06	0.56
1:A:165:ARG:HB3	1:A:165:ARG:NH2	2.21	0.56
1:G:259:ARG:NH1	6:G:1373:HOH:O	2.13	0.56
1:D:323:SER:OG	6:D:664:HOH:O	2.11	0.56
1:H:251:VAL:HA	1:H:254:GLN:NE2	2.17	0.56
1:A:124:THR:OG1	1:A:126:GLU:OE2	2.16	0.56
1:A:347:ARG:NH2	1:A:354:GLU:OE2	2.39	0.56
1:D:342:LEU:HD21	1:D:350:ARG:NH1	2.20	0.56
1:E:337:MSE:HG2	6:E:628:HOH:O	2.04	0.56
1:H:199:ILE:HG23	1:H:244:LEU:HG	1.87	0.56
1:H:213:ARG:NH2	6:H:565:HOH:O	2.38	0.56
1:F:123:THR:HG22	1:F:153:VAL:HG22	1.87	0.56
1:H:259:ARG:NH2	6:H:623:HOH:O	2.38	0.56
1:D:100:TYR:N	1:D:143:GLU:OE1	2.31	0.56
1:E:35:GLU:OE2	1:E:36:ARG:N	2.39	0.56
1:A:319:THR:HB	1:A:330:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:PHE:HA	1:A:9:ARG:NH1	2.21	0.56
1:H:245:HIS:HE1	6:H:533:HOH:O	1.86	0.56
1:B:16:ARG:NH1	6:B:677:HOH:O	2.39	0.56
1:F:309:GLU:HG3	1:F:336:LEU:HD13	1.87	0.56
1:G:213:ARG:NH2	3:G:402:GOL:O2	2.23	0.56
1:B:120:ALA:HB3	1:B:131:ALA:HB2	1.86	0.56
1:D:36:ARG:O	1:D:39:GLN:HB2	2.05	0.56
1:C:314:ARG:NH1	1:C:380:GLY:HA2	2.20	0.56
1:C:41:GLU:N	6:C:612:HOH:O	2.32	0.56
1:D:264:ARG:NH2	1:D:367:GLN:HE22	2.04	0.56
1:A:168:ARG:HH22	3:A:402:GOL:H31	1.71	0.56
1:C:358:ARG:NH2	2:C:401:MES:O3S	2.40	0.56
1:G:113:GLN:HB3	1:H:113:GLN:OE1	2.05	0.56
1:E:124:THR:OG1	1:E:126:GLU:HG2	2.05	0.56
1:E:131:ALA:O	1:E:132:LEU:HB2	2.06	0.56
1:E:3:GLY:C	1:E:4:MSE:SE	2.95	0.56
1:H:6:PHE:HA	1:H:9:ARG:HG3	1.88	0.56
1:B:104:ASP:OD2	1:B:119:TYR:OH	2.24	0.56
1:B:345:GLU:OE2	1:B:345:GLU:N	2.39	0.56
1:H:150:LEU:HD22	1:H:175:PHE:HE2	1.69	0.56
1:C:64:LEU:HD11	1:C:244:LEU:HD11	1.87	0.55
1:D:292:MSE:HE1	1:D:295:PRO:HA	1.87	0.55
1:G:131:ALA:O	1:G:133:ALA:N	2.39	0.55
1:H:319:THR:HB	1:H:330:LEU:HD23	1.88	0.55
1:C:97:ASP:HB3	6:C:664:HOH:O	2.06	0.55
1:G:284:GLN:HB2	1:G:287:VAL:HB	1.88	0.55
1:B:282:HIS:O	1:B:284:GLN:N	2.39	0.55
1:D:175:PHE:CZ	1:D:298:ILE:HB	2.41	0.55
1:A:333:CYS:N	1:A:337:MSE:HE1	2.21	0.55
1:C:298:ILE:HD12	1:C:324:LEU:HD22	1.88	0.55
1:D:134:GLU:O	1:D:165:ARG:NH1	2.39	0.55
1:B:180:LEU:HD22	1:B:294:ALA:HB3	1.88	0.55
1:G:3:GLY:C	1:G:4:MSE:HG2	2.25	0.55
1:E:94:VAL:HG11	1:E:131:ALA:HB1	1.86	0.55
1:A:336:LEU:HB2	1:A:337:MSE:HG3	1.87	0.55
1:F:347:ARG:O	1:F:352:ILE:HD12	2.06	0.55
1:B:94:VAL:HG22	1:B:118:ARG:HB3	1.88	0.55
1:D:43:ARG:HG3	1:D:44:TYR:CE2	2.40	0.55
1:G:83:LEU:HD11	1:G:190:VAL:HG11	1.86	0.55
1:B:160:ARG:O	1:B:164:GLU:HG3	2.06	0.55
1:C:199:ILE:HA	1:C:247:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:ASP:OD2	1:G:29:HIS:ND1	2.29	0.55
1:G:180:LEU:HD22	1:G:294:ALA:HB3	1.88	0.55
1:E:334:PRO:O	1:E:339:HIS:N	2.29	0.55
1:G:340:ARG:HA	1:G:347:ARG:NH2	2.18	0.55
1:C:191:SER:HB3	1:C:193:TYR:CE2	2.40	0.55
1:E:310:ARG:HH21	1:E:314:ARG:HH22	1.54	0.55
1:G:55:GLU:O	1:G:59:GLU:HG3	2.06	0.55
1:H:159:SER:O	1:H:163:HIS:ND1	2.39	0.55
1:B:84:LEU:O	6:B:558:HOH:O	2.17	0.55
1:D:288:VAL:O	1:D:292:MSE:HG3	2.07	0.55
1:G:131:ALA:O	1:G:133:ALA:N	2.39	0.55
1:D:342:LEU:HD22	1:D:350:ARG:CZ	2.37	0.55
1:C:94:VAL:HA	1:C:118:ARG:O	2.06	0.55
1:F:332:GLU:OE2	1:F:338:THR:OG1	2.21	0.55
1:E:97:ASP:HB2	1:E:119:TYR:HB3	1.88	0.55
1:F:310:ARG:O	1:F:314:ARG:NH1	2.39	0.55
1:F:9:ARG:HH22	1:F:66:ARG:HG3	1.70	0.55
1:H:11:VAL:HA	1:H:245:HIS:CD2	2.40	0.55
1:A:236:ASP:OD2	6:A:632:HOH:O	2.18	0.55
1:B:56:GLU:OE1	3:B:405:GOL:O2	2.15	0.55
1:G:260:VAL:HG13	6:G:667:HOH:O	2.06	0.55
1:E:294:ALA:O	1:E:296:GLY:N	2.38	0.55
1:G:3:GLY:O	6:G:1441:HOH:O	2.18	0.55
1:E:348:ALA:HB3	6:E:694:HOH:O	2.05	0.55
1:A:112:ARG:HG2	1:E:116:ARG:NH1	2.21	0.55
1:A:18:SER:OG	1:A:18:SER:O	2.22	0.55
1:D:340:ARG:HB2	1:D:341:PRO:HD3	1.87	0.55
1:D:347:ARG:HD2	1:D:352:ILE:O	2.07	0.55
1:E:217:LEU:HB2	4:E:404:CL:CL	2.43	0.55
1:F:123:THR:HG22	1:F:153:VAL:HG22	1.88	0.55
1:H:157:GLU:HA	1:H:160:ARG:HH12	1.71	0.55
1:E:350:ARG:NH1	6:E:675:HOH:O	2.40	0.55
1:B:39:GLN:O	1:B:42:PRO:HD3	2.06	0.55
1:H:333:CYS:H	1:H:337:MSE:SE	2.40	0.55
1:F:9:ARG:HH12	1:F:66:ARG:CZ	2.19	0.55
1:E:126:GLU:N	1:E:126:GLU:OE2	2.38	0.55
1:F:342:LEU:O	1:F:347:ARG:NH1	2.40	0.55
1:F:59:GLU:O	6:F:557:HOH:O	2.18	0.55
1:G:180:LEU:HB3	1:G:292:MSE:SE	2.57	0.55
1:E:347:ARG:O	1:E:352:ILE:N	2.38	0.55
1:H:11:VAL:HA	1:H:245:HIS:HD2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:335:ALA:HA	1:H:347:ARG:HD2	1.88	0.55
1:C:248:SER:HB2	5:C:404:GOL:O1	2.05	0.55
1:D:353:GLY:O	6:D:587:HOH:O	2.17	0.55
1:D:40:ASP:O	1:D:42:PRO:HD3	2.05	0.55
1:C:161:ARG:HA	1:C:164:GLU:OE1	2.06	0.55
1:D:168:ARG:NH2	4:D:405:CL:CL	2.76	0.55
1:D:197:LLP:NZ	1:D:197:LLP:O3	2.35	0.55
1:D:322:VAL:HG12	1:D:337:MSE:HG2	1.89	0.55
1:F:379:GLY:HA2	6:F:651:HOH:O	2.05	0.55
1:C:180:LEU:HD22	1:C:294:ALA:HB3	1.89	0.55
1:D:104:ASP:OD2	1:D:119:TYR:OH	2.15	0.55
1:E:276:TYR:OH	1:E:295:PRO:HB2	2.07	0.55
1:F:224:TYR:OH	6:F:557:HOH:O	2.14	0.55
1:G:108:ASP:O	1:G:112:ARG:HD2	2.06	0.55
1:A:44:TYR:OH	1:A:55:GLU:OE2	2.13	0.55
1:D:339:HIS:O	1:D:347:ARG:HD3	2.06	0.55
1:E:278:GLY:HA2	1:E:285:HIS:HE1	1.70	0.55
1:F:202:HIS:NE2	6:F:516:HOH:O	2.33	0.55
1:B:254:GLN:HG2	1:B:361:VAL:O	2.06	0.55
1:A:180:LEU:HD22	1:A:294:ALA:HB3	1.89	0.55
1:H:236:ASP:OD1	6:H:653:HOH:O	2.18	0.55
1:D:120:ALA:O	6:D:682:HOH:O	2.18	0.55
1:D:264:ARG:NH1	1:D:367:GLN:OE1	2.39	0.55
1:E:213:ARG:NH1	3:E:402:GOL:H2	2.20	0.55
1:E:43:ARG:NH2	1:E:44:TYR:OH	2.30	0.55
1:B:288:VAL:O	1:B:292:MSE:HG2	2.06	0.55
1:C:29:HIS:CD2	1:C:52:PRO:HB2	2.42	0.55
1:F:122:LEU:O	1:F:128:ILE:HD11	2.06	0.55
1:D:254:GLN:HB3	1:D:297:ALA:CB	2.36	0.55
1:H:161:ARG:HD3	1:H:164:GLU:OE1	2.07	0.55
1:D:110:ALA:HB1	1:D:115:VAL:HB	1.87	0.55
1:G:43:ARG:NH2	6:G:586:HOH:O	2.38	0.55
1:H:343:SER:O	1:H:347:ARG:HB2	2.07	0.55
1:H:332:GLU:OE2	1:H:338:THR:OG1	2.23	0.55
2:H:401:MES:O1S	6:H:538:HOH:O	2.18	0.55
1:F:54:ARG:HD3	6:F:652:HOH:O	2.05	0.55
1:E:288:VAL:HG13	1:E:292:MSE:HG2	1.88	0.55
1:E:8:THR:HG23	1:H:364:GLU:HB3	1.89	0.55
1:G:337:MSE:O	1:G:341:PRO:HD3	2.06	0.55
1:G:276:TYR:OH	1:G:295:PRO:HB2	2.06	0.55
1:D:5:ARG:O	1:D:9:ARG:N	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ALA:HB1	1:A:350:ARG:HE	1.72	0.55
1:C:253:ARG:HG2	1:C:363:ILE:HG22	1.88	0.55
1:F:334:PRO:HA	1:F:338:THR:HG22	1.88	0.55
1:E:257:THR:HG21	1:E:369:LEU:HD12	1.88	0.55
1:A:150:LEU:HD22	1:A:175:PHE:HE2	1.72	0.55
1:E:303:TYR:O	6:E:600:HOH:O	2.18	0.55
1:E:9:ARG:NH2	1:E:66:ARG:HG2	2.22	0.55
1:B:338:THR:HG22	2:B:401:MES:H32	1.89	0.55
1:F:146:THR:O	1:F:146:THR:OG1	2.22	0.55
1:G:116:ARG:HH11	1:G:134:GLU:HG2	1.72	0.55
1:D:292:MSE:HE2	6:D:656:HOH:O	2.07	0.55
1:D:347:ARG:HB3	1:D:352:ILE:HB	1.89	0.55
1:E:109:LEU:HA	1:E:112:ARG:HD2	1.89	0.55
1:A:18:SER:HB2	1:A:23:ASP:HB2	1.89	0.55
1:C:312:LEU:HD13	1:C:337:MSE:HE1	1.89	0.55
1:A:46:TYR:CD2	2:B:401:MES:H61	2.42	0.55
1:C:321:GLY:HA2	1:C:337:MSE:CE	2.36	0.55
1:E:14:GLY:HA2	1:E:59:GLU:OE2	2.07	0.55
3:E:402:GOL:H12	6:E:543:HOH:O	2.07	0.55
1:H:264:ARG:NH2	1:H:374:SER:OG	2.40	0.55
1:H:298:ILE:HD11	1:H:324:LEU:HD13	1.89	0.55
1:B:330:LEU:HB2	1:B:360:SER:HB3	1.88	0.55
1:D:145:PRO:CD	1:D:292:MSE:HE1	2.36	0.55
1:E:367:GLN:HG3	6:H:635:HOH:O	2.06	0.55
1:A:14:GLY:O	1:A:16:ARG:N	2.40	0.55
1:A:180:LEU:HD22	1:A:294:ALA:HB3	1.88	0.55
1:B:323:SER:HA	2:B:401:MES:O1S	2.07	0.55
1:C:252:HIS:HD2	6:C:546:HOH:O	1.90	0.55
1:B:109:LEU:HD23	1:B:112:ARG:HH11	1.72	0.55
1:B:43:ARG:NH2	6:B:590:HOH:O	2.40	0.55
1:E:62:ALA:HB1	1:E:67:ALA:O	2.07	0.55
1:E:112:ARG:HD2	6:E:619:HOH:O	2.06	0.55
1:E:342:LEU:O	1:E:347:ARG:NH1	2.40	0.55
1:B:173:ASN:HB3	1:B:193:TYR:CE1	2.41	0.55
1:F:181:GLN:HE21	1:F:291:GLN:HG3	1.72	0.55
1:G:277:PRO:HB2	1:G:295:PRO:HB2	1.87	0.55
1:H:173:ASN:HB3	1:H:193:TYR:CE1	2.41	0.55
1:G:100:TYR:O	1:G:104:ASP:N	2.37	0.55
1:G:4:MSE:HE3	6:G:684:HOH:O	2.06	0.55
1:B:339:HIS:O	1:B:347:ARG:NH1	2.37	0.55
1:B:54:ARG:HD2	1:B:225:ARG:HH12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:ALA:O	1:G:133:ALA:N	2.40	0.55
1:A:118:ARG:HD2	6:A:553:HOH:O	2.07	0.55
1:F:144:THR:OG1	1:F:152:VAL:HG13	2.07	0.55
1:C:180:LEU:HD22	1:C:294:ALA:HB3	1.88	0.55
1:D:95:SER:HB2	1:D:141:TRP:HB3	1.89	0.55
1:E:279:LEU:HB3	1:E:281:GLU:OE1	2.06	0.55
1:H:6:PHE:HD1	1:H:9:ARG:NH1	2.05	0.55
1:A:282:HIS:CG	1:A:283:PRO:HD2	2.42	0.55
1:D:252:HIS:HB3	6:D:660:HOH:O	2.06	0.55
1:A:122:LEU:HD22	1:A:128:ILE:HG12	1.89	0.54
1:A:4:MSE:HB3	1:A:8:THR:HG21	1.88	0.54
1:A:99:VAL:O	6:A:584:HOH:O	2.18	0.54
1:C:236:ASP:HB3	6:C:626:HOH:O	2.06	0.54
1:E:285:HIS:CD2	6:E:502:HOH:O	2.59	0.54
3:F:405:GOL:H2	1:G:249:LEU:HD23	1.88	0.54
1:G:86:LEU:HD13	4:G:406:FMT:H	1.88	0.54
1:A:323:SER:OG	1:A:324:LEU:N	2.39	0.54
1:C:186:LEU:HD11	1:C:291:GLN:HB2	1.88	0.54
1:E:4:MSE:SE	1:E:4:MSE:N	2.90	0.54
1:F:175:PHE:CE2	1:F:298:ILE:HB	2.42	0.54
1:D:180:LEU:HD22	1:D:294:ALA:HB3	1.88	0.54
1:F:56:GLU:OE1	6:F:536:HOH:O	2.18	0.54
1:C:96:THR:C	1:C:98:ASP:H	2.10	0.54
1:C:107:PHE:HB3	1:C:117:VAL:HG21	1.89	0.54
1:F:54:ARG:HG3	1:F:237:CYS:SG	2.47	0.54
1:G:190:VAL:HG22	1:G:212:TYR:HB3	1.89	0.54
1:D:292:MSE:HE1	1:D:295:PRO:CA	2.37	0.54
1:E:120:ALA:HB2	1:E:131:ALA:HB2	1.89	0.54
1:B:40:ASP:OD1	1:B:40:ASP:N	2.32	0.54
1:C:160:ARG:HB3	1:C:161:ARG:NH2	2.21	0.54
1:G:36:ARG:HH11	1:G:36:ARG:CG	2.19	0.54
1:C:18:SER:OG	6:C:660:HOH:O	2.18	0.54
1:F:180:LEU:HD22	1:F:294:ALA:HB3	1.90	0.54
1:A:379:GLY:HA3	6:A:651:HOH:O	2.07	0.54
1:B:84:LEU:HD23	1:B:106:LEU:HB3	1.88	0.54
1:D:132:LEU:HD22	1:D:137:LEU:HD21	1.90	0.54
1:F:100:TYR:CE1	2:F:401:MES:H62	2.42	0.54
1:E:282:HIS:CD2	1:E:283:PRO:HD2	2.42	0.54
1:E:332:GLU:O	1:E:334:PRO:HD3	2.07	0.54
1:H:118:ARG:NH1	1:H:130:ALA:O	2.40	0.54
1:E:39:GLN:HE21	1:G:21:THR:C	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:THR:OG1	1:D:339:HIS:ND1	2.39	0.54
1:A:346:ALA:HA	1:A:349:ARG:CZ	2.37	0.54
1:F:334:PRO:O	1:F:338:THR:N	2.40	0.54
1:B:84:LEU:HD23	1:B:106:LEU:HB3	1.89	0.54
1:B:4:MSE:HE1	1:C:317:LEU:HB2	1.89	0.54
2:C:401:MES:H61	1:D:46:TYR:CD2	2.42	0.54
1:G:3:GLY:C	1:G:4:MSE:SE	2.95	0.54
1:G:95:SER:OG	1:G:96:THR:N	2.39	0.54
1:A:37:ARG:HG3	6:A:693:HOH:O	2.07	0.54
1:H:332:GLU:OE2	1:H:337:MSE:HG3	2.08	0.54
1:C:339:HIS:O	1:C:347:ARG:HD3	2.07	0.54
1:F:197:LLP:O3	6:F:584:HOH:O	2.18	0.54
1:F:96:THR:O	1:F:98:ASP:N	2.35	0.54
1:E:4:MSE:O	1:E:9:ARG:NH2	2.40	0.54
1:D:338:THR:OG1	1:D:339:HIS:N	2.39	0.54
1:H:96:THR:HB	1:H:98:ASP:OD1	2.07	0.54
1:D:6:PHE:CE2	1:D:179:VAL:HA	2.42	0.54
1:F:175:PHE:C	1:F:175:PHE:CD1	2.81	0.54
1:H:333:CYS:HB3	1:H:337:MSE:SE	2.58	0.54
1:A:43:ARG:NH1	6:A:638:HOH:O	2.39	0.54
1:C:3:GLY:C	1:C:4:MSE:SE	2.96	0.54
1:D:180:LEU:HD22	1:D:294:ALA:HB3	1.87	0.54
1:D:92:CYS:HA	1:D:116:ARG:O	2.07	0.54
1:B:54:ARG:HD2	1:B:225:ARG:NH1	2.23	0.54
1:D:98:ASP:HB2	1:D:146:THR:HB	1.89	0.54
1:E:100:TYR:OH	2:E:401:MES:H62	2.08	0.54
1:F:336:LEU:O	1:F:340:ARG:HD2	2.07	0.54
1:E:46:TYR:CD2	2:F:401:MES:H61	2.42	0.54
1:H:277:PRO:O	1:H:288:VAL:HG11	2.07	0.54
1:H:281:GLU:N	6:H:666:HOH:O	2.37	0.54
1:A:43:ARG:O	1:A:50:GLU:HG2	2.08	0.54
1:E:180:LEU:HD22	1:E:294:ALA:HB3	1.88	0.54
1:E:333:CYS:SG	1:E:336:LEU:HB2	2.48	0.54
1:B:332:GLU:OE2	1:B:337:MSE:HB2	2.08	0.54
1:C:199:ILE:HG23	1:C:244:LEU:HD13	1.88	0.54
1:F:4:MSE:HB3	1:F:66:ARG:HH12	1.72	0.54
1:G:180:LEU:HD22	1:G:294:ALA:HB3	1.89	0.54
1:H:178:PRO:HD3	1:H:193:TYR:CZ	2.42	0.54
1:A:124:THR:HG23	1:A:127:GLY:H	1.72	0.54
1:B:93:VAL:HG22	1:B:139:LEU:HB3	1.89	0.54
1:G:84:LEU:HD12	1:G:106:LEU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:ARG:NH1	6:H:667:HOH:O	2.40	0.54
1:D:88:ARG:H	1:D:91:GLN:HE21	1.56	0.54
1:A:180:LEU:HD22	1:A:294:ALA:HB3	1.89	0.54
1:D:178:PRO:HD3	1:D:193:TYR:CE1	2.41	0.54
1:E:347:ARG:HB2	1:E:352:ILE:HB	1.90	0.54
1:F:124:THR:HG23	1:F:127:GLY:H	1.71	0.54
1:F:342:LEU:HB3	1:F:346:ALA:HB3	1.90	0.54
1:F:347:ARG:HB3	1:F:352:ILE:HB	1.89	0.54
1:F:96:THR:HG21	6:F:659:HOH:O	2.08	0.54
1:C:145:PRO:HD2	1:C:175:PHE:HD1	1.73	0.54
1:E:343:SER:OG	1:E:346:ALA:N	2.26	0.54
1:H:11:VAL:HA	1:H:245:HIS:CD2	2.41	0.54
1:B:29:HIS:CE1	3:B:405:GOL:H12	2.43	0.54
1:A:340:ARG:NH2	6:A:644:HOH:O	2.40	0.54
1:C:277:PRO:HA	1:C:282:HIS:CD2	2.42	0.54
1:C:337:MSE:CE	1:D:36:ARG:HD2	2.38	0.54
1:B:19:ALA:O	6:B:680:HOH:O	2.18	0.54
1:D:116:ARG:NH1	1:D:135:PRO:HD2	2.23	0.54
1:F:124:THR:O	1:F:126:GLU:N	2.41	0.54
1:F:319:THR:HB	1:F:330:LEU:HD12	1.88	0.54
1:F:168:ARG:NH2	3:F:403:GOL:O3	2.40	0.54
1:G:316:THR:OG1	1:G:375:ARG:NH1	2.41	0.54
1:A:16:ARG:HB2	1:A:56:GLU:CG	2.35	0.54
1:D:342:LEU:HD21	1:D:350:ARG:HH11	1.73	0.54
1:E:39:GLN:HB2	1:E:42:PRO:HG3	1.89	0.54
1:A:95:SER:O	1:A:120:ALA:N	2.39	0.54
1:C:295:PRO:HG3	6:C:663:HOH:O	2.08	0.54
1:G:104:ASP:OD1	1:G:119:TYR:OH	2.18	0.54
1:E:33:THR:HA	6:E:694:HOH:O	2.08	0.54
1:C:148:PRO:O	1:C:300:SER:OG	2.23	0.54
1:E:285:HIS:NE2	6:E:501:HOH:O	2.34	0.54
1:E:35:GLU:OE2	1:E:37:ARG:NE	2.34	0.54
1:C:175:PHE:CZ	1:C:298:ILE:HB	2.43	0.54
1:A:346:ALA:N	6:A:622:HOH:O	2.36	0.54
1:B:94:VAL:HG21	1:B:131:ALA:O	2.08	0.54
1:G:157:GLU:OE1	1:G:161:ARG:NH1	2.38	0.54
1:C:100:TYR:OH	2:C:401:MES:H62	2.08	0.54
1:B:90:GLY:HA2	1:E:88:ARG:NH2	2.22	0.54
1:C:43:ARG:NH1	6:C:658:HOH:O	2.39	0.54
1:G:198:SER:HB3	6:G:657:HOH:O	2.06	0.54
1:E:5:ARG:NH1	1:H:368:ASP:OD1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ILE:O	1:C:132:LEU:HG	2.08	0.54
1:H:333:CYS:HB2	1:H:357:ILE:HD13	1.89	0.54
1:B:5:ARG:O	1:B:9:ARG:HG3	2.07	0.54
1:F:132:LEU:HD23	1:F:161:ARG:HB3	1.90	0.54
1:B:342:LEU:HD12	1:B:347:ARG:HG2	1.90	0.54
1:A:116:ARG:HH21	1:E:112:ARG:HG2	1.72	0.54
1:F:342:LEU:HB3	1:F:346:ALA:HB3	1.90	0.54
1:B:337:MSE:SE	6:B:681:HOH:O	2.75	0.54
1:B:95:SER:HB2	1:B:141:TRP:HB3	1.90	0.54
1:E:197:LLP:HB2	1:E:324:LEU:HD12	1.88	0.54
1:H:367:GLN:HG2	6:H:662:HOH:O	2.06	0.54
1:A:135:PRO:HA	1:A:165:ARG:HH12	1.72	0.54
1:G:332:GLU:O	1:G:357:ILE:HA	2.07	0.54
1:H:349:ARG:C	1:H:351:GLY:H	2.11	0.54
1:H:34:TYR:CE1	1:H:44:TYR:HB3	2.43	0.54
1:H:354:GLU:HG2	6:H:584:HOH:O	2.08	0.54
1:D:62:ALA:HB1	1:D:67:ALA:O	2.08	0.54
1:B:96:THR:HG22	6:B:680:HOH:O	2.08	0.54
1:E:150:LEU:HD12	1:E:277:PRO:HD3	1.89	0.54
1:A:180:LEU:HD22	1:A:294:ALA:HB3	1.90	0.54
1:E:213:ARG:HE	3:E:402:GOL:H2	1.71	0.54
1:G:113:GLN:HB3	1:H:113:GLN:OE1	2.08	0.54
1:A:113:GLN:NE2	1:B:113:GLN:HB3	2.22	0.54
1:H:92:CYS:SG	1:H:116:ARG:NH2	2.81	0.54
1:G:68:PRO:HG2	1:G:213:ARG:HA	1.90	0.54
1:H:65:GLU:OE1	6:H:559:HOH:O	2.18	0.54
1:E:214:ASP:OD1	1:E:217:LEU:N	2.25	0.54
1:H:350:ARG:NH2	6:H:683:HOH:O	2.35	0.54
1:A:343:SER:O	1:A:347:ARG:HG3	2.07	0.54
1:D:109:LEU:O	1:D:113:GLN:HG2	2.07	0.54
2:E:401:MES:H61	1:F:46:TYR:CD2	2.42	0.54
1:A:337:MSE:SE	4:A:406:CL:CL	3.13	0.54
1:B:88:ARG:NE	1:E:136:ASP:OD1	2.40	0.54
1:F:252:HIS:CD2	6:F:666:HOH:O	2.60	0.54
1:C:4:MSE:HG2	1:C:8:THR:HG21	1.90	0.54
1:E:282:HIS:CG	1:E:283:PRO:HD2	2.43	0.54
1:E:46:TYR:OH	1:F:196:THR:HG21	2.08	0.54
1:A:322:VAL:HG13	1:A:337:MSE:HE2	1.89	0.54
1:G:134:GLU:H	1:G:165:ARG:HH12	1.56	0.54
1:G:100:TYR:CE1	1:G:101:ALA:HB3	2.43	0.54
1:H:289:LYS:HD2	6:H:655:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:VAL:HA	1:F:118:ARG:O	2.08	0.54
1:G:197:LLP:HD3	1:G:324:LEU:HG	1.90	0.54
1:H:143:GLU:HG3	1:H:172:ASP:HB3	1.89	0.54
1:G:46:TYR:CD2	2:H:401:MES:H61	2.42	0.54
1:H:42:PRO:HB2	1:H:45:PHE:CE1	2.42	0.54
1:C:111:ALA:HA	1:C:115:VAL:O	2.07	0.53
1:H:251:VAL:HA	1:H:254:GLN:HE21	1.73	0.53
1:E:145:PRO:HD2	1:E:175:PHE:CD1	2.44	0.53
1:A:37:ARG:HD2	1:B:320:CYS:HB3	1.91	0.53
1:D:223:ALA:O	1:D:227:THR:HG23	2.07	0.53
1:H:4:MSE:HB3	1:H:9:ARG:HD2	1.91	0.53
1:C:338:THR:HG23	1:C:339:HIS:ND1	2.23	0.53
1:G:264:ARG:HH11	1:G:367:GLN:HE22	1.55	0.53
1:A:37:ARG:NH1	6:A:609:HOH:O	2.41	0.53
1:B:99:VAL:O	6:B:605:HOH:O	2.19	0.53
1:C:300:SER:HB2	1:C:356:LEU:HD11	1.89	0.53
1:B:332:GLU:OE2	1:B:338:THR:HG23	2.08	0.53
1:B:60:CYS:SG	1:B:244:LEU:HD13	2.48	0.53
1:E:336:LEU:C	1:E:337:MSE:SE	2.96	0.53
1:F:15:ARG:HD2	1:F:24:VAL:O	2.09	0.53
1:G:119:TYR:CE1	6:G:1480:HOH:O	2.53	0.53
1:G:276:TYR:OH	1:G:295:PRO:HB2	2.08	0.53
1:G:354:GLU:OE1	6:G:1472:HOH:O	2.18	0.53
1:B:154:ASP:OD2	6:B:537:HOH:O	2.18	0.53
1:A:64:LEU:HD11	1:A:244:LEU:HD11	1.89	0.53
1:B:36:ARG:O	1:B:38:ALA:N	2.41	0.53
1:H:118:ARG:HH21	1:H:120:ALA:HB2	1.72	0.53
1:C:131:ALA:C	1:C:133:ALA:H	2.10	0.53
1:C:16:ARG:HB3	1:C:17:PRO:CD	2.38	0.53
1:D:180:LEU:HD13	1:D:294:ALA:O	2.08	0.53
1:E:39:GLN:OE1	1:G:21:THR:HA	2.09	0.53
1:D:342:LEU:O	1:D:347:ARG:HD3	2.07	0.53
1:F:98:ASP:N	1:F:98:ASP:OD1	2.39	0.53
1:H:104:ASP:OD2	6:H:619:HOH:O	2.18	0.53
1:C:322:VAL:O	1:C:323:SER:HB2	2.07	0.53
1:F:181:GLN:HE21	1:F:291:GLN:HG3	1.73	0.53
1:A:347:ARG:NH2	1:A:354:GLU:OE1	2.40	0.53
1:D:213:ARG:HH11	3:D:402:GOL:H2	1.72	0.53
1:C:122:LEU:O	1:C:153:VAL:HG22	2.08	0.53
1:E:225:ARG:HG2	1:E:231:VAL:HG22	1.90	0.53
1:F:96:THR:C	1:F:98:ASP:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:292:MSE:HG2	6:G:1364:HOH:O	2.07	0.53
1:E:6:PHE:HB2	6:E:626:HOH:O	2.07	0.53
1:F:197:LLP:O3	6:F:565:HOH:O	2.18	0.53
1:H:3:GLY:O	1:H:4:MSE:HG2	2.08	0.53
1:G:101:ALA:HA	1:G:104:ASP:HB2	1.89	0.53
1:B:300:SER:HB3	1:B:356:LEU:HD11	1.90	0.53
1:C:277:PRO:HA	1:C:282:HIS:CD2	2.43	0.53
1:E:146:THR:OG1	1:E:151:THR:HB	2.08	0.53
1:G:152:VAL:H	1:G:284:GLN:NE2	2.06	0.53
1:B:90:GLY:N	1:B:114:GLY:O	2.37	0.53
1:E:132:LEU:O	6:E:572:HOH:O	2.18	0.53
1:E:285:HIS:HB3	6:E:638:HOH:O	2.07	0.53
1:F:96:THR:C	1:F:98:ASP:H	2.10	0.53
1:D:150:LEU:HD22	1:D:175:PHE:CE2	2.41	0.53
1:D:168:ARG:NE	4:D:405:CL:CL	2.78	0.53
1:A:335:ALA:HB2	1:A:347:ARG:HD3	1.90	0.53
1:C:146:THR:OG1	1:C:151:THR:HG22	2.08	0.53
1:C:224:TYR:OH	6:C:675:HOH:O	2.17	0.53
1:G:100:TYR:CE1	2:G:401:MES:H81	2.40	0.53
1:D:169:VAL:N	1:D:189:ASP:OD2	2.40	0.53
1:F:161:ARG:N	1:F:161:ARG:HD2	2.24	0.53
1:G:268:SER:O	6:G:617:HOH:O	2.19	0.53
1:G:36:ARG:CZ	1:H:337:MSE:HE3	2.38	0.53
1:B:16:ARG:HG3	1:B:56:GLU:OE1	2.09	0.53
1:F:251:VAL:HA	1:F:254:GLN:OE1	2.08	0.53
1:G:6:PHE:N	6:G:619:HOH:O	2.28	0.53
1:E:180:LEU:HD22	1:E:294:ALA:HB3	1.89	0.53
1:D:4:MSE:O	1:D:9:ARG:NH2	2.41	0.53
1:F:332:GLU:OE1	1:F:338:THR:HG23	2.08	0.53
1:H:95:SER:OG	1:H:141:TRP:HB3	2.09	0.53
1:A:262:VAL:HG11	1:A:279:LEU:HD21	1.91	0.53
1:E:289:LYS:HB3	6:E:592:HOH:O	2.09	0.53
1:A:336:LEU:O	1:A:340:ARG:HD3	2.07	0.53
1:H:110:ALA:HB1	1:H:115:VAL:HG21	1.91	0.53
1:E:33:THR:HG23	1:G:24:VAL:HB	1.90	0.53
1:A:95:SER:HB2	1:A:141:TRP:HB3	1.91	0.53
1:E:277:PRO:HA	1:E:282:HIS:CD2	2.43	0.53
1:F:214:ASP:OD1	4:F:408:CL:CL	2.63	0.53
1:H:47:GLY:O	1:H:54:ARG:NH2	2.41	0.53
1:A:37:ARG:NH1	1:B:312:LEU:O	2.41	0.53
1:E:347:ARG:HA	1:E:350:ARG:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ARG:HB3	6:B:602:HOH:O	2.08	0.53
1:C:236:ASP:OD1	6:C:573:HOH:O	2.18	0.53
1:D:285:HIS:HA	1:D:288:VAL:HB	1.90	0.53
1:D:91:GLN:HA	1:D:136:ASP:HB3	1.89	0.53
1:E:333:CYS:O	1:E:337:MSE:N	2.41	0.53
1:H:276:TYR:CZ	1:H:295:PRO:HB2	2.43	0.53
1:D:338:THR:HG21	2:D:401:MES:O3S	2.08	0.53
1:G:9:ARG:NH1	6:G:612:HOH:O	2.26	0.53
1:G:36:ARG:NH2	1:H:322:VAL:HG13	2.23	0.53
1:D:105:GLY:O	1:D:108:ASP:HB2	2.08	0.53
1:D:253:ARG:NH2	1:D:257:THR:OG1	2.41	0.53
1:H:93:VAL:HG22	1:H:139:LEU:HB3	1.90	0.53
1:E:95:SER:O	1:E:120:ALA:N	2.41	0.53
1:D:346:ALA:O	1:D:349:ARG:HB3	2.08	0.53
1:F:367:GLN:NE2	1:F:371:GLU:OE2	2.40	0.53
1:A:108:ASP:O	1:A:112:ARG:HG2	2.08	0.53
1:F:4:MSE:HG2	1:F:9:ARG:HA	1.91	0.53
1:B:367:GLN:HG2	1:C:5:ARG:NH2	2.23	0.53
1:E:368:ASP:OD2	1:H:5:ARG:N	2.29	0.53
1:F:372:ASP:OD1	1:F:375:ARG:NH1	2.41	0.53
1:B:17:PRO:HB3	6:B:675:HOH:O	2.07	0.53
1:G:252:HIS:CE1	6:G:663:HOH:O	2.62	0.53
1:E:143:GLU:O	1:E:146:THR:HG22	2.09	0.53
1:G:206:LEU:HD23	1:H:32:THR:HG22	1.91	0.53
1:A:18:SER:OG	3:A:403:GOL:O3	2.23	0.53
1:E:372:ASP:HA	1:E:375:ARG:NH1	2.24	0.53
1:G:282:HIS:CG	1:G:283:PRO:HD2	2.44	0.53
1:B:26:PRO:HB3	3:B:405:GOL:H31	1.91	0.53
1:B:344:ALA:HB2	1:B:347:ARG:NH2	2.23	0.53
1:C:350:ARG:NH1	6:C:657:HOH:O	2.41	0.53
1:A:292:MSE:SE	1:A:295:PRO:HA	2.59	0.53
1:A:344:ALA:HB2	1:A:347:ARG:NH2	2.24	0.53
1:H:344:ALA:HA	1:H:347:ARG:HH21	1.74	0.53
1:A:343:SER:N	1:A:346:ALA:HB3	2.22	0.53
1:F:173:ASN:HB3	1:F:193:TYR:CE1	2.44	0.53
1:F:339:HIS:O	1:F:347:ARG:NH1	2.36	0.53
1:F:150:LEU:HD22	1:F:175:PHE:CE2	2.42	0.53
1:B:16:ARG:NH1	6:B:663:HOH:O	2.21	0.53
1:E:94:VAL:HG11	1:E:131:ALA:HB1	1.90	0.53
1:H:124:THR:HG22	1:H:125:PRO:HD2	1.91	0.53
1:A:132:LEU:HD23	1:A:161:ARG:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:CYS:HA	1:A:116:ARG:O	2.08	0.53
1:B:323:SER:HA	2:B:401:MES:O1S	2.08	0.53
1:B:96:THR:O	1:B:119:TYR:HD1	1.90	0.53
1:D:94:VAL:HG21	1:D:131:ALA:O	2.09	0.53
1:C:48:ARG:O	6:C:572:HOH:O	2.19	0.53
1:C:52:PRO:HA	1:C:55:GLU:OE1	2.09	0.53
1:A:179:VAL:HG21	1:A:251:VAL:HG11	1.90	0.53
1:A:181:GLN:NE2	6:A:536:HOH:O	2.41	0.53
1:C:345:GLU:O	1:C:348:ALA:N	2.42	0.53
1:F:39:GLN:HE22	1:F:44:TYR:HB2	1.73	0.53
1:G:225:ARG:HG2	1:G:231:VAL:HG12	1.90	0.53
1:E:197:LLP:HD3	1:E:324:LEU:HG	1.91	0.53
1:F:95:SER:OG	1:F:96:THR:N	2.42	0.53
1:C:11:VAL:HA	1:C:245:HIS:ND1	2.24	0.53
1:A:347:ARG:O	1:A:352:ILE:N	2.35	0.53
1:B:283:PRO:HB2	1:B:284:GLN:NE2	2.23	0.53
1:B:284:GLN:HG2	6:B:669:HOH:O	2.08	0.53
1:D:140:VAL:HB	1:D:169:VAL:HG22	1.90	0.53
1:B:88:ARG:NH1	1:E:136:ASP:OD2	2.40	0.53
1:D:36:ARG:HB2	1:D:42:PRO:HB3	1.90	0.53
1:E:123:THR:OG1	6:E:602:HOH:O	2.19	0.53
1:E:43:ARG:NH2	1:E:44:TYR:OH	2.41	0.53
1:G:97:ASP:C	1:G:99:VAL:H	2.12	0.53
1:A:36:ARG:HH22	1:B:337:MSE:HG2	1.74	0.53
1:A:14:GLY:HA2	1:A:59:GLU:OE1	2.09	0.53
1:B:180:LEU:HA	1:B:293:SER:HB3	1.91	0.53
1:E:16:ARG:HD3	6:E:633:HOH:O	2.09	0.53
1:F:150:LEU:HD22	1:F:175:PHE:HZ	1.74	0.53
1:H:84:LEU:HD23	1:H:141:TRP:CZ3	2.44	0.53
1:G:97:ASP:HB3	1:G:119:TYR:CG	2.44	0.53
1:H:333:CYS:O	1:H:337:MSE:SE	2.77	0.53
1:G:346:ALA:O	1:G:350:ARG:N	2.42	0.53
1:F:14:GLY:HA2	1:F:59:GLU:HG2	1.91	0.53
1:H:110:ALA:O	1:H:115:VAL:N	2.35	0.53
1:A:112:ARG:NH2	1:E:135:PRO:HG3	2.24	0.53
1:H:29:HIS:CD2	1:H:52:PRO:HB2	2.44	0.53
1:F:353:GLY:O	6:F:573:HOH:O	2.18	0.53
1:D:332:GLU:HB2	1:D:337:MSE:HE2	1.91	0.53
1:E:128:ILE:O	1:E:132:LEU:HB2	2.09	0.53
1:G:264:ARG:NH2	1:G:374:SER:OG	2.40	0.53
1:C:4:MSE:HG2	1:C:8:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:PRO:HD3	1:F:339:HIS:CE1	2.44	0.53
1:A:18:SER:HA	3:A:403:GOL:O1	2.09	0.53
1:F:298:ILE:HD12	6:F:662:HOH:O	2.09	0.53
1:C:285:HIS:CE1	6:C:652:HOH:O	2.61	0.53
1:A:334:PRO:HG2	1:A:356:LEU:HD23	1.91	0.53
1:H:11:VAL:HA	1:H:245:HIS:CD2	2.42	0.53
1:B:337:MSE:O	1:B:340:ARG:HG2	2.09	0.53
1:B:346:ALA:HA	1:B:349:ARG:HD3	1.89	0.53
1:H:3:GLY:CA	6:H:650:HOH:O	2.55	0.53
2:G:401:MES:H61	1:H:46:TYR:CE2	2.44	0.53
1:F:100:TYR:CE2	1:F:102:GLY:HA3	2.44	0.53
1:F:4:MSE:SE	1:F:9:ARG:HA	2.58	0.53
1:D:314:ARG:CZ	1:D:379:GLY:HA2	2.39	0.53
1:E:4:MSE:O	1:E:9:ARG:NE	2.39	0.53
1:D:91:GLN:C	1:D:116:ARG:HD3	2.30	0.53
1:H:322:VAL:HB	2:H:401:MES:H72	1.90	0.53
1:B:222:ARG:NH1	6:B:583:HOH:O	2.42	0.53
1:E:100:TYR:OH	2:E:401:MES:H62	2.09	0.53
1:B:197:LLP:HD3	1:B:324:LEU:HG	1.91	0.53
1:C:375:ARG:HD2	6:C:640:HOH:O	2.07	0.53
1:E:319:THR:HG23	1:F:35:GLU:OE1	2.08	0.53
1:H:11:VAL:HA	1:H:245:HIS:HD2	1.74	0.53
1:C:347:ARG:HG2	1:C:352:ILE:HB	1.89	0.53
1:D:288:VAL:O	1:D:292:MSE:HB2	2.09	0.53
1:F:84:LEU:HD12	1:F:106:LEU:HB3	1.91	0.53
1:A:40:ASP:N	1:A:40:ASP:OD1	2.41	0.53
1:E:66:ARG:CZ	6:E:666:HOH:O	2.49	0.53
1:D:216:ASP:N	1:D:216:ASP:OD1	2.40	0.53
1:D:264:ARG:NH2	1:D:374:SER:OG	2.42	0.53
1:G:213:ARG:HG2	1:G:213:ARG:HH11	1.74	0.53
1:G:263:GLU:HG2	6:G:514:HOH:O	2.09	0.53
1:E:18:SER:OG	1:E:23:ASP:N	2.41	0.53
1:E:376:ALA:O	6:E:655:HOH:O	2.18	0.53
1:F:342:LEU:O	1:F:347:ARG:NH1	2.42	0.53
1:G:206:LEU:HD23	1:H:32:THR:HG22	1.91	0.53
1:A:135:PRO:HG3	1:E:112:ARG:HH21	1.74	0.52
1:G:333:CYS:HA	1:G:356:LEU:O	2.09	0.52
1:B:180:LEU:HD22	1:B:294:ALA:HB3	1.91	0.52
1:D:347:ARG:O	1:D:351:GLY:N	2.41	0.52
1:D:168:ARG:HH22	3:D:403:GOL:H32	1.73	0.52
1:F:339:HIS:O	1:F:347:ARG:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:ASP:O	1:G:112:ARG:HD2	2.09	0.52
1:D:124:THR:O	1:D:128:ILE:HG13	2.08	0.52
1:B:365:ASP:N	1:C:8:THR:HG22	2.19	0.52
1:A:189:ASP:HA	1:A:213:ARG:NH2	2.23	0.52
1:B:91:GLN:HA	1:B:136:ASP:HB3	1.91	0.52
1:F:122:LEU:HD22	1:F:128:ILE:HD13	1.91	0.52
1:F:335:ALA:HA	1:F:347:ARG:NH1	2.24	0.52
1:F:9:ARG:NH1	6:F:642:HOH:O	2.36	0.52
1:B:134:GLU:O	1:B:165:ARG:NH1	2.43	0.52
1:C:197:LLP:O3	6:C:555:HOH:O	2.18	0.52
1:C:174:THR:HB	1:C:197:LLP:H2'2	1.91	0.52
1:D:285:HIS:O	1:D:288:VAL:HB	2.09	0.52
1:B:119:TYR:HE1	6:B:687:HOH:O	1.92	0.52
1:H:43:ARG:NH2	6:H:651:HOH:O	2.33	0.52
1:C:327:VAL:HG12	1:C:328:HIS:CE1	2.45	0.52
1:H:16:ARG:HG2	1:H:17:PRO:HD2	1.92	0.52
1:G:46:TYR:CD2	2:H:401:MES:H61	2.44	0.52
1:E:3:GLY:HA2	6:E:669:HOH:O	2.08	0.52
1:C:149:LEU:HD11	1:C:351:GLY:HA3	1.91	0.52
1:D:104:ASP:O	1:D:108:ASP:HB2	2.09	0.52
1:A:168:ARG:HH22	3:A:402:GOL:HO3	1.55	0.52
1:F:197:LLP:HB2	1:F:324:LEU:HD12	1.91	0.52
1:H:32:THR:OG1	1:H:33:THR:OG1	2.25	0.52
1:F:282:HIS:CG	1:F:283:PRO:HD2	2.44	0.52
1:F:277:PRO:HG2	1:F:292:MSE:HE1	1.92	0.52
1:B:133:ALA:CA	1:B:165:ARG:HH11	2.22	0.52
1:G:213:ARG:HB3	3:G:402:GOL:O1	2.09	0.52
1:A:22:GLY:HA2	1:C:38:ALA:HB3	1.92	0.52
1:B:17:PRO:O	1:B:18:SER:HB2	2.09	0.52
1:E:345:GLU:C	1:E:347:ARG:H	2.12	0.52
1:E:339:HIS:O	1:E:347:ARG:HD3	2.09	0.52
1:H:168:ARG:NH2	3:H:404:GOL:H32	2.25	0.52
1:C:309:GLU:HG3	1:C:310:ARG:NH2	2.24	0.52
1:F:95:SER:OG	1:F:96:THR:N	2.42	0.52
1:C:227:THR:O	1:D:77:GLN:NE2	2.42	0.52
1:C:100:TYR:OH	2:C:401:MES:H62	2.10	0.52
1:C:46:TYR:CG	2:D:401:MES:H52	2.44	0.52
1:F:44:TYR:O	1:F:45:PHE:HD1	1.91	0.52
1:B:343:SER:O	1:B:347:ARG:N	2.26	0.52
1:C:309:GLU:OE1	1:C:310:ARG:NH2	2.43	0.52
1:G:157:GLU:O	1:G:161:ARG:HD2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:168:ARG:HH22	3:H:404:GOL:H32	1.74	0.52
1:A:9:ARG:NH2	1:A:64:LEU:HA	2.24	0.52
1:C:180:LEU:HD22	1:C:294:ALA:HB3	1.91	0.52
1:C:96:THR:OG1	1:C:99:VAL:HB	2.10	0.52
1:F:192:LEU:HD12	1:F:193:TYR:N	2.24	0.52
1:G:293:SER:OG	6:G:660:HOH:O	2.19	0.52
1:F:54:ARG:HG3	1:F:237:CYS:SG	2.48	0.52
1:A:68:PRO:HG2	1:A:213:ARG:HA	1.91	0.52
1:D:334:PRO:HG2	1:D:356:LEU:HD23	1.92	0.52
1:G:337:MSE:C	1:G:339:HIS:N	2.61	0.52
1:H:53:THR:HA	1:H:56:GLU:OE1	2.09	0.52
1:A:180:LEU:HD22	1:A:294:ALA:HB3	1.91	0.52
1:E:241:ARG:NE	6:E:539:HOH:O	2.40	0.52
1:D:176:ALA:HB1	1:D:180:LEU:HB2	1.92	0.52
1:F:35:GLU:HG3	1:F:38:ALA:HB2	1.91	0.52
1:B:131:ALA:C	1:B:133:ALA:H	2.12	0.52
1:H:157:GLU:OE1	1:H:160:ARG:NH1	2.42	0.52
1:A:54:ARG:NH1	6:A:586:HOH:O	2.41	0.52
1:F:3:GLY:C	1:F:4:MSE:HG2	2.29	0.52
5:F:407:FMT:H	6:F:547:HOH:O	2.08	0.52
1:B:97:ASP:HB3	6:B:681:HOH:O	2.08	0.52
1:D:291:GLN:HG3	1:D:292:MSE:HG2	1.91	0.52
1:E:317:LEU:O	6:E:509:HOH:O	2.19	0.52
1:F:4:MSE:N	6:F:598:HOH:O	2.42	0.52
1:F:4:MSE:SE	1:F:5:ARG:O	2.78	0.52
1:G:14:GLY:HA2	1:G:59:GLU:OE2	2.10	0.52
1:A:95:SER:HB2	1:A:141:TRP:HB3	1.91	0.52
1:D:11:VAL:HA	1:D:245:HIS:ND1	2.24	0.52
1:E:108:ASP:HB3	1:E:112:ARG:HH11	1.73	0.52
1:E:346:ALA:O	1:E:349:ARG:N	2.35	0.52
1:H:168:ARG:HH22	3:H:405:GOL:H32	1.74	0.52
1:D:94:VAL:HA	1:D:118:ARG:O	2.09	0.52
1:F:134:GLU:HB2	1:F:137:LEU:HD13	1.92	0.52
1:H:133:ALA:O	1:H:165:ARG:NH1	2.42	0.52
1:H:3:GLY:HA3	1:H:8:THR:HG21	1.92	0.52
1:F:241:ARG:HA	1:F:244:LEU:HD12	1.91	0.52
1:C:100:TYR:CZ	2:C:401:MES:H72	2.45	0.52
1:G:121:ASP:CG	6:G:685:HOH:O	2.48	0.52
1:G:233:GLY:HA3	6:G:659:HOH:O	2.09	0.52
1:A:6:PHE:CZ	1:A:179:VAL:HA	2.44	0.52
1:A:338:THR:HG22	6:A:686:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:THR:O	1:B:99:VAL:HB	2.10	0.52
1:E:6:PHE:O	1:E:6:PHE:CD2	2.62	0.52
1:H:231:VAL:HG12	1:H:232:PRO:HD2	1.90	0.52
1:A:90:GLY:N	1:A:114:GLY:O	2.29	0.52
1:F:332:GLU:OE1	1:F:338:THR:HG22	2.09	0.52
1:D:4:MSE:SE	1:D:8:THR:HG21	2.60	0.52
1:E:277:PRO:HA	1:E:282:HIS:CD2	2.44	0.52
1:B:5:ARG:HD3	1:C:368:ASP:OD1	2.10	0.52
1:A:344:ALA:HA	1:A:347:ARG:HB2	1.91	0.52
1:D:248:SER:OG	1:D:252:HIS:NE2	2.43	0.52
1:E:128:ILE:O	1:E:132:LEU:HB2	2.09	0.52
1:E:32:THR:OG1	1:E:33:THR:HG23	2.09	0.52
1:C:344:ALA:O	1:C:347:ARG:HB2	2.10	0.52
1:B:9:ARG:NH1	6:B:664:HOH:O	2.42	0.52
1:C:18:SER:OG	6:C:612:HOH:O	2.18	0.52
1:B:88:ARG:NE	1:E:136:ASP:OD1	2.42	0.52
1:A:108:ASP:O	1:A:112:ARG:HG3	2.10	0.52
1:A:19:ALA:O	1:A:21:THR:N	2.43	0.52
1:A:206:LEU:HD23	1:B:32:THR:HG22	1.92	0.52
1:E:309:GLU:N	1:E:309:GLU:CD	2.63	0.52
1:H:178:PRO:HD3	1:H:193:TYR:CE1	2.45	0.52
1:E:297:ALA:HB3	6:E:658:HOH:O	2.10	0.52
1:G:104:ASP:OD1	1:G:119:TYR:OH	2.21	0.52
1:E:43:ARG:HB3	1:E:44:TYR:CD2	2.44	0.52
1:G:96:THR:HG23	6:G:667:HOH:O	2.09	0.52
1:H:101:ALA:HA	1:H:104:ASP:HB2	1.91	0.52
1:A:337:MSE:HE3	1:B:36:ARG:CZ	2.39	0.52
1:D:6:PHE:HD2	1:D:9:ARG:HH11	1.58	0.52
1:H:259:ARG:NE	6:H:591:HOH:O	2.14	0.52
1:H:95:SER:OG	1:H:96:THR:N	2.41	0.52
1:H:9:ARG:HD3	1:H:63:GLY:O	2.09	0.52
1:A:150:LEU:HD22	1:A:175:PHE:HE2	1.74	0.52
1:F:103:THR:O	1:F:107:PHE:N	2.41	0.52
1:A:9:ARG:NH1	1:A:66:ARG:HE	2.06	0.52
1:C:108:ASP:O	1:C:112:ARG:HD2	2.10	0.52
1:E:320:CYS:CB	1:F:37:ARG:HD2	2.40	0.52
1:H:342:LEU:HD21	1:H:350:ARG:HE	1.74	0.52
1:D:213:ARG:NE	6:D:653:HOH:O	2.40	0.52
1:F:368:ASP:OD2	1:G:5:ARG:N	2.27	0.52
1:G:36:ARG:NE	6:G:685:HOH:O	2.42	0.52
1:H:180:LEU:HD22	1:H:294:ALA:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:ARG:O	1:H:7:GLY:N	2.42	0.52
1:H:259:ARG:CZ	6:H:665:HOH:O	2.57	0.52
1:F:9:ARG:NH2	1:F:64:LEU:HA	2.24	0.52
1:A:65:GLU:OE1	6:A:533:HOH:O	2.19	0.52
1:G:352:ILE:HG23	1:G:356:LEU:HD23	1.91	0.52
1:G:9:ARG:NH1	1:G:66:ARG:HH11	2.08	0.52
1:E:72:VAL:HG23	1:E:232:PRO:HG3	1.92	0.52
1:E:205:VAL:HG23	1:E:236:ASP:OD2	2.10	0.52
1:G:292:MSE:CE	1:G:295:PRO:HA	2.30	0.52
1:B:265:LEU:O	6:B:581:HOH:O	2.18	0.52
1:F:37:ARG:HB2	1:F:37:ARG:HH11	1.74	0.52
1:A:32:THR:HG22	1:B:206:LEU:HD12	1.91	0.52
1:E:109:LEU:O	1:E:113:GLN:HG2	2.10	0.52
1:H:92:CYS:HA	1:H:116:ARG:O	2.10	0.52
1:C:178:PRO:HD3	1:C:193:TYR:CE1	2.45	0.52
1:A:17:PRO:HA	6:A:628:HOH:O	2.10	0.52
1:E:150:LEU:HD22	1:E:175:PHE:HE2	1.75	0.52
1:F:254:GLN:HB3	1:F:297:ALA:HB2	1.92	0.52
1:H:333:CYS:H	1:H:337:MSE:CE	2.22	0.52
1:H:65:GLU:HG2	1:H:182:GLN:OE1	2.10	0.52
1:B:157:GLU:HA	1:B:160:ARG:HE	1.75	0.52
1:G:307:PRO:HB3	1:G:309:GLU:OE2	2.09	0.52
1:A:342:LEU:HD13	1:A:350:ARG:CZ	2.40	0.52
1:C:68:PRO:HG2	1:C:213:ARG:HA	1.92	0.52
1:D:95:SER:OG	1:D:96:THR:N	2.43	0.52
1:G:100:TYR:OH	2:G:401:MES:H51	2.10	0.52
1:A:322:VAL:O	1:A:323:SER:HB3	2.08	0.52
1:F:105:GLY:HA3	3:F:402:GOL:O3	2.09	0.52
1:C:42:PRO:HB2	1:C:45:PHE:HE1	1.75	0.52
1:B:121:ASP:HB3	1:B:127:GLY:HA3	1.92	0.52
1:B:214:ASP:HB3	6:B:605:HOH:O	2.09	0.52
1:B:245:HIS:HB3	1:C:327:VAL:HG21	1.92	0.52
1:E:345:GLU:HB3	1:E:349:ARG:NH1	2.25	0.52
1:E:43:ARG:O	1:E:50:GLU:HG2	2.10	0.52
1:B:16:ARG:NH2	6:B:663:HOH:O	2.36	0.52
1:B:332:GLU:OE2	1:B:358:ARG:NH2	2.42	0.52
1:D:61:LEU:HD21	1:D:244:LEU:HD11	1.92	0.52
1:G:156:ALA:O	1:G:160:ARG:HG2	2.10	0.52
1:H:178:PRO:HD3	1:H:193:TYR:CE1	2.45	0.52
2:C:401:MES:H61	1:D:46:TYR:CD2	2.45	0.52
1:G:343:SER:O	1:G:346:ALA:N	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:GLN:HE21	1:D:113:GLN:NE2	2.08	0.52
1:H:298:ILE:HD11	1:H:324:LEU:HD13	1.91	0.52
1:E:91:GLN:HB3	1:E:138:ALA:HB2	1.90	0.52
1:C:175:PHE:CZ	1:C:298:ILE:HB	2.45	0.52
1:G:268:SER:O	6:G:606:HOH:O	2.19	0.52
1:E:95:SER:HB2	1:E:141:TRP:HB3	1.91	0.52
1:B:214:ASP:HB3	1:B:217:LEU:HB3	1.92	0.52
1:G:159:SER:HA	1:G:169:VAL:HG21	1.92	0.52
1:G:9:ARG:NE	6:G:649:HOH:O	2.43	0.52
1:A:365:ASP:OD1	1:A:367:GLN:HB2	2.09	0.52
1:B:310:ARG:HB3	1:B:314:ARG:HH11	1.75	0.52
1:A:18:SER:HB2	3:A:403:GOL:H31	1.92	0.52
1:C:43:ARG:HB2	6:C:643:HOH:O	2.09	0.52
1:B:124:THR:O	1:B:128:ILE:N	2.43	0.51
1:E:147:ASN:ND2	1:E:148:PRO:HA	2.25	0.51
1:E:350:ARG:HD2	6:E:634:HOH:O	2.09	0.51
1:G:264:ARG:HH11	1:G:367:GLN:NE2	2.08	0.51
1:D:168:ARG:NE	4:D:405:CL:CL	2.80	0.51
1:E:116:ARG:NH1	1:E:135:PRO:O	2.41	0.51
1:H:340:ARG:H	1:H:341:PRO:HD2	1.76	0.51
1:C:133:ALA:HA	1:C:165:ARG:HH11	1.75	0.51
1:A:98:ASP:N	1:A:98:ASP:OD1	2.43	0.51
1:C:14:GLY:HA2	1:C:59:GLU:OE1	2.10	0.51
1:D:28:ILE:HG21	1:D:235:LEU:HD23	1.92	0.51
1:C:253:ARG:NH1	1:C:257:THR:OG1	2.43	0.51
1:G:116:ARG:NH1	1:G:134:GLU:HG3	2.24	0.51
1:A:109:LEU:O	1:A:113:GLN:HG2	2.10	0.51
1:A:24:VAL:HG21	1:C:33:THR:HG22	1.92	0.51
1:G:277:PRO:HA	1:G:282:HIS:CD2	2.45	0.51
1:H:147:ASN:HD21	1:H:358:ARG:HD3	1.76	0.51
1:H:292:MSE:SE	1:H:294:ALA:O	2.78	0.51
1:B:238:PHE:HA	6:B:602:HOH:O	2.11	0.51
1:D:28:ILE:HG21	1:D:235:LEU:HD23	1.92	0.51
1:C:236:ASP:OD1	6:C:623:HOH:O	2.18	0.51
1:E:18:SER:OG	1:E:23:ASP:HB2	2.10	0.51
1:F:339:HIS:HA	6:F:654:HOH:O	2.08	0.51
1:B:6:PHE:HE2	1:B:179:VAL:HG22	1.75	0.51
1:F:189:ASP:HB3	3:F:406:CL:CL	2.48	0.51
1:G:101:ALA:HA	1:G:104:ASP:HB2	1.91	0.51
1:B:4:MSE:N	1:B:4:MSE:SE	2.88	0.51
1:G:367:GLN:O	1:G:371:GLU:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:GLU:OE1	1:E:135:PRO:HD2	2.11	0.51
1:G:148:PRO:HD3	1:G:339:HIS:CE1	2.45	0.51
1:D:168:ARG:NH1	6:D:558:HOH:O	2.42	0.51
1:D:152:VAL:HG11	1:D:288:VAL:HG22	1.92	0.51
1:D:152:VAL:CG1	1:D:284:GLN:HB2	2.41	0.51
1:A:213:ARG:NE	3:A:404:GOL:O2	2.40	0.51
1:D:9:ARG:HD3	6:D:672:HOH:O	2.11	0.51
1:F:94:VAL:HA	1:F:118:ARG:O	2.10	0.51
1:A:9:ARG:NH1	6:A:605:HOH:O	2.36	0.51
1:A:198:SER:OG	6:A:523:HOH:O	2.19	0.51
1:B:38:ALA:O	6:B:657:HOH:O	2.19	0.51
1:C:288:VAL:HA	1:C:292:MSE:HG3	1.91	0.51
1:D:145:PRO:HG3	1:D:292:MSE:HE1	1.91	0.51
1:H:9:ARG:NH1	6:H:649:HOH:O	2.39	0.51
1:C:333:CYS:HB2	1:C:357:ILE:HD13	1.92	0.51
1:E:3:GLY:O	1:E:4:MSE:HB3	2.10	0.51
1:E:313:ASP:O	1:F:37:ARG:NH2	2.44	0.51
1:G:160:ARG:HB3	1:G:161:ARG:NE	2.25	0.51
1:D:56:GLU:OE2	6:D:570:HOH:O	2.19	0.51
1:G:122:LEU:N	6:G:640:HOH:O	2.43	0.51
1:H:323:SER:O	1:H:330:LEU:HD12	2.11	0.51
1:B:152:VAL:O	1:B:284:GLN:NE2	2.43	0.51
1:B:276:TYR:CZ	1:B:295:PRO:HB2	2.45	0.51
1:C:143:GLU:HG3	1:C:172:ASP:HB3	1.92	0.51
1:G:214:ASP:HB3	1:G:217:LEU:HB3	1.92	0.51
1:G:277:PRO:HA	1:G:282:HIS:CD2	2.46	0.51
1:E:285:HIS:CD2	1:E:289:LYS:HG3	2.45	0.51
1:E:313:ASP:CG	6:E:663:HOH:O	2.48	0.51
1:H:245:HIS:HE1	6:H:533:HOH:O	1.93	0.51
1:E:180:LEU:HD22	1:E:294:ALA:HB3	1.92	0.51
1:H:86:LEU:HD13	3:H:403:GOL:H32	1.92	0.51
1:B:12:HIS:CE1	1:B:15:ARG:NH1	2.79	0.51
1:C:310:ARG:NH1	1:C:313:ASP:OD2	2.43	0.51
1:C:380:GLY:CA	6:C:506:HOH:O	2.58	0.51
1:E:178:PRO:HG3	1:E:193:TYR:CZ	2.46	0.51
1:A:226:THR:HG22	4:A:405:GOL:H11	1.92	0.51
1:C:112:ARG:HD2	6:C:603:HOH:O	2.10	0.51
1:C:310:ARG:HA	1:C:310:ARG:NE	2.26	0.51
1:G:372:ASP:OD1	1:G:375:ARG:NH1	2.44	0.51
1:A:42:PRO:HG3	6:A:683:HOH:O	2.09	0.51
1:H:222:ARG:O	1:H:226:THR:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ARG:H	1:D:91:GLN:HE21	1.57	0.51
1:B:20:GLY:N	6:B:657:HOH:O	2.33	0.51
1:D:322:VAL:HG21	2:D:401:MES:H52	1.93	0.51
1:F:358:ARG:HH22	2:F:401:MES:H71	1.74	0.51
4:E:404:GOL:H12	6:E:686:HOH:O	2.10	0.51
1:G:157:GLU:O	1:G:161:ARG:HD2	2.10	0.51
1:G:134:GLU:N	1:G:165:ARG:HH12	2.08	0.51
1:C:309:GLU:HB3	1:C:310:ARG:NH1	2.26	0.51
1:D:279:LEU:O	1:D:281:GLU:N	2.44	0.51
1:D:36:ARG:O	1:D:39:GLN:HB2	2.09	0.51
1:G:341:PRO:HD3	6:G:662:HOH:O	2.09	0.51
1:E:312:LEU:HD11	1:E:333:CYS:HB2	1.92	0.51
1:G:91:GLN:HA	1:G:136:ASP:HB3	1.91	0.51
1:D:4:MSE:HG3	6:D:670:HOH:O	2.11	0.51
1:E:309:GLU:N	1:E:309:GLU:OE1	2.44	0.51
1:F:334:PRO:O	1:F:339:HIS:N	2.33	0.51
1:F:375:ARG:HD3	6:F:660:HOH:O	2.10	0.51
1:A:160:ARG:HE	1:A:161:ARG:NH1	2.06	0.51
1:C:199:ILE:HG23	1:C:244:LEU:CD2	2.37	0.51
1:E:346:ALA:O	1:E:350:ARG:HG2	2.10	0.51
1:H:339:HIS:CD2	1:H:352:ILE:HD13	2.45	0.51
1:D:335:ALA:HB1	1:D:347:ARG:HD2	1.93	0.51
1:D:91:GLN:O	1:D:116:ARG:N	2.40	0.51
1:C:137:LEU:HG	1:C:167:ALA:HB2	1.93	0.51
1:E:347:ARG:O	1:E:352:ILE:N	2.44	0.51
1:G:108:ASP:O	1:G:112:ARG:HD2	2.10	0.51
1:A:113:GLN:HG3	1:B:113:GLN:HB3	1.91	0.51
1:B:6:PHE:HA	1:B:9:ARG:NE	2.24	0.51
1:F:97:ASP:HA	1:F:119:TYR:CD2	2.38	0.51
1:H:259:ARG:NH1	6:H:589:HOH:O	2.41	0.51
1:B:118:ARG:HG2	1:B:134:GLU:HG3	1.91	0.51
1:B:9:ARG:NE	1:B:66:ARG:HH11	2.08	0.51
1:E:347:ARG:O	1:E:351:GLY:N	2.43	0.51
1:F:168:ARG:NE	4:F:408:CL:CL	2.81	0.51
1:F:118:ARG:NH2	1:F:134:GLU:OE2	2.39	0.51
1:G:91:GLN:HA	1:G:136:ASP:HB3	1.93	0.51
1:H:354:GLU:O	6:H:604:HOH:O	2.19	0.51
1:A:88:ARG:NH1	6:A:654:HOH:O	2.43	0.51
1:A:236:ASP:OD1	1:A:236:ASP:N	2.44	0.51
1:E:16:ARG:O	6:E:555:HOH:O	2.19	0.51
1:E:143:GLU:HG3	1:E:172:ASP:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:GLU:OE2	1:H:37:ARG:N	2.33	0.51
1:B:120:ALA:HB1	6:B:580:HOH:O	2.10	0.51
6:A:617:HOH:O	1:D:4:MSE:HE1	2.09	0.51
1:F:147:ASN:N	6:F:666:HOH:O	2.44	0.51
1:E:161:ARG:NH2	1:E:164:GLU:OE2	2.43	0.51
1:E:178:PRO:HG3	1:E:193:TYR:OH	2.10	0.51
1:H:285:HIS:HA	1:H:288:VAL:HB	1.92	0.51
1:C:41:GLU:OE1	1:C:42:PRO:HD2	2.11	0.51
1:C:44:TYR:HA	1:C:50:GLU:HB2	1.93	0.51
1:B:368:ASP:OD2	1:C:8:THR:HG21	2.11	0.51
1:C:100:TYR:OH	2:C:401:MES:H62	2.11	0.51
1:F:84:LEU:HD12	1:F:106:LEU:HB3	1.93	0.51
1:G:132:LEU:C	1:G:134:GLU:H	2.13	0.51
1:G:66:ARG:O	3:G:402:GOL:H31	2.10	0.51
1:F:173:ASN:HB3	1:F:193:TYR:CE1	2.45	0.51
1:E:339:HIS:O	1:E:347:ARG:NH1	2.38	0.51
1:G:147:ASN:HD21	1:G:358:ARG:NH1	2.07	0.51
1:D:60:CYS:SG	1:D:244:LEU:HD13	2.51	0.51
1:E:150:LEU:HD13	1:E:277:PRO:HD3	1.92	0.51
1:E:322:VAL:O	1:E:323:SER:OG	2.19	0.51
1:F:128:ILE:O	1:F:132:LEU:HB2	2.10	0.51
1:C:334:PRO:HA	1:C:338:THR:HG22	1.92	0.51
1:E:148:PRO:HD3	1:E:339:HIS:CE1	2.46	0.51
1:D:160:ARG:HB3	1:D:161:ARG:HE	1.76	0.51
1:G:213:ARG:NE	3:G:402:GOL:H11	2.26	0.51
1:C:293:SER:OG	6:C:673:HOH:O	2.08	0.51
1:F:109:LEU:O	1:F:113:GLN:HG2	2.11	0.51
1:H:148:PRO:HD3	1:H:339:HIS:CE1	2.46	0.51
1:H:35:GLU:OE2	1:H:37:ARG:NE	2.27	0.51
3:B:404:GOL:O1	3:B:404:GOL:O3	2.27	0.51
1:C:343:SER:O	1:C:346:ALA:N	2.44	0.51
1:D:339:HIS:HD2	1:D:352:ILE:HD13	1.74	0.51
1:F:95:SER:HB2	1:F:141:TRP:HB3	1.92	0.51
1:G:319:THR:HG23	1:H:35:GLU:OE1	2.11	0.51
1:H:375:ARG:NH2	6:H:638:HOH:O	2.20	0.51
1:H:39:GLN:OE1	1:H:44:TYR:HB2	2.11	0.51
1:B:116:ARG:NH2	1:B:134:GLU:OE2	2.42	0.51
1:G:95:SER:O	1:G:120:ALA:N	2.44	0.51
1:C:340:ARG:O	1:C:342:LEU:N	2.41	0.51
1:H:180:LEU:HB3	1:H:292:MSE:HE3	1.93	0.51
1:C:64:LEU:HB2	6:C:537:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ARG:N	1:D:368:ASP:OD1	2.44	0.51
1:H:122:LEU:N	6:H:680:HOH:O	2.27	0.51
1:H:39:GLN:NE2	1:H:44:TYR:HB2	2.21	0.51
1:C:100:TYR:OH	2:C:401:MES:H62	2.11	0.51
1:D:95:SER:O	1:D:120:ALA:N	2.43	0.51
1:F:124:THR:C	1:F:126:GLU:H	2.13	0.51
1:F:43:ARG:HD3	1:F:44:TYR:CE2	2.46	0.51
1:F:9:ARG:HG3	1:F:64:LEU:HD23	1.91	0.51
1:B:3:GLY:HA3	1:B:66:ARG:HH22	1.76	0.51
1:C:36:ARG:HD2	6:D:648:HOH:O	2.10	0.51
1:H:44:TYR:OH	1:H:55:GLU:OE2	2.23	0.51
1:E:280:PRO:HA	1:E:285:HIS:CD2	2.39	0.51
1:H:11:VAL:HA	1:H:245:HIS:CD2	2.41	0.51
1:A:309:GLU:OE1	1:A:309:GLU:N	2.25	0.51
1:G:260:VAL:O	1:G:263:GLU:HG2	2.10	0.51
1:G:4:MSE:O	1:G:9:ARG:NE	2.38	0.51
1:B:105:GLY:HA2	1:B:108:ASP:OD2	2.11	0.51
1:F:31:SER:HB2	1:H:25:VAL:HB	1.93	0.51
1:E:94:VAL:HG21	1:E:131:ALA:O	2.11	0.51
1:C:338:THR:HB	2:C:401:MES:C7	2.41	0.51
1:A:198:SER:OG	6:A:563:HOH:O	2.19	0.51
1:F:5:ARG:NH1	1:G:368:ASP:OD1	2.39	0.51
1:D:337:MSE:O	1:D:338:THR:C	2.48	0.51
1:G:152:VAL:CG1	1:G:284:GLN:HB2	2.41	0.51
1:G:159:SER:HA	1:G:169:VAL:HG21	1.93	0.51
1:G:332:GLU:OE2	1:G:358:ARG:NH2	2.44	0.51
1:B:9:ARG:HD3	1:B:66:ARG:NH2	2.26	0.51
1:G:116:ARG:NH2	6:G:501:HOH:O	1.96	0.51
1:G:152:VAL:HG21	1:G:288:VAL:HG22	1.93	0.51
1:H:60:CYS:SG	1:H:244:LEU:HD13	2.51	0.51
1:C:43:ARG:NH1	1:C:55:GLU:OE2	2.43	0.51
1:C:4:MSE:SE	1:C:8:THR:O	2.79	0.51
1:F:161:ARG:NE	1:F:164:GLU:OE2	2.44	0.51
1:B:345:GLU:O	1:B:349:ARG:HD3	2.11	0.51
1:B:111:ALA:HA	1:B:115:VAL:O	2.11	0.51
1:B:116:ARG:NH2	1:B:135:PRO:O	2.43	0.51
1:C:233:GLY:HA3	1:D:236:ASP:OD1	2.11	0.51
1:D:17:PRO:HA	6:D:622:HOH:O	2.10	0.51
1:G:84:LEU:HD12	1:G:106:LEU:HB3	1.92	0.51
1:G:320:CYS:SG	1:H:36:ARG:HG3	2.51	0.51
1:E:84:LEU:HD11	1:E:107:PHE:HD1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ARG:NH1	6:A:502:HOH:O	2.43	0.51
1:F:6:PHE:CZ	1:F:179:VAL:HG22	2.45	0.51
1:A:111:ALA:O	1:E:116:ARG:HD3	2.11	0.51
1:G:123:THR:O	1:G:123:THR:OG1	2.28	0.51
1:H:289:LYS:HB2	6:H:642:HOH:O	2.11	0.51
1:B:249:LEU:HD21	1:C:253:ARG:HD2	1.92	0.51
1:B:5:ARG:NH2	1:C:371:GLU:OE2	2.40	0.51
1:A:350:ARG:HD2	1:A:352:ILE:HD11	1.92	0.51
1:E:43:ARG:HB3	1:E:43:ARG:HH11	1.76	0.51
1:A:367:GLN:OE1	6:A:682:HOH:O	2.18	0.51
1:A:36:ARG:NH1	1:B:337:MSE:SE	2.94	0.51
1:E:281:GLU:OE1	6:E:501:HOH:O	2.19	0.51
1:H:347:ARG:HH21	1:H:354:GLU:CD	2.14	0.51
1:B:84:LEU:HD23	1:B:106:LEU:HB3	1.93	0.51
1:C:101:ALA:O	1:C:104:ASP:HB2	2.11	0.51
1:D:123:THR:HB	1:D:284:GLN:NE2	2.26	0.51
1:B:43:ARG:HD3	1:B:44:TYR:CE2	2.46	0.51
1:D:254:GLN:OE1	6:D:622:HOH:O	2.19	0.51
1:H:144:THR:OG1	1:H:152:VAL:HG13	2.11	0.51
1:B:259:ARG:NE	6:B:630:HOH:O	2.43	0.51
1:E:347:ARG:O	1:E:351:GLY:N	2.44	0.51
1:A:35:GLU:HB3	1:A:38:ALA:HB3	1.94	0.51
1:G:148:PRO:O	1:G:149:LEU:HD23	2.11	0.51
1:A:16:ARG:O	1:A:18:SER:N	2.44	0.51
1:G:352:ILE:HG23	1:G:356:LEU:HD23	1.93	0.51
1:A:336:LEU:O	1:A:340:ARG:HB2	2.11	0.50
1:A:5:ARG:H	1:D:368:ASP:CG	2.14	0.50
1:F:35:GLU:HG2	1:F:38:ALA:HB2	1.92	0.50
1:G:164:GLU:O	6:G:671:HOH:O	2.19	0.50
2:C:401:MES:H61	1:D:46:TYR:CG	2.46	0.50
1:E:368:ASP:OD1	1:H:5:ARG:NH1	2.40	0.50
1:G:276:TYR:HB3	1:G:279:LEU:HG	1.92	0.50
1:G:88:ARG:HH21	1:G:88:ARG:HB2	1.76	0.50
1:D:93:VAL:HG22	1:D:139:LEU:HB3	1.92	0.50
1:A:45:PHE:HD2	1:A:50:GLU:OE1	1.94	0.50
1:D:18:SER:OG	1:D:21:THR:OG1	2.28	0.50
1:F:149:LEU:HD11	1:F:350:ARG:O	2.11	0.50
1:A:33:THR:HG22	1:B:203:ALA:HB1	1.92	0.50
1:E:367:GLN:CD	6:E:671:HOH:O	2.48	0.50
1:G:266:ARG:NH2	1:G:279:LEU:HD22	2.26	0.50
2:C:401:MES:H61	1:D:46:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:SER:OG	6:D:617:HOH:O	2.18	0.50
1:E:339:HIS:HD2	1:E:342:LEU:HD12	1.76	0.50
2:C:401:MES:H61	1:D:46:TYR:CD2	2.47	0.50
1:G:100:TYR:CD1	1:G:101:ALA:N	2.79	0.50
1:G:332:GLU:CB	1:G:358:ARG:HB3	2.40	0.50
1:H:346:ALA:O	1:H:349:ARG:N	2.30	0.50
1:D:132:LEU:HA	1:D:137:LEU:HD22	1.93	0.50
1:E:143:GLU:HG3	1:E:172:ASP:HB3	1.94	0.50
1:H:100:TYR:CE1	2:H:401:MES:H31	2.46	0.50
1:H:100:TYR:OH	2:H:401:MES:H62	2.11	0.50
1:E:89:PRO:HA	1:E:114:GLY:C	2.31	0.50
6:A:683:HOH:O	1:B:233:GLY:HA3	2.10	0.50
1:B:40:ASP:N	1:B:40:ASP:OD2	2.35	0.50
1:E:284:GLN:NE2	6:E:657:HOH:O	2.35	0.50
1:C:84:LEU:HD21	1:C:107:PHE:HE1	1.75	0.50
1:G:132:LEU:CD1	1:G:161:ARG:HB3	2.41	0.50
1:G:380:GLY:N	6:G:634:HOH:O	2.33	0.50
1:A:344:ALA:N	6:A:663:HOH:O	2.43	0.50
1:C:339:HIS:CD2	1:C:352:ILE:HD13	2.46	0.50
1:C:157:GLU:OE2	1:C:161:ARG:NH1	2.38	0.50
1:C:316:THR:HG1	1:C:375:ARG:NH1	2.09	0.50
1:C:96:THR:HA	1:C:120:ALA:H	1.75	0.50
1:E:5:ARG:NH1	1:H:367:GLN:HB3	2.26	0.50
1:D:108:ASP:OD2	6:D:657:HOH:O	2.19	0.50
1:H:92:CYS:SG	1:H:93:VAL:N	2.84	0.50
1:D:254:GLN:NE2	6:D:560:HOH:O	2.20	0.50
1:E:84:LEU:HD13	1:E:110:ALA:HB2	1.92	0.50
1:E:94:VAL:HA	1:E:118:ARG:O	2.12	0.50
1:F:27:PRO:HB2	1:H:27:PRO:HB2	1.93	0.50
1:G:142:ILE:HA	6:G:667:HOH:O	2.11	0.50
1:A:240:VAL:O	1:A:244:LEU:HD23	2.12	0.50
1:G:107:PHE:CG	1:G:117:VAL:HG11	2.46	0.50
1:A:367:GLN:HG2	1:D:5:ARG:NH1	2.25	0.50
1:E:16:ARG:HB2	1:E:56:GLU:OE1	2.11	0.50
1:G:97:ASP:OD1	6:G:657:HOH:O	2.19	0.50
1:H:334:PRO:HB3	1:H:339:HIS:CD2	2.45	0.50
1:B:197:LLP:H6	6:B:559:HOH:O	2.11	0.50
1:C:163:HIS:HE1	1:C:187:GLY:O	1.94	0.50
1:A:323:SER:N	2:A:401:MES:O2S	2.36	0.50
1:B:95:SER:O	1:B:120:ALA:N	2.34	0.50
1:D:168:ARG:HH12	3:D:404:GOL:H32	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:ASN:HD21	1:E:358:ARG:HH11	1.59	0.50
1:F:292:MSE:CE	1:F:295:PRO:HA	2.40	0.50
1:D:277:PRO:HB2	1:D:292:MSE:HE1	1.93	0.50
1:D:333:CYS:O	1:D:337:MSE:HB2	2.12	0.50
1:A:341:PRO:O	1:A:342:LEU:HD12	2.11	0.50
1:D:147:ASN:HD21	1:D:358:ARG:HH11	1.59	0.50
1:G:332:GLU:CG	1:G:337:MSE:HG2	2.41	0.50
1:B:342:LEU:HB3	6:B:675:HOH:O	2.12	0.50
1:E:345:GLU:O	1:E:347:ARG:N	2.44	0.50
1:B:365:ASP:H	1:C:8:THR:HG23	1.76	0.50
1:H:99:VAL:HG21	1:H:107:PHE:HE2	1.77	0.50
1:F:5:ARG:NH1	1:G:368:ASP:OD1	2.44	0.50
1:A:343:SER:H	1:A:346:ALA:HB3	1.77	0.50
1:C:128:ILE:HG12	1:C:158:VAL:HG22	1.94	0.50
1:F:360:SER:OG	6:F:541:HOH:O	2.18	0.50
1:G:319:THR:HG23	1:H:35:GLU:OE1	2.12	0.50
1:H:157:GLU:OE1	1:H:161:ARG:NH1	2.44	0.50
1:H:197:LLP:HB2	1:H:324:LEU:HD12	1.93	0.50
1:E:213:ARG:HH11	3:E:402:GOL:C2	2.12	0.50
1:G:285:HIS:CD2	6:G:1467:HOH:O	2.63	0.50
1:B:15:ARG:HG2	6:B:593:HOH:O	2.10	0.50
1:D:142:ILE:HG22	1:D:144:THR:HB	1.92	0.50
1:E:116:ARG:NH2	1:E:136:ASP:HB2	2.24	0.50
1:E:40:ASP:O	1:E:42:PRO:HD3	2.11	0.50
1:F:189:ASP:HB3	3:F:406:CL:CL	2.48	0.50
1:G:137:LEU:H	1:G:165:ARG:NH2	2.09	0.50
1:G:132:LEU:HD12	1:G:161:ARG:HB3	1.93	0.50
1:H:105:GLY:O	1:H:109:LEU:N	2.38	0.50
1:H:168:ARG:NE	4:H:406:CL:CL	2.76	0.50
1:C:33:THR:HG21	6:D:656:HOH:O	2.12	0.50
1:E:131:ALA:O	1:E:134:GLU:HG2	2.12	0.50
1:F:259:ARG:HH12	1:F:295:PRO:HD2	1.76	0.50
1:D:264:ARG:NH1	1:D:370:ALA:HB1	2.27	0.50
1:F:180:LEU:HD22	1:F:294:ALA:HB3	1.94	0.50
1:A:199:ILE:HG23	1:A:244:LEU:CD2	2.35	0.50
1:C:285:HIS:HD2	6:C:621:HOH:O	1.95	0.50
1:C:276:TYR:OH	1:C:295:PRO:HG2	2.11	0.50
1:E:276:TYR:OH	1:E:295:PRO:HG2	2.12	0.50
1:D:43:ARG:NH1	1:D:43:ARG:HG3	2.25	0.50
1:A:135:PRO:HG2	1:E:112:ARG:HD3	1.93	0.50
1:G:288:VAL:HG22	1:G:292:MSE:SE	2.61	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:NH2	1:A:130:ALA:O	2.43	0.50
1:F:27:PRO:HB2	1:H:27:PRO:HB2	1.92	0.50
1:B:96:THR:O	1:B:119:TYR:HD1	1.93	0.50
1:E:181:GLN:HB2	1:E:292:MSE:HG2	1.93	0.50
1:D:77:GLN:OE1	1:D:102:GLY:HA3	2.12	0.50
1:G:121:ASP:OD1	1:G:123:THR:OG1	2.24	0.50
1:E:131:ALA:O	1:E:134:GLU:HG2	2.12	0.50
1:H:264:ARG:NH2	1:H:374:SER:HG	2.10	0.50
1:A:113:GLN:NE2	1:B:113:GLN:HB3	2.26	0.50
1:F:222:ARG:O	1:F:226:THR:HG23	2.11	0.50
1:B:40:ASP:N	6:B:660:HOH:O	1.99	0.50
1:C:175:PHE:HD1	1:C:175:PHE:C	2.15	0.50
1:D:84:LEU:HD12	1:D:106:LEU:HB3	1.92	0.50
1:F:285:HIS:HA	1:F:288:VAL:HB	1.93	0.50
1:C:28:ILE:HG21	1:C:235:LEU:HD23	1.93	0.50
1:E:100:TYR:HE1	2:E:401:MES:H31	1.77	0.50
1:F:96:THR:O	1:F:98:ASP:N	2.45	0.50
1:C:145:PRO:HD3	1:C:292:MSE:HE2	1.93	0.50
1:B:3:GLY:C	1:B:4:MSE:SE	3.00	0.50
1:H:197:LLP:O3	1:H:197:LLP:NZ	2.37	0.50
1:A:20:GLY:O	1:C:39:GLN:HB3	2.12	0.50
1:F:214:ASP:HB2	1:F:217:LEU:HB3	1.94	0.50
1:H:160:ARG:HB3	1:H:161:ARG:HH22	1.75	0.50
1:H:253:ARG:HG2	1:H:363:ILE:HG22	1.94	0.50
1:B:145:PRO:HD2	1:B:175:PHE:CD1	2.47	0.50
1:A:20:GLY:O	1:C:39:GLN:HG2	2.12	0.50
1:E:259:ARG:NE	6:E:572:HOH:O	2.30	0.50
1:B:58:GLU:OE1	6:B:573:HOH:O	2.18	0.50
1:F:339:HIS:HA	6:F:640:HOH:O	2.11	0.50
1:H:124:THR:OG1	1:H:126:GLU:HG2	2.11	0.50
1:E:95:SER:HB2	1:E:141:TRP:HB3	1.93	0.50
1:H:295:PRO:HG3	6:H:607:HOH:O	2.10	0.50
1:H:173:ASN:HB3	1:H:193:TYR:CE1	2.46	0.50
1:A:368:ASP:OD1	1:D:5:ARG:NH1	2.42	0.50
1:E:97:ASP:OD2	1:E:98:ASP:N	2.44	0.50
1:G:107:PHE:CG	1:G:117:VAL:HG11	2.47	0.50
1:H:322:VAL:HB	2:H:401:MES:H32	1.93	0.50
1:A:99:VAL:HG13	1:A:103:THR:HB	1.94	0.50
1:B:55:GLU:OE1	6:B:605:HOH:O	2.17	0.50
1:C:276:TYR:OH	1:C:295:PRO:HG2	2.11	0.50
1:G:98:ASP:OD1	1:G:98:ASP:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:VAL:O	1:B:292:MSE:HB3	2.11	0.50
1:D:314:ARG:HH22	1:D:379:GLY:HA2	1.77	0.50
1:B:9:ARG:HD3	1:B:66:ARG:NH2	2.26	0.50
1:D:277:PRO:HG2	1:D:292:MSE:HE1	1.94	0.50
1:G:322:VAL:O	1:G:323:SER:OG	2.28	0.50
1:H:110:ALA:HB1	1:H:115:VAL:HG21	1.94	0.50
1:B:180:LEU:HD22	1:B:294:ALA:HB3	1.93	0.50
1:E:95:SER:OG	1:E:99:VAL:HG11	2.11	0.50
1:B:367:GLN:HB2	6:B:697:HOH:O	2.11	0.50
1:F:181:GLN:HE21	1:F:291:GLN:HG3	1.77	0.50
1:A:36:ARG:NH1	1:B:337:MSE:HG3	2.23	0.50
1:F:100:TYR:HE1	2:F:401:MES:H71	1.76	0.50
1:F:181:GLN:HE21	1:F:291:GLN:HG3	1.76	0.50
1:F:16:ARG:HG3	1:F:56:GLU:HG2	1.93	0.50
1:G:9:ARG:NH2	1:G:66:ARG:HE	2.10	0.50
1:B:118:ARG:NH2	1:B:119:TYR:O	2.45	0.50
1:C:161:ARG:NE	6:C:674:HOH:O	2.43	0.50
1:F:288:VAL:HA	1:F:292:MSE:HE3	1.94	0.50
1:F:118:ARG:NH1	1:F:130:ALA:O	2.45	0.50
1:F:259:ARG:NH1	6:F:597:HOH:O	2.30	0.50
1:B:263:GLU:O	6:B:501:HOH:O	2.19	0.50
1:E:178:PRO:HD3	1:E:193:TYR:CE1	2.47	0.50
1:E:332:GLU:OE1	1:E:338:THR:OG1	2.19	0.50
1:A:249:LEU:HD21	1:D:253:ARG:HD2	1.94	0.50
1:B:133:ALA:HA	1:B:165:ARG:HH11	1.76	0.50
1:D:372:ASP:HA	1:D:375:ARG:HH11	1.77	0.50
1:C:303:TYR:O	1:C:355:SER:OG	2.27	0.50
1:G:157:GLU:O	1:G:161:ARG:HD2	2.11	0.50
1:B:29:HIS:CD2	3:B:405:GOL:HO3	2.30	0.50
1:D:341:PRO:O	1:D:343:SER:N	2.44	0.50
1:G:275:HIS:HB2	1:G:300:SER:OG	2.12	0.50
1:F:288:VAL:HG13	1:F:292:MSE:SE	2.61	0.50
1:A:36:ARG:NH2	6:A:597:HOH:O	2.44	0.50
1:E:332:GLU:HB2	1:E:337:MSE:CE	2.41	0.50
1:F:255:VAL:O	1:F:259:ARG:HG2	2.11	0.50
1:F:277:PRO:O	1:F:288:VAL:HG11	2.12	0.50
1:F:372:ASP:OD1	1:F:375:ARG:NH1	2.44	0.50
1:G:43:ARG:HB2	6:G:659:HOH:O	2.11	0.50
1:B:335:ALA:HB1	1:B:354:GLU:OE1	2.12	0.50
1:C:350:ARG:NH2	6:C:652:HOH:O	2.45	0.50
1:C:375:ARG:NH1	6:C:582:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ARG:NH1	6:D:514:HOH:O	2.20	0.50
1:F:33:THR:HG23	1:H:24:VAL:HB	1.93	0.50
1:G:98:ASP:OD1	1:G:98:ASP:N	2.43	0.50
1:H:11:VAL:HA	1:H:245:HIS:CD2	2.46	0.50
1:H:152:VAL:O	1:H:284:GLN:NE2	2.44	0.50
1:E:100:TYR:CE1	2:E:401:MES:H31	2.47	0.50
1:E:128:ILE:HG23	1:E:132:LEU:HD22	1.94	0.50
1:G:152:VAL:H	1:G:284:GLN:HE21	1.60	0.50
1:B:334:PRO:O	1:B:339:HIS:N	2.43	0.50
1:C:338:THR:C	1:C:341:PRO:HD2	2.32	0.50
1:D:264:ARG:NH2	6:D:651:HOH:O	2.45	0.50
1:E:100:TYR:CZ	2:E:401:MES:H51	2.46	0.50
1:E:32:THR:OG1	1:E:33:THR:HG22	2.12	0.50
1:F:98:ASP:OD2	1:F:98:ASP:N	2.44	0.50
1:G:266:ARG:HH22	1:G:279:LEU:HD22	1.76	0.50
1:B:245:HIS:HB3	1:C:327:VAL:HG21	1.94	0.50
1:B:36:ARG:NH2	1:B:45:PHE:HD1	2.10	0.50
1:C:16:ARG:HA	6:C:648:HOH:O	2.12	0.50
1:E:338:THR:OG1	1:E:339:HIS:ND1	2.36	0.50
1:A:77:GLN:OE1	1:A:102:GLY:HA3	2.12	0.50
1:D:346:ALA:O	1:D:350:ARG:HG3	2.11	0.50
1:A:124:THR:HG23	1:A:127:GLY:H	1.77	0.50
1:B:148:PRO:HD3	1:B:339:HIS:CE1	2.46	0.50
1:A:342:LEU:HD21	1:A:350:ARG:NH2	2.27	0.50
1:C:143:GLU:HG3	1:C:172:ASP:HB3	1.94	0.50
1:C:253:ARG:NH1	6:C:641:HOH:O	2.31	0.50
1:D:346:ALA:O	1:D:348:ALA:N	2.45	0.49
1:D:91:GLN:OE1	1:D:138:ALA:HB2	2.12	0.49
1:H:277:PRO:HA	1:H:282:HIS:CD2	2.47	0.49
1:D:252:HIS:HB3	6:D:669:HOH:O	2.11	0.49
1:E:323:SER:N	2:E:401:MES:O2S	2.41	0.49
1:G:334:PRO:C	1:G:339:HIS:HB2	2.33	0.49
1:D:39:GLN:O	1:D:42:PRO:HD3	2.12	0.49
1:E:35:GLU:OE1	1:E:37:ARG:NH2	2.35	0.49
1:H:157:GLU:HA	1:H:160:ARG:HH12	1.75	0.49
1:F:364:GLU:HB2	1:F:369:LEU:HD11	1.93	0.49
1:C:342:LEU:HB3	1:C:347:ARG:HG3	1.93	0.49
1:G:190:VAL:HG22	1:G:212:TYR:HB3	1.93	0.49
1:A:68:PRO:HG2	1:A:213:ARG:HA	1.93	0.49
1:C:148:PRO:HD3	1:C:339:HIS:NE2	2.27	0.49
1:C:199:ILE:HA	1:C:247:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:PHE:O	1:D:10:LEU:N	2.42	0.49
1:F:128:ILE:O	1:F:132:LEU:HD13	2.11	0.49
1:G:292:MSE:SE	1:G:293:SER:H	2.45	0.49
1:D:97:ASP:HB3	1:D:119:TYR:HB3	1.93	0.49
1:H:367:GLN:NE2	6:H:611:HOH:O	2.38	0.49
1:E:5:ARG:N	1:H:368:ASP:OD2	2.33	0.49
1:F:97:ASP:HA	1:F:119:TYR:CD2	2.47	0.49
1:G:18:SER:N	6:G:616:HOH:O	2.44	0.49
1:F:124:THR:HG23	1:F:127:GLY:HA3	1.94	0.49
1:D:253:ARG:NH2	6:D:598:HOH:O	2.16	0.49
1:E:147:ASN:ND2	6:E:542:HOH:O	2.45	0.49
1:G:101:ALA:O	6:G:674:HOH:O	2.19	0.49
1:B:332:GLU:OE2	1:B:338:THR:OG1	2.29	0.49
1:D:276:TYR:OH	1:D:295:PRO:HG2	2.12	0.49
4:A:405:GOL:C1	1:B:105:GLY:HA3	2.43	0.49
1:D:314:ARG:NH2	1:D:379:GLY:HA2	2.27	0.49
1:E:7:GLY:N	6:E:594:HOH:O	2.44	0.49
1:A:146:THR:O	1:A:150:LEU:HA	2.11	0.49
1:D:292:MSE:SE	6:D:631:HOH:O	2.80	0.49
1:F:9:ARG:CZ	1:F:66:ARG:HD3	2.42	0.49
1:H:92:CYS:HB2	1:H:116:ARG:NH1	2.27	0.49
1:C:43:ARG:HB2	1:C:44:TYR:CE1	2.47	0.49
1:F:38:ALA:HB3	1:H:22:GLY:HA2	1.93	0.49
1:C:340:ARG:HG2	1:C:341:PRO:HD3	1.94	0.49
1:H:213:ARG:NH2	6:H:633:HOH:O	2.44	0.49
1:D:161:ARG:NH2	1:D:164:GLU:OE2	2.45	0.49
1:F:29:HIS:CD2	1:F:52:PRO:HB2	2.47	0.49
1:B:43:ARG:HB2	6:B:684:HOH:O	2.12	0.49
1:B:88:ARG:NE	1:E:136:ASP:OD1	2.42	0.49
1:F:340:ARG:H	1:F:341:PRO:CD	2.20	0.49
1:C:348:ALA:O	6:C:628:HOH:O	2.18	0.49
1:G:263:GLU:HG2	6:G:510:HOH:O	2.12	0.49
1:B:16:ARG:NE	6:B:652:HOH:O	2.21	0.49
3:B:406:GOL:O1	3:B:406:GOL:O3	2.27	0.49
1:F:37:ARG:NH1	6:F:667:HOH:O	2.45	0.49
1:A:37:ARG:HH22	1:B:320:CYS:N	1.98	0.49
1:B:99:VAL:CG1	1:B:103:THR:HB	2.43	0.49
1:D:277:PRO:O	6:D:612:HOH:O	2.19	0.49
1:G:97:ASP:HA	1:G:119:TYR:CD1	2.48	0.49
1:C:92:CYS:SG	1:C:116:ARG:NH2	2.85	0.49
1:A:36:ARG:NH2	1:B:337:MSE:HE3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:TYR:CE1	2:E:401:MES:H82	2.45	0.49
1:G:147:ASN:ND2	1:G:358:ARG:HH11	2.09	0.49
1:H:7:GLY:HA2	1:H:10:LEU:HD12	1.94	0.49
1:H:168:ARG:HH12	3:H:405:GOL:H32	1.78	0.49
1:H:348:ALA:O	1:H:351:GLY:N	2.37	0.49
1:F:16:ARG:NE	1:F:59:GLU:OE2	2.46	0.49
1:E:27:PRO:HB2	1:G:27:PRO:HB2	1.93	0.49
1:C:175:PHE:CZ	1:C:298:ILE:HB	2.47	0.49
1:C:175:PHE:CD1	1:C:175:PHE:C	2.85	0.49
1:G:95:SER:HB2	1:G:141:TRP:HB3	1.93	0.49
1:A:316:THR:HG1	1:A:375:ARG:HH11	1.51	0.49
1:B:322:VAL:HB	2:B:401:MES:H72	1.93	0.49
1:B:367:GLN:OE1	6:B:666:HOH:O	2.20	0.49
1:B:36:ARG:HB2	1:B:36:ARG:HH21	1.77	0.49
1:C:337:MSE:CG	1:D:36:ARG:HE	2.25	0.49
1:F:96:THR:HG23	1:F:122:LEU:HD12	1.93	0.49
1:B:4:MSE:HG2	1:B:8:THR:HG21	1.93	0.49
1:C:3:GLY:O	1:C:4:MSE:SE	2.80	0.49
1:B:157:GLU:O	1:B:161:ARG:HD2	2.12	0.49
1:B:346:ALA:O	1:B:350:ARG:HB2	2.12	0.49
1:D:252:HIS:CD2	6:D:638:HOH:O	2.65	0.49
6:F:606:HOH:O	1:G:3:GLY:HA3	2.12	0.49
1:H:319:THR:HB	1:H:330:LEU:HD23	1.93	0.49
1:F:143:GLU:HG3	1:F:172:ASP:HB3	1.95	0.49
1:A:18:SER:HA	3:A:403:GOL:H11	1.93	0.49
1:B:339:HIS:O	1:B:347:ARG:HD3	2.13	0.49
1:F:277:PRO:CG	1:F:292:MSE:HE1	2.42	0.49
1:G:17:PRO:HA	6:G:683:HOH:O	2.11	0.49
1:B:3:GLY:C	1:B:66:ARG:HH12	2.16	0.49
1:E:16:ARG:NE	6:E:667:HOH:O	2.45	0.49
1:E:283:PRO:HB2	1:E:284:GLN:NE2	2.27	0.49
1:G:277:PRO:HA	1:G:282:HIS:CD2	2.48	0.49
1:G:332:GLU:OE2	1:G:338:THR:HG23	2.12	0.49
1:E:84:LEU:HD12	1:E:106:LEU:HB3	1.93	0.49
1:G:6:PHE:CZ	1:G:64:LEU:HD22	2.48	0.49
1:H:324:LEU:HD13	2:H:401:MES:O1S	2.13	0.49
1:A:199:ILE:HG23	1:A:244:LEU:HD13	1.93	0.49
1:A:98:ASP:HA	1:A:350:ARG:NH2	2.27	0.49
1:H:342:LEU:HD12	1:H:347:ARG:HG2	1.95	0.49
1:C:371:GLU:O	1:C:375:ARG:HB2	2.13	0.49
1:E:159:SER:HA	1:E:169:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:ASP:HA	6:H:678:HOH:O	2.12	0.49
1:H:88:ARG:O	1:H:115:VAL:HG22	2.13	0.49
1:E:97:ASP:OD1	1:E:97:ASP:N	2.40	0.49
1:H:197:LLP:HD3	1:H:324:LEU:HG	1.95	0.49
1:H:6:PHE:HZ	1:H:178:PRO:HB2	1.76	0.49
1:A:16:ARG:NE	1:A:59:GLU:OE1	2.43	0.49
1:D:122:LEU:O	1:D:153:VAL:HG22	2.13	0.49
1:F:126:GLU:HG3	1:F:127:GLY:H	1.77	0.49
1:H:4:MSE:O	1:H:9:ARG:NH1	2.45	0.49
6:C:696:HOH:O	1:D:37:ARG:CD	2.53	0.49
1:D:9:ARG:HB3	6:D:518:HOH:O	2.13	0.49
1:A:343:SER:HB2	6:A:663:HOH:O	2.12	0.49
1:B:44:TYR:CE2	1:D:21:THR:HG22	2.47	0.49
1:C:285:HIS:HB2	6:C:596:HOH:O	2.12	0.49
1:D:145:PRO:HG2	1:D:175:PHE:CE1	2.48	0.49
1:E:347:ARG:HD2	1:E:352:ILE:HB	1.94	0.49
1:H:255:VAL:O	1:H:259:ARG:HG3	2.11	0.49
1:G:66:ARG:O	3:G:402:GOL:H32	2.12	0.49
1:B:180:LEU:HD22	1:B:294:ALA:HB3	1.94	0.49
1:C:343:SER:O	1:C:346:ALA:N	2.44	0.49
1:C:43:ARG:O	1:C:50:GLU:HG2	2.12	0.49
1:B:180:LEU:HA	1:B:293:SER:OG	2.11	0.49
1:D:180:LEU:HD22	1:D:294:ALA:HB3	1.93	0.49
1:D:343:SER:O	1:D:347:ARG:N	2.45	0.49
1:D:344:ALA:HA	1:D:347:ARG:HB2	1.95	0.49
1:F:180:LEU:HD22	1:F:294:ALA:HB3	1.93	0.49
1:A:36:ARG:NH2	1:B:337:MSE:HG2	2.28	0.49
1:B:367:GLN:HG3	6:B:666:HOH:O	2.13	0.49
1:D:134:GLU:HB2	1:D:137:LEU:HB2	1.94	0.49
1:F:6:PHE:HA	1:F:9:ARG:HE	1.77	0.49
1:H:244:LEU:HD23	1:H:247:LEU:HB2	1.93	0.49
1:F:214:ASP:OD1	4:F:408:CL:CL	2.68	0.49
1:G:95:SER:O	1:G:120:ALA:N	2.44	0.49
1:E:97:ASP:C	1:E:99:VAL:H	2.15	0.49
1:H:174:THR:HB	1:H:197:LLP:H2'2	1.95	0.49
1:D:16:ARG:C	6:D:657:HOH:O	2.50	0.49
1:H:6:PHE:O	1:H:9:ARG:HB2	2.13	0.49
1:D:279:LEU:HB3	1:D:281:GLU:CG	2.42	0.49
1:F:174:THR:HB	1:F:197:LLP:H2'2	1.95	0.49
1:F:9:ARG:NH2	1:F:66:ARG:HH11	2.11	0.49
6:E:585:HOH:O	1:G:29:HIS:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HD12	1:B:161:ARG:HB3	1.95	0.49
1:B:288:VAL:HG22	1:B:292:MSE:HE1	1.94	0.49
1:E:35:GLU:OE2	1:E:36:ARG:N	2.46	0.49
1:B:17:PRO:HA	6:B:688:HOH:O	2.12	0.49
1:D:108:ASP:OD1	6:D:650:HOH:O	2.20	0.49
1:D:335:ALA:HB1	1:D:354:GLU:OE1	2.13	0.49
1:C:113:GLN:OE1	6:C:650:HOH:O	2.20	0.49
1:F:145:PRO:HD2	1:F:175:PHE:CD1	2.48	0.49
1:F:100:TYR:HE1	2:F:401:MES:H82	1.76	0.49
1:C:161:ARG:HD3	1:C:164:GLU:OE1	2.12	0.49
1:E:156:ALA:HB1	1:E:160:ARG:NH2	2.28	0.49
1:E:146:THR:OG1	1:E:151:THR:HG22	2.11	0.49
1:G:333:CYS:H	1:G:337:MSE:CE	2.26	0.49
1:F:34:TYR:CD1	1:F:44:TYR:HB3	2.46	0.49
1:A:346:ALA:O	1:A:350:ARG:HG3	2.13	0.49
1:E:276:TYR:CZ	1:E:295:PRO:HB2	2.47	0.49
1:E:333:CYS:O	1:E:335:ALA:N	2.46	0.49
1:H:253:ARG:HH11	1:H:253:ARG:HB2	1.78	0.49
1:D:198:SER:HA	1:D:325:GLY:O	2.12	0.49
1:E:213:ARG:HH11	3:E:402:GOL:H2	1.77	0.49
1:H:41:GLU:CB	6:H:512:HOH:O	2.60	0.49
1:H:97:ASP:C	1:H:99:VAL:H	2.15	0.49
1:C:11:VAL:HA	1:C:245:HIS:ND1	2.27	0.49
1:H:341:PRO:HA	6:H:648:HOH:O	2.13	0.49
1:A:102:GLY:HA2	3:B:403:GOL:H31	1.95	0.49
1:A:180:LEU:HD22	1:A:294:ALA:HB3	1.95	0.49
1:C:358:ARG:NH1	2:C:401:MES:O3S	2.43	0.49
1:B:214:ASP:HB2	6:B:516:HOH:O	2.12	0.49
1:B:364:GLU:HB3	1:C:8:THR:HG23	1.93	0.49
1:F:54:ARG:HG3	1:F:237:CYS:SG	2.53	0.49
1:E:3:GLY:C	1:E:4:MSE:HG2	2.33	0.49
1:E:45:PHE:HE2	6:F:649:HOH:O	1.94	0.49
1:F:254:GLN:HB3	1:F:297:ALA:HB2	1.95	0.49
1:G:287:VAL:HG23	6:G:678:HOH:O	2.12	0.49
1:A:214:ASP:OD2	1:A:217:LEU:N	2.41	0.49
1:A:29:HIS:NE2	3:A:403:GOL:H2	2.28	0.49
1:B:36:ARG:HH21	1:B:36:ARG:HB2	1.75	0.49
1:D:213:ARG:HE	3:D:402:GOL:H12	1.78	0.49
1:G:320:CYS:O	1:H:35:GLU:HA	2.13	0.49
1:H:6:PHE:CZ	1:H:178:PRO:HB2	2.48	0.49
1:C:327:VAL:HG23	1:C:363:ILE:CG1	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:LEU:HG	1:G:141:TRP:CZ3	2.48	0.49
1:B:173:ASN:HB3	1:B:193:TYR:CE1	2.47	0.49
1:E:333:CYS:O	1:E:336:LEU:N	2.32	0.49
1:E:35:GLU:OE1	1:F:319:THR:HG23	2.13	0.49
1:G:292:MSE:SE	1:G:294:ALA:H	2.45	0.49
1:C:320:CYS:O	1:D:35:GLU:HA	2.12	0.49
1:G:312:LEU:HD13	1:H:36:ARG:HH12	1.78	0.49
1:B:33:THR:HG23	1:D:24:VAL:HB	1.94	0.49
1:D:5:ARG:C	1:D:9:ARG:HE	2.16	0.49
2:E:401:MES:H61	1:F:46:TYR:CD2	2.48	0.49
1:E:4:MSE:HB3	6:E:652:HOH:O	2.13	0.49
1:F:358:ARG:NH2	6:F:507:HOH:O	2.45	0.49
1:H:344:ALA:O	1:H:347:ARG:HB2	2.13	0.49
1:B:199:ILE:HG23	1:B:244:LEU:HD21	1.94	0.49
1:G:121:ASP:OD1	1:G:123:THR:OG1	2.29	0.49
1:B:206:LEU:HD23	1:B:206:LEU:N	2.27	0.49
1:C:282:HIS:O	1:C:285:HIS:HB3	2.12	0.49
1:G:4:MSE:HB2	6:G:684:HOH:O	2.12	0.49
1:D:52:PRO:O	1:D:56:GLU:HG3	2.12	0.49
1:E:35:GLU:OE2	1:E:37:ARG:N	2.38	0.49
1:F:236:ASP:CG	6:F:676:HOH:O	2.51	0.49
1:B:18:SER:HA	3:B:405:GOL:O2	2.13	0.49
1:E:346:ALA:O	1:E:349:ARG:N	2.45	0.49
1:B:197:LLP:O3	6:B:550:HOH:O	2.20	0.49
1:B:367:GLN:HA	1:B:367:GLN:NE2	2.28	0.49
1:G:101:ALA:O	1:G:105:GLY:N	2.46	0.49
1:E:310:ARG:HH21	1:E:314:ARG:NH2	2.09	0.49
1:G:334:PRO:HD2	1:G:356:LEU:O	2.13	0.49
1:G:40:ASP:N	6:G:678:HOH:O	2.28	0.49
2:A:401:MES:H61	1:B:46:TYR:CD2	2.48	0.49
6:A:661:HOH:O	1:E:112:ARG:HD3	2.12	0.49
1:F:368:ASP:HB3	1:G:3:GLY:HA3	1.94	0.49
1:A:35:GLU:OE2	1:A:37:ARG:HG2	2.13	0.49
1:B:282:HIS:O	1:B:285:HIS:N	2.44	0.49
1:C:157:GLU:OE2	1:C:161:ARG:NH1	2.45	0.49
1:G:36:ARG:HG3	1:H:337:MSE:HE3	1.94	0.49
1:D:143:GLU:HG3	1:D:172:ASP:HB3	1.95	0.49
1:E:100:TYR:OH	2:E:401:MES:H62	2.13	0.49
1:F:100:TYR:CZ	2:F:401:MES:H62	2.48	0.49
1:G:121:ASP:O	1:G:123:THR:N	2.41	0.49
1:D:55:GLU:OE2	6:D:664:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:THR:HG23	1:F:35:GLU:OE1	2.13	0.49
1:F:16:ARG:HA	6:F:679:HOH:O	2.12	0.49
1:G:343:SER:O	1:G:347:ARG:NH1	2.46	0.49
1:C:84:LEU:HD21	1:C:107:PHE:HE1	1.78	0.49
1:G:312:LEU:HD13	1:H:36:ARG:NH1	2.28	0.49
1:E:198:SER:N	6:E:556:HOH:O	2.45	0.49
1:H:9:ARG:HD3	6:H:606:HOH:O	2.12	0.49
1:F:56:GLU:OE2	6:F:583:HOH:O	2.20	0.48
1:B:95:SER:HB2	1:B:141:TRP:HB3	1.95	0.48
1:B:6:PHE:HA	1:B:9:ARG:HE	1.78	0.48
1:D:124:THR:C	1:D:126:GLU:H	2.17	0.48
1:F:152:VAL:HG11	1:F:292:MSE:HE1	1.93	0.48
1:A:288:VAL:O	1:A:292:MSE:HB3	2.12	0.48
1:B:266:ARG:HG2	1:B:266:ARG:HH21	1.78	0.48
1:C:319:THR:HB	1:C:330:LEU:HD23	1.94	0.48
1:D:251:VAL:O	1:D:255:VAL:HG23	2.13	0.48
1:H:9:ARG:N	1:H:9:ARG:HD3	2.28	0.48
1:B:17:PRO:HB2	1:B:18:SER:H	1.37	0.48
1:C:100:TYR:CE1	2:C:401:MES:H72	2.48	0.48
1:D:6:PHE:HZ	1:D:178:PRO:HB2	1.77	0.48
1:D:180:LEU:O	1:D:293:SER:N	2.45	0.48
1:F:360:SER:OG	6:F:546:HOH:O	2.20	0.48
1:B:342:LEU:O	1:B:347:ARG:NH1	2.46	0.48
1:C:56:GLU:OE1	6:C:533:HOH:O	2.20	0.48
1:C:32:THR:HG22	1:D:206:LEU:HD23	1.95	0.48
1:D:332:GLU:HG2	1:D:358:ARG:HH21	1.78	0.48
1:E:11:VAL:HA	1:E:245:HIS:ND1	2.28	0.48
1:H:245:HIS:HE1	6:H:535:HOH:O	1.95	0.48
1:C:134:GLU:CD	1:C:135:PRO:HD2	2.33	0.48
1:C:214:ASP:HB3	1:C:217:LEU:HB3	1.95	0.48
1:A:181:GLN:HB2	1:A:292:MSE:SE	2.63	0.48
1:F:333:CYS:O	1:F:336:LEU:N	2.46	0.48
1:H:275:HIS:HE1	6:H:648:HOH:O	1.96	0.48
1:B:175:PHE:HB3	6:B:515:HOH:O	2.12	0.48
1:B:93:VAL:HG22	1:B:139:LEU:HB3	1.95	0.48
1:B:95:SER:HB2	1:B:141:TRP:HB3	1.95	0.48
1:G:156:ALA:O	1:G:160:ARG:HG2	2.12	0.48
1:B:373:LEU:O	1:B:377:LEU:HG	2.13	0.48
1:A:346:ALA:O	1:A:350:ARG:N	2.46	0.48
1:D:88:ARG:H	1:D:91:GLN:HE21	1.59	0.48
1:C:309:GLU:HG3	1:C:336:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ARG:HH21	1:C:89:PRO:HD2	1.77	0.48
1:D:36:ARG:O	1:D:38:ALA:N	2.46	0.48
1:E:54:ARG:HD3	6:E:600:HOH:O	2.11	0.48
1:B:146:THR:OG1	1:B:151:THR:N	2.42	0.48
1:E:44:TYR:CE2	1:G:21:THR:HG22	2.48	0.48
1:C:91:GLN:O	1:C:116:ARG:N	2.43	0.48
1:B:173:ASN:HB3	1:B:193:TYR:CE1	2.48	0.48
1:B:337:MSE:SE	1:B:338:THR:HG23	2.63	0.48
1:B:368:ASP:OD1	1:C:5:ARG:NH1	2.45	0.48
1:D:150:LEU:HD22	1:D:175:PHE:HE2	1.79	0.48
1:D:143:GLU:HG3	1:D:172:ASP:HB3	1.96	0.48
1:C:332:GLU:OE2	1:C:338:THR:N	2.40	0.48
1:C:54:ARG:HG3	1:C:237:CYS:SG	2.53	0.48
1:C:9:ARG:NH2	1:C:63:GLY:O	2.35	0.48
1:A:5:ARG:O	1:A:9:ARG:HG3	2.12	0.48
1:C:16:ARG:HD2	1:C:56:GLU:HG3	1.94	0.48
1:E:309:GLU:HA	1:E:312:LEU:HD12	1.95	0.48
1:E:181:GLN:NE2	1:E:292:MSE:SE	2.96	0.48
1:E:332:GLU:O	1:E:334:PRO:HD3	2.13	0.48
1:G:129:ALA:HB2	6:G:606:HOH:O	2.13	0.48
1:D:142:ILE:O	1:D:171:VAL:HA	2.12	0.48
1:B:15:ARG:HB2	1:B:15:ARG:NH2	2.27	0.48
1:D:43:ARG:HG3	1:D:44:TYR:CD2	2.49	0.48
1:G:96:THR:HG22	1:G:120:ALA:O	2.12	0.48
1:H:9:ARG:HB3	1:H:64:LEU:HD23	1.95	0.48
1:A:341:PRO:O	1:A:342:LEU:HG	2.13	0.48
1:D:94:VAL:HG11	1:D:131:ALA:HB1	1.95	0.48
1:E:180:LEU:HD22	1:E:294:ALA:HB3	1.94	0.48
1:A:9:ARG:HH21	1:A:64:LEU:HA	1.76	0.48
1:C:84:LEU:HD21	1:C:107:PHE:CE1	2.48	0.48
1:G:134:GLU:O	1:G:165:ARG:NH2	2.37	0.48
1:H:6:PHE:HE2	1:H:179:VAL:HG22	1.76	0.48
1:H:98:ASP:OD1	1:H:98:ASP:N	2.47	0.48
1:D:143:GLU:HG3	1:D:172:ASP:HB3	1.94	0.48
1:F:338:THR:HG23	1:F:339:HIS:CE1	2.48	0.48
1:G:292:MSE:HE2	6:G:1364:HOH:O	2.13	0.48
1:H:44:TYR:C	1:H:45:PHE:HD1	2.16	0.48
1:C:285:HIS:CG	1:C:286:ALA:N	2.82	0.48
1:E:84:LEU:HD13	1:E:110:ALA:HB2	1.95	0.48
1:A:16:ARG:HG3	6:A:653:HOH:O	2.12	0.48
1:E:332:GLU:O	1:E:334:PRO:HD3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:GLY:HA2	3:E:405:GOL:H31	1.95	0.48
1:F:100:TYR:HB2	6:F:639:HOH:O	2.14	0.48
1:F:95:SER:HB2	1:F:141:TRP:HB3	1.94	0.48
1:B:322:VAL:O	1:B:323:SER:OG	2.28	0.48
1:D:92:CYS:HA	1:D:116:ARG:O	2.13	0.48
1:E:277:PRO:HB3	1:E:288:VAL:HG21	1.94	0.48
1:G:4:MSE:HG2	1:G:9:ARG:HG2	1.95	0.48
1:H:347:ARG:NH1	1:H:354:GLU:OE2	2.46	0.48
1:A:281:GLU:CD	1:A:281:GLU:H	2.17	0.48
1:D:54:ARG:HG3	1:D:237:CYS:SG	2.54	0.48
1:A:108:ASP:HB3	1:A:112:ARG:NH1	2.27	0.48
1:D:97:ASP:H	1:D:119:TYR:HB3	1.78	0.48
1:E:314:ARG:NH1	1:E:375:ARG:O	2.40	0.48
1:G:132:LEU:HD12	1:G:161:ARG:HB3	1.95	0.48
1:G:288:VAL:HG13	1:G:292:MSE:SE	2.63	0.48
1:G:16:ARG:HA	1:G:16:ARG:NE	2.27	0.48
1:A:90:GLY:N	1:A:114:GLY:O	2.33	0.48
1:F:197:LLP:HD3	1:F:324:LEU:HG	1.96	0.48
1:G:113:GLN:NE2	1:H:113:GLN:OE1	2.40	0.48
1:B:97:ASP:O	1:B:350:ARG:NH2	2.46	0.48
1:C:283:PRO:HB3	6:C:671:HOH:O	2.13	0.48
1:D:339:HIS:HD2	1:D:352:ILE:HD13	1.79	0.48
1:G:112:ARG:NH2	6:G:503:HOH:O	2.46	0.48
1:H:213:ARG:HE	3:H:402:GOL:C2	2.25	0.48
1:F:6:PHE:CE2	1:F:179:VAL:HG22	2.48	0.48
1:B:3:GLY:HA2	1:B:66:ARG:CZ	2.43	0.48
1:C:84:LEU:HD23	1:C:106:LEU:HB3	1.94	0.48
1:D:332:GLU:CD	1:D:338:THR:HB	2.32	0.48
1:A:131:ALA:O	1:A:134:GLU:HG2	2.12	0.48
2:C:401:MES:H81	2:C:401:MES:H51	1.77	0.48
1:B:66:ARG:HH21	1:B:66:ARG:HB3	1.78	0.48
1:D:132:LEU:O	1:D:165:ARG:NE	2.44	0.48
1:D:66:ARG:NH2	6:D:625:HOH:O	2.47	0.48
1:G:100:TYR:CG	1:G:101:ALA:N	2.81	0.48
1:B:118:ARG:HE	1:B:131:ALA:HB2	1.79	0.48
1:C:180:LEU:HD22	1:C:294:ALA:HB3	1.95	0.48
1:D:104:ASP:HA	1:D:107:PHE:HB2	1.96	0.48
1:D:116:ARG:NH1	1:D:135:PRO:O	2.47	0.48
1:D:186:LEU:HD11	1:D:291:GLN:HB2	1.95	0.48
1:G:347:ARG:HA	1:G:352:ILE:HD12	1.94	0.48
1:H:145:PRO:HG3	1:H:292:MSE:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ASP:O	1:C:112:ARG:HG2	2.13	0.48
1:C:124:THR:HG23	1:C:127:GLY:H	1.79	0.48
1:G:252:HIS:HE1	6:G:575:HOH:O	1.96	0.48
1:B:282:HIS:HA	3:B:406:GOL:H11	1.94	0.48
1:E:367:GLN:NE2	6:E:649:HOH:O	2.46	0.48
1:F:298:ILE:HD11	1:F:324:LEU:HB2	1.95	0.48
1:C:293:SER:HB3	6:C:654:HOH:O	2.13	0.48
1:D:9:ARG:HH22	1:D:66:ARG:HG3	1.79	0.48
1:D:6:PHE:HE1	1:D:179:VAL:HG22	1.79	0.48
1:A:337:MSE:O	1:A:338:THR:HG23	2.13	0.48
1:F:94:VAL:HG21	1:F:131:ALA:O	2.13	0.48
1:A:285:HIS:ND1	6:A:571:HOH:O	2.34	0.48
1:C:320:CYS:HA	1:C:331:VAL:O	2.13	0.48
1:D:95:SER:N	1:D:118:ARG:O	2.35	0.48
1:F:160:ARG:HE	1:F:161:ARG:NH1	2.10	0.48
1:G:4:MSE:O	6:G:629:HOH:O	2.20	0.48
1:A:264:ARG:HD3	6:A:502:HOH:O	2.14	0.48
1:C:314:ARG:NH2	6:C:549:HOH:O	2.46	0.48
1:F:4:MSE:HA	1:F:8:THR:HB	1.94	0.48
1:A:4:MSE:C	1:A:9:ARG:HE	2.16	0.48
1:D:319:THR:HB	1:D:330:LEU:HD23	1.94	0.48
1:D:333:CYS:HB3	1:D:337:MSE:HE3	1.96	0.48
1:G:371:GLU:HB3	1:G:375:ARG:NH2	2.29	0.48
1:G:50:GLU:HA	6:G:569:HOH:O	2.13	0.48
1:A:21:THR:HG22	1:C:44:TYR:CE1	2.48	0.48
1:E:43:ARG:NH2	6:E:678:HOH:O	2.46	0.48
1:F:288:VAL:HG22	1:F:292:MSE:HE3	1.95	0.48
1:A:191:SER:HB3	1:A:193:TYR:CE2	2.48	0.48
1:C:173:ASN:HB3	1:C:193:TYR:CE1	2.47	0.48
1:F:49:GLY:O	1:F:54:ARG:NH2	2.46	0.48
1:G:98:ASP:O	6:G:538:HOH:O	2.20	0.48
1:H:99:VAL:HG21	1:H:107:PHE:CE2	2.48	0.48
1:B:282:HIS:CD2	3:B:405:GOL:H12	2.47	0.48
1:E:42:PRO:HB2	1:E:45:PHE:HE2	1.79	0.48
1:F:168:ARG:HH22	3:F:402:GOL:C1	2.25	0.48
1:G:213:ARG:NH2	3:G:402:GOL:O2	2.28	0.48
1:H:285:HIS:HD2	6:H:661:HOH:O	1.92	0.48
1:B:264:ARG:CZ	1:B:370:ALA:HB1	2.44	0.48
1:B:6:PHE:CE2	1:B:179:VAL:HG22	2.48	0.48
1:E:109:LEU:HA	1:E:112:ARG:HH11	1.78	0.48
1:C:33:THR:HG21	1:D:203:ALA:HB1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:CYS:SG	1:D:336:LEU:HD12	2.53	0.48
1:F:333:CYS:HB3	1:F:336:LEU:HB2	1.96	0.48
1:B:104:ASP:OD1	1:B:119:TYR:OH	2.23	0.48
1:D:310:ARG:NH1	6:D:502:HOH:O	2.23	0.48
1:D:322:VAL:CG1	1:D:338:THR:HG23	2.44	0.48
1:B:100:TYR:OH	2:B:401:MES:H62	2.14	0.48
1:D:108:ASP:O	1:D:112:ARG:HG2	2.14	0.48
1:A:206:LEU:HD11	1:B:48:ARG:HA	1.95	0.48
1:C:16:ARG:HH22	1:C:55:GLU:HB3	1.79	0.48
1:E:152:VAL:HG21	1:E:288:VAL:HG22	1.95	0.48
1:E:95:SER:OG	1:E:99:VAL:HG11	2.13	0.48
1:D:95:SER:O	1:D:120:ALA:N	2.46	0.48
1:G:325:GLY:O	6:G:527:HOH:O	2.20	0.48
1:E:21:THR:HG22	1:G:44:TYR:CE2	2.49	0.48
1:A:116:ARG:HD3	1:E:111:ALA:O	2.13	0.48
1:A:189:ASP:HA	1:A:213:ARG:HH22	1.78	0.48
1:G:323:SER:O	6:G:546:HOH:O	2.20	0.48
3:F:404:GOL:H12	6:F:583:HOH:O	2.14	0.48
1:H:92:CYS:HB2	1:H:116:ARG:NH2	2.29	0.48
1:E:32:THR:OG1	1:E:33:THR:HG22	2.14	0.48
1:G:43:ARG:HD3	1:G:44:TYR:CE2	2.48	0.48
1:G:46:TYR:CG	2:H:401:MES:H61	2.48	0.48
1:B:43:ARG:HG3	6:B:672:HOH:O	2.13	0.48
1:B:4:MSE:HG2	6:B:674:HOH:O	2.14	0.48
1:E:347:ARG:HA	1:E:350:ARG:CB	2.44	0.48
1:B:152:VAL:H	1:B:284:GLN:NE2	2.11	0.48
1:A:33:THR:HG23	1:B:203:ALA:HB1	1.94	0.48
1:A:184:LEU:HB3	3:A:404:GOL:H32	1.95	0.48
1:C:116:ARG:HB2	1:C:116:ARG:HH21	1.77	0.48
1:E:340:ARG:CA	1:E:347:ARG:HH12	2.26	0.48
1:F:120:ALA:HB3	1:F:131:ALA:HB2	1.95	0.48
1:H:118:ARG:HG2	1:H:134:GLU:HG3	1.95	0.48
1:E:288:VAL:HG22	1:E:292:MSE:SE	2.63	0.48
1:B:29:HIS:NE2	3:B:405:GOL:H2	2.29	0.48
1:C:9:ARG:HB3	1:C:64:LEU:HD23	1.95	0.48
1:E:35:GLU:HG3	1:E:36:ARG:O	2.13	0.48
3:G:404:GOL:H11	1:H:320:CYS:SG	2.54	0.48
1:G:112:ARG:O	1:H:88:ARG:NH2	2.34	0.48
1:A:18:SER:HA	3:A:403:GOL:H11	1.96	0.48
1:B:54:ARG:HH11	1:B:232:PRO:HD2	1.79	0.48
1:G:277:PRO:HB2	1:G:295:PRO:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:348:ALA:O	1:G:351:GLY:N	2.42	0.48
1:B:352:ILE:HG23	1:B:356:LEU:HD23	1.95	0.48
1:B:197:LLP:O3	2:B:401:MES:O1S	2.27	0.48
1:G:277:PRO:HA	1:G:282:HIS:CD2	2.49	0.48
1:H:84:LEU:HD11	1:H:107:PHE:CD1	2.49	0.48
1:F:100:TYR:CE1	2:F:401:MES:H31	2.49	0.48
1:G:43:ARG:NH2	1:G:44:TYR:CZ	2.82	0.48
1:C:312:LEU:HD11	1:C:333:CYS:HB2	1.94	0.48
1:C:66:ARG:NE	6:C:661:HOH:O	2.46	0.48
1:B:173:ASN:HB3	1:B:193:TYR:CE1	2.48	0.48
1:C:264:ARG:NH1	1:C:367:GLN:HE22	2.11	0.48
1:F:143:GLU:HG3	1:F:172:ASP:HB3	1.96	0.48
1:H:35:GLU:OE2	1:H:36:ARG:N	2.47	0.48
1:E:113:GLN:HA	1:E:113:GLN:HE21	1.79	0.48
1:F:159:SER:HA	1:F:169:VAL:HG21	1.96	0.48
1:A:259:ARG:O	6:A:591:HOH:O	2.20	0.48
1:A:266:ARG:NH1	6:A:597:HOH:O	2.47	0.48
1:C:264:ARG:HD2	1:C:374:SER:OG	2.12	0.48
1:D:121:ASP:HB3	1:D:127:GLY:HA3	1.95	0.48
1:D:251:VAL:HA	1:D:254:GLN:HE21	1.78	0.48
2:G:401:MES:H61	1:H:46:TYR:CD2	2.49	0.48
1:A:204:ASP:OD2	1:D:242:ARG:NE	2.26	0.48
1:D:339:HIS:O	1:D:347:ARG:HD3	2.13	0.48
1:D:253:ARG:HG2	1:D:363:ILE:HG22	1.95	0.48
1:D:294:ALA:O	1:D:296:GLY:N	2.38	0.48
1:H:277:PRO:HA	1:H:282:HIS:CD2	2.49	0.48
1:A:322:VAL:O	1:A:323:SER:HB3	2.14	0.48
1:C:339:HIS:CD2	6:C:656:HOH:O	2.66	0.48
1:C:288:VAL:HG22	1:C:292:MSE:CE	2.43	0.48
1:C:151:THR:HG23	1:C:284:GLN:OE1	2.14	0.48
1:E:192:LEU:HD12	1:E:193:TYR:N	2.29	0.48
1:E:344:ALA:HA	1:E:347:ARG:CZ	2.44	0.48
1:F:4:MSE:HE1	1:F:8:THR:HB	1.95	0.48
1:A:203:ALA:HB1	1:B:33:THR:HG23	1.95	0.48
1:C:339:HIS:CD2	6:C:657:HOH:O	2.66	0.48
1:D:184:LEU:HB3	3:D:402:GOL:H2	1.96	0.48
1:D:65:GLU:O	3:D:402:GOL:H31	2.14	0.48
1:E:314:ARG:HB3	1:E:376:ALA:HA	1.96	0.48
1:D:314:ARG:NH2	1:D:379:GLY:HA2	2.29	0.48
1:F:213:ARG:NH1	3:F:406:GOL:O2	2.42	0.48
1:H:367:GLN:NE2	6:H:672:HOH:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:VAL:HG22	1:A:118:ARG:HD3	1.95	0.48
1:A:116:ARG:NH2	1:A:136:ASP:HB2	2.29	0.48
1:A:197:LLP:HD3	1:A:324:LEU:HG	1.96	0.48
1:D:94:VAL:HG21	1:D:131:ALA:O	2.14	0.48
1:H:222:ARG:O	1:H:226:THR:HG22	2.14	0.48
1:A:307:PRO:HB3	1:A:309:GLU:OE1	2.13	0.48
1:B:173:ASN:HB3	1:B:193:TYR:CE1	2.48	0.48
1:B:92:CYS:O	1:B:138:ALA:N	2.46	0.48
1:D:88:ARG:HB2	1:D:91:GLN:HG3	1.96	0.48
1:F:225:ARG:HG2	1:F:231:VAL:HG23	1.96	0.48
1:F:83:LEU:HD22	1:F:210:LEU:HD22	1.94	0.48
1:G:236:ASP:OD1	6:G:615:HOH:O	2.19	0.48
1:G:17:PRO:HG3	6:G:669:HOH:O	2.14	0.48
1:G:232:PRO:HA	6:H:586:HOH:O	2.13	0.48
1:D:292:MSE:SE	1:D:295:PRO:HA	2.63	0.48
1:B:10:LEU:HD22	1:B:244:LEU:HD22	1.96	0.48
1:E:282:HIS:CB	1:E:285:HIS:HB2	2.39	0.48
1:F:99:VAL:HB	1:F:103:THR:HB	1.96	0.48
1:F:204:ASP:OD2	1:G:242:ARG:NE	2.37	0.48
1:A:251:VAL:HA	1:A:254:GLN:OE1	2.14	0.48
1:B:43:ARG:NH1	1:B:44:TYR:OH	2.47	0.48
1:E:249:LEU:HD21	1:H:253:ARG:HD2	1.96	0.48
1:D:291:GLN:HG3	1:D:292:MSE:HG3	1.94	0.48
1:D:313:ASP:HB3	6:D:642:HOH:O	2.13	0.48
1:F:103:THR:HG22	1:F:107:PHE:CE2	2.49	0.48
1:B:354:GLU:HG2	6:B:659:HOH:O	2.13	0.48
1:A:46:TYR:CD2	2:B:401:MES:H61	2.48	0.48
1:B:97:ASP:C	1:B:99:VAL:H	2.16	0.48
1:C:253:ARG:HG3	1:C:253:ARG:NH1	2.20	0.48
1:A:371:GLU:O	1:A:375:ARG:HB2	2.13	0.48
1:E:322:VAL:O	1:E:330:LEU:HD13	2.13	0.48
1:E:343:SER:HG	1:E:346:ALA:H	1.55	0.48
1:F:54:ARG:NH1	6:F:664:HOH:O	2.47	0.48
1:A:320:CYS:SG	1:A:337:MSE:HE1	2.54	0.47
1:C:130:ALA:O	1:C:133:ALA:N	2.40	0.47
1:C:157:GLU:O	1:C:161:ARG:HG2	2.13	0.47
1:C:332:GLU:HB3	1:C:337:MSE:SE	2.64	0.47
1:G:262:VAL:O	1:G:266:ARG:HG2	2.14	0.47
1:H:226:THR:HG23	6:H:661:HOH:O	2.13	0.47
1:A:46:TYR:CD2	2:B:401:MES:H61	2.49	0.47
1:D:254:GLN:HB3	1:D:297:ALA:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:665:HOH:O	1:F:109:LEU:HD13	2.13	0.47
1:F:137:LEU:HB3	1:F:165:ARG:HH11	1.78	0.47
1:F:152:VAL:N	1:F:284:GLN:OE1	2.34	0.47
1:B:132:LEU:HD12	1:B:161:ARG:HB3	1.94	0.47
1:B:99:VAL:HG23	1:B:104:ASP:HB2	1.95	0.47
1:F:37:ARG:CZ	6:F:663:HOH:O	2.54	0.47
1:G:168:ARG:HH22	4:G:407:FMT:H	1.78	0.47
1:H:351:GLY:O	6:H:600:HOH:O	2.20	0.47
1:A:36:ARG:NH1	1:A:45:PHE:HB3	2.29	0.47
1:E:100:TYR:HB2	6:E:667:HOH:O	2.14	0.47
1:F:338:THR:O	1:F:341:PRO:HD2	2.14	0.47
1:B:4:MSE:HB3	1:B:8:THR:HB	1.96	0.47
1:G:4:MSE:N	1:G:4:MSE:SE	2.97	0.47
1:H:322:VAL:HB	2:H:401:MES:C7	2.43	0.47
1:B:350:ARG:O	1:B:352:ILE:N	2.47	0.47
1:D:104:ASP:OD2	1:D:119:TYR:HE2	1.97	0.47
1:B:92:CYS:HB3	1:B:137:LEU:HA	1.96	0.47
1:C:66:ARG:CD	6:C:661:HOH:O	2.62	0.47
1:D:338:THR:HG1	1:D:339:HIS:CE1	2.29	0.47
1:B:4:MSE:HE1	6:C:684:HOH:O	2.13	0.47
1:C:88:ARG:HH21	1:C:88:ARG:HB3	1.78	0.47
1:G:52:PRO:O	1:G:56:GLU:HG3	2.14	0.47
1:F:146:THR:HG23	1:F:151:THR:O	2.14	0.47
1:F:41:GLU:HA	1:F:42:PRO:HD3	1.79	0.47
1:G:336:LEU:HB3	6:H:570:HOH:O	2.13	0.47
1:H:355:SER:OG	6:H:647:HOH:O	2.17	0.47
1:C:344:ALA:HA	1:C:347:ARG:HH11	1.79	0.47
1:D:336:LEU:HB3	1:D:337:MSE:SE	2.64	0.47
1:H:222:ARG:O	1:H:226:THR:HG22	2.15	0.47
1:D:88:ARG:N	1:D:91:GLN:HE21	2.12	0.47
1:F:150:LEU:HD22	1:F:175:PHE:CZ	2.49	0.47
1:F:98:ASP:CG	6:F:659:HOH:O	2.52	0.47
1:D:94:VAL:HG21	1:D:131:ALA:O	2.14	0.47
1:D:332:GLU:OE2	1:D:337:MSE:HB2	2.12	0.47
1:E:287:VAL:O	1:E:291:GLN:HG2	2.13	0.47
1:E:37:ARG:O	1:E:39:GLN:N	2.47	0.47
1:G:128:ILE:O	1:G:132:LEU:HB2	2.14	0.47
1:B:99:VAL:HG13	1:B:103:THR:HB	1.96	0.47
1:D:334:PRO:HA	1:D:338:THR:HB	1.96	0.47
1:D:6:PHE:CE1	1:D:179:VAL:HG22	2.49	0.47
1:E:150:LEU:HD13	1:E:277:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:PHE:HA	1:F:9:ARG:HD2	1.96	0.47
1:H:180:LEU:HD22	1:H:294:ALA:HB3	1.96	0.47
1:D:333:CYS:SG	1:D:336:LEU:HB2	2.54	0.47
1:A:16:ARG:HA	1:A:17:PRO:HD2	1.39	0.47
1:E:260:VAL:HG13	6:E:655:HOH:O	2.14	0.47
1:G:345:GLU:HA	1:G:348:ALA:HB3	1.97	0.47
1:C:11:VAL:HA	1:C:245:HIS:ND1	2.29	0.47
1:D:37:ARG:C	1:D:39:GLN:H	2.17	0.47
1:E:214:ASP:HB3	1:E:217:LEU:HB3	1.95	0.47
1:F:94:VAL:HG21	1:F:131:ALA:O	2.14	0.47
1:F:249:LEU:HD23	3:F:403:GOL:H12	1.96	0.47
1:G:43:ARG:HD3	1:G:44:TYR:CE2	2.49	0.47
1:D:177:SER:HB2	1:D:178:PRO:HD2	1.96	0.47
1:E:213:ARG:NH2	6:E:577:HOH:O	2.41	0.47
1:A:50:GLU:HA	6:A:553:HOH:O	2.14	0.47
1:C:11:VAL:HA	1:C:245:HIS:ND1	2.30	0.47
1:D:310:ARG:HG3	1:D:314:ARG:NH1	2.30	0.47
1:H:322:VAL:HG11	4:H:406:CL:CL	2.51	0.47
1:C:156:ALA:HA	1:C:186:LEU:O	2.14	0.47
1:C:350:ARG:O	1:C:350:ARG:HG2	2.14	0.47
1:H:113:GLN:NE2	6:H:649:HOH:O	2.34	0.47
1:H:6:PHE:HD1	1:H:9:ARG:HH22	1.62	0.47
1:B:16:ARG:HH11	3:B:405:GOL:H12	1.78	0.47
1:B:83:LEU:HD13	1:B:210:LEU:HD13	1.95	0.47
1:C:176:ALA:HB3	1:C:292:MSE:HE3	1.96	0.47
1:C:88:ARG:NH1	1:D:112:ARG:HG3	2.27	0.47
1:E:323:SER:N	2:E:401:MES:O2S	2.46	0.47
1:C:121:ASP:O	1:C:122:LEU:HD23	2.14	0.47
1:F:123:THR:HG22	1:F:153:VAL:HG22	1.96	0.47
1:G:36:ARG:HD2	1:G:45:PHE:CE1	2.49	0.47
1:A:9:ARG:NH1	6:A:607:HOH:O	2.47	0.47
1:B:213:ARG:NH2	6:B:612:HOH:O	2.47	0.47
1:C:42:PRO:HB3	1:C:45:PHE:CE1	2.48	0.47
1:C:161:ARG:N	1:C:161:ARG:HD2	2.29	0.47
1:F:336:LEU:C	1:F:340:ARG:HB2	2.35	0.47
1:H:92:CYS:SG	1:H:116:ARG:CZ	3.02	0.47
1:C:174:THR:HB	1:C:197:LLP:H2'2	1.96	0.47
1:D:213:ARG:NH2	6:D:606:HOH:O	2.46	0.47
1:E:354:GLU:O	6:E:614:HOH:O	2.20	0.47
1:G:137:LEU:H	1:G:165:ARG:HH21	1.61	0.47
1:H:341:PRO:HA	6:H:659:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLU:OE1	1:B:338:THR:HG23	2.14	0.47
1:B:18:SER:OG	6:B:603:HOH:O	2.20	0.47
1:B:87:VAL:HG11	1:B:93:VAL:HG23	1.97	0.47
1:C:197:LLP:HD3	1:C:324:LEU:HG	1.96	0.47
1:E:277:PRO:HA	1:E:282:HIS:CD2	2.49	0.47
1:G:282:HIS:CG	1:G:283:PRO:HD2	2.50	0.47
1:H:145:PRO:HG2	1:H:175:PHE:CE1	2.49	0.47
1:H:213:ARG:NH1	3:H:402:GOL:O2	2.43	0.47
1:B:367:GLN:O	1:B:371:GLU:HG3	2.14	0.47
1:A:46:TYR:CD2	2:B:401:MES:H61	2.49	0.47
3:G:403:GOL:O1	3:G:403:GOL:O3	2.32	0.47
6:F:624:HOH:O	1:G:371:GLU:HG3	2.14	0.47
2:D:401:MES:H51	2:D:401:MES:H81	1.46	0.47
1:E:14:GLY:HA2	1:E:59:GLU:OE1	2.14	0.47
1:F:15:ARG:HG3	6:F:648:HOH:O	2.13	0.47
1:A:197:LLP:NZ	1:A:197:LLP:O3	2.40	0.47
1:C:252:HIS:CD2	3:C:403:GOL:HO1	2.33	0.47
1:F:310:ARG:O	1:F:314:ARG:NH1	2.47	0.47
1:H:180:LEU:HD22	1:H:294:ALA:HB3	1.95	0.47
1:A:225:ARG:HG2	1:A:231:VAL:HG12	1.94	0.47
1:E:16:ARG:HA	1:E:17:PRO:HD3	1.69	0.47
1:E:195:THR:HA	1:E:199:ILE:HB	1.96	0.47
1:F:89:PRO:HB3	1:F:114:GLY:HA3	1.95	0.47
1:H:118:ARG:CZ	1:H:131:ALA:HA	2.44	0.47
1:A:277:PRO:HA	1:A:282:HIS:CD2	2.50	0.47
1:F:152:VAL:HG21	1:F:288:VAL:CG2	2.44	0.47
1:F:332:GLU:HG3	1:F:333:CYS:N	2.29	0.47
1:G:178:PRO:HD3	1:G:193:TYR:CE1	2.50	0.47
1:B:179:VAL:HG11	1:B:252:HIS:CE1	2.50	0.47
1:B:6:PHE:CA	1:B:9:ARG:HE	2.27	0.47
1:D:99:VAL:HG21	1:D:103:THR:HG21	1.96	0.47
1:F:100:TYR:CE1	2:F:401:MES:H82	2.49	0.47
1:D:309:GLU:HG3	1:D:336:LEU:HD11	1.97	0.47
1:F:215:ALA:O	1:F:218:HIS:HB3	2.15	0.47
1:H:180:LEU:HD22	1:H:294:ALA:HB3	1.97	0.47
1:F:280:PRO:HA	1:F:285:HIS:CD2	2.49	0.47
1:F:364:GLU:HB3	1:G:8:THR:HG22	1.95	0.47
1:C:178:PRO:HD3	1:C:193:TYR:CE1	2.50	0.47
1:D:145:PRO:HB2	1:D:175:PHE:CE2	2.50	0.47
1:D:337:MSE:O	1:D:339:HIS:N	2.47	0.47
1:F:128:ILE:HD12	1:F:158:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLU:O	1:B:165:ARG:NH1	2.42	0.47
1:B:292:MSE:HB3	1:B:292:MSE:HE3	1.71	0.47
1:B:100:TYR:CE1	2:B:401:MES:H81	2.49	0.47
1:A:282:HIS:CG	1:A:283:PRO:HD2	2.49	0.47
1:C:327:VAL:HG13	1:C:363:ILE:CG1	2.39	0.47
1:D:132:LEU:CB	1:D:165:ARG:HG3	2.45	0.47
1:F:275:HIS:HB2	1:F:300:SER:OG	2.15	0.47
1:B:148:PRO:HD3	1:B:339:HIS:NE2	2.29	0.47
1:D:41:GLU:O	1:D:43:ARG:HG2	2.15	0.47
1:G:374:SER:OG	6:G:619:HOH:O	2.20	0.47
1:H:275:HIS:HE1	6:H:639:HOH:O	1.97	0.47
1:F:282:HIS:HB3	1:F:285:HIS:HB2	1.96	0.47
1:F:95:SER:OG	1:F:96:THR:N	2.47	0.47
1:G:266:ARG:NH2	6:G:588:HOH:O	2.40	0.47
1:G:348:ALA:C	1:G:350:ARG:H	2.17	0.47
1:G:10:LEU:HD22	1:G:244:LEU:HD22	1.95	0.47
1:G:292:MSE:SE	1:G:295:PRO:N	2.98	0.47
1:H:96:THR:O	1:H:98:ASP:N	2.46	0.47
1:B:225:ARG:HG2	1:B:231:VAL:HG12	1.96	0.47
1:C:178:PRO:HD3	1:C:193:TYR:CE1	2.50	0.47
1:F:124:THR:OG1	1:F:126:GLU:OE2	2.25	0.47
1:B:11:VAL:HG13	1:C:327:VAL:HG13	1.96	0.47
1:E:102:GLY:CA	3:E:405:GOL:H11	2.43	0.47
1:H:42:PRO:HB3	1:H:45:PHE:CE2	2.49	0.47
1:E:40:ASP:O	1:E:42:PRO:HD3	2.15	0.47
1:G:84:LEU:HD12	1:G:106:LEU:HB3	1.97	0.47
1:A:68:PRO:HG2	1:A:213:ARG:HA	1.97	0.47
1:D:254:GLN:HG2	1:D:361:VAL:O	2.15	0.47
1:E:263:GLU:OE1	1:E:266:ARG:NH1	2.48	0.47
1:F:255:VAL:HG12	1:F:259:ARG:NH1	2.30	0.47
1:G:132:LEU:O	1:G:137:LEU:HD22	2.15	0.47
1:H:264:ARG:NE	1:H:370:ALA:HB1	2.30	0.47
1:H:180:LEU:HD22	1:H:294:ALA:HB3	1.97	0.47
1:E:96:THR:O	1:E:99:VAL:HG22	2.14	0.47
1:F:100:TYR:CE1	2:F:401:MES:H31	2.47	0.47
1:B:5:ARG:HH12	1:C:371:GLU:CD	2.17	0.47
1:E:150:LEU:HD22	1:E:175:PHE:HE2	1.80	0.47
1:G:344:ALA:O	1:G:348:ALA:N	2.38	0.47
1:D:145:PRO:HD2	1:D:175:PHE:CG	2.50	0.47
1:E:111:ALA:HA	1:E:115:VAL:O	2.14	0.47
1:F:9:ARG:NH2	1:F:63:GLY:O	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:PRO:HB2	1:H:45:PHE:HE1	1.77	0.47
1:A:18:SER:HB2	6:A:647:HOH:O	2.14	0.47
1:A:35:GLU:CD	1:A:37:ARG:HE	2.18	0.47
1:A:95:SER:OG	1:A:96:THR:N	2.45	0.47
1:A:367:GLN:HB3	1:D:5:ARG:NH1	2.30	0.47
1:A:292:MSE:HE2	1:A:295:PRO:HA	1.97	0.47
1:B:84:LEU:HD13	1:B:141:TRP:CZ3	2.50	0.47
1:E:112:ARG:NH1	6:E:619:HOH:O	2.34	0.47
1:H:110:ALA:HB1	1:H:115:VAL:HG21	1.96	0.47
1:H:34:TYR:CD1	1:H:44:TYR:HB3	2.49	0.47
1:G:292:MSE:O	6:G:596:HOH:O	2.20	0.47
1:H:375:ARG:HB2	1:H:375:ARG:HE	1.57	0.47
1:H:3:GLY:C	1:H:4:MSE:HG3	2.34	0.47
1:H:9:ARG:HD3	1:H:9:ARG:H	1.79	0.47
1:A:88:ARG:NH2	6:A:619:HOH:O	2.47	0.47
1:D:168:ARG:NH1	6:D:508:HOH:O	2.28	0.47
1:F:277:PRO:HA	1:F:282:HIS:CD2	2.50	0.47
1:H:97:ASP:N	1:H:119:TYR:HD2	2.12	0.47
1:C:46:TYR:CD2	2:D:401:MES:H52	2.50	0.47
1:F:16:ARG:HD3	6:F:578:HOH:O	2.15	0.47
1:H:264:ARG:HD3	1:H:374:SER:OG	2.15	0.47
1:C:259:ARG:NH2	6:C:598:HOH:O	2.08	0.47
1:D:96:THR:HG22	1:D:122:LEU:HG	1.97	0.47
1:F:180:LEU:HD22	1:F:294:ALA:HB3	1.96	0.47
1:G:4:MSE:HA	1:G:8:THR:HG21	1.96	0.47
1:A:43:ARG:HD3	1:A:44:TYR:CE2	2.50	0.47
1:B:347:ARG:HB3	1:B:352:ILE:O	2.14	0.47
1:A:116:ARG:HH21	1:E:112:ARG:HG2	1.78	0.47
1:D:143:GLU:O	1:D:146:THR:HG22	2.13	0.47
1:E:168:ARG:NH1	3:E:403:GOL:O2	2.40	0.47
1:E:96:THR:O	1:E:99:VAL:HG13	2.15	0.47
1:H:281:GLU:HB2	6:H:666:HOH:O	2.14	0.47
1:H:29:HIS:HB3	6:H:552:HOH:O	2.15	0.47
1:H:336:LEU:O	1:H:337:MSE:HG3	2.15	0.47
1:A:36:ARG:NH2	1:A:36:ARG:HB2	2.26	0.47
1:B:43:ARG:NH2	1:B:55:GLU:OE1	2.47	0.47
1:H:367:GLN:HG2	1:H:367:GLN:H	1.54	0.47
1:B:345:GLU:H	1:B:345:GLU:CD	2.18	0.47
1:B:16:ARG:HH22	1:B:55:GLU:HB3	1.79	0.47
1:C:150:LEU:N	1:C:150:LEU:HD23	2.30	0.47
1:F:309:GLU:HG3	1:F:309:GLU:H	1.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:ARG:NE	1:F:59:GLU:OE1	2.48	0.47
1:E:213:ARG:HE	3:E:402:GOL:H2	1.79	0.47
1:F:322:VAL:O	1:F:323:SER:HB3	2.15	0.47
1:A:110:ALA:HB1	1:A:115:VAL:HG21	1.95	0.47
1:A:19:ALA:O	1:A:21:THR:N	2.45	0.47
1:C:263:GLU:OE1	1:C:266:ARG:NH1	2.47	0.47
1:C:33:THR:CG2	1:D:203:ALA:HB1	2.44	0.47
1:H:102:GLY:HA2	3:H:403:GOL:H31	1.96	0.47
1:H:264:ARG:CZ	1:H:370:ALA:HB1	2.45	0.47
1:A:277:PRO:HA	1:A:282:HIS:CD2	2.50	0.47
1:C:277:PRO:HA	1:C:282:HIS:CD2	2.49	0.47
1:D:180:LEU:HD22	1:D:294:ALA:HB3	1.95	0.47
1:E:278:GLY:HA2	1:E:285:HIS:CE1	2.49	0.47
1:E:339:HIS:O	1:E:342:LEU:HB2	2.15	0.47
1:F:9:ARG:HH22	1:F:66:ARG:HH11	1.61	0.47
1:G:113:GLN:HB3	1:H:113:GLN:OE1	2.13	0.47
1:C:309:GLU:HG2	6:C:659:HOH:O	2.13	0.47
1:D:155:VAL:HB	1:D:186:LEU:HD13	1.97	0.47
1:E:19:ALA:C	1:E:21:THR:H	2.18	0.47
1:E:303:TYR:OH	1:E:310:ARG:NH2	2.47	0.47
1:G:294:ALA:O	1:G:296:GLY:N	2.35	0.47
1:H:179:VAL:HG22	6:H:682:HOH:O	2.15	0.47
1:A:179:VAL:HG22	1:A:251:VAL:HG11	1.96	0.47
1:C:180:LEU:HD22	1:C:294:ALA:HB3	1.95	0.47
1:E:263:GLU:OE1	6:E:502:HOH:O	2.20	0.47
1:F:145:PRO:HD2	1:F:175:PHE:HD1	1.79	0.47
1:G:111:ALA:HA	1:G:115:VAL:O	2.15	0.47
1:H:245:HIS:HE1	6:H:540:HOH:O	1.98	0.47
1:A:284:GLN:NE2	6:A:640:HOH:O	2.39	0.47
1:B:340:ARG:HA	1:B:347:ARG:HH12	1.80	0.47
1:H:178:PRO:HD3	1:H:193:TYR:CE1	2.49	0.47
1:B:338:THR:CG2	2:B:401:MES:H32	2.39	0.47
1:C:43:ARG:HA	1:C:45:PHE:CZ	2.50	0.47
1:G:333:CYS:O	1:G:337:MSE:HE3	2.15	0.47
1:E:3:GLY:O	1:H:317:LEU:HD22	2.15	0.47
1:G:282:HIS:O	1:G:284:GLN:N	2.47	0.47
1:G:340:ARG:HA	1:G:347:ARG:NH1	2.30	0.47
1:H:288:VAL:HG13	1:H:292:MSE:SE	2.64	0.47
1:F:95:SER:HB2	1:F:141:TRP:HB3	1.97	0.47
1:F:98:ASP:N	1:F:98:ASP:OD2	2.47	0.47
1:D:285:HIS:O	1:D:288:VAL:HB	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:THR:O	6:F:661:HOH:O	2.21	0.47
1:E:18:SER:HB3	6:E:585:HOH:O	2.15	0.47
1:B:110:ALA:O	1:B:115:VAL:HB	2.15	0.47
1:C:15:ARG:O	1:C:16:ARG:O	2.33	0.47
1:D:96:THR:O	1:D:99:VAL:N	2.47	0.47
1:E:147:ASN:HD21	1:E:324:LEU:CD2	2.28	0.47
1:E:60:CYS:SG	1:E:244:LEU:HD13	2.55	0.47
1:G:345:GLU:O	1:G:349:ARG:N	2.47	0.47
1:A:118:ARG:HE	1:A:120:ALA:HB2	1.80	0.47
1:E:312:LEU:O	1:F:37:ARG:NH2	2.43	0.47
1:H:252:HIS:HD2	6:H:572:HOH:O	1.98	0.47
1:D:147:ASN:CG	1:D:358:ARG:HH11	2.17	0.47
6:E:653:HOH:O	1:F:337:MSE:HE3	2.15	0.47
1:B:96:THR:C	1:B:98:ASP:H	2.18	0.47
1:D:156:ALA:O	1:D:160:ARG:HG3	2.15	0.47
1:G:36:ARG:HG3	3:G:404:GOL:H31	1.96	0.47
1:H:107:PHE:O	1:H:111:ALA:N	2.47	0.47
1:A:36:ARG:O	1:A:38:ALA:N	2.48	0.47
1:B:251:VAL:HA	1:B:254:GLN:OE1	2.15	0.47
1:B:300:SER:HB3	1:B:356:LEU:HD11	1.97	0.47
1:D:281:GLU:H	1:D:281:GLU:HG2	1.59	0.47
1:D:282:HIS:HB3	1:D:285:HIS:HB2	1.96	0.47
1:E:97:ASP:HA	1:E:119:TYR:HD1	1.79	0.47
1:F:11:VAL:HA	1:F:245:HIS:ND1	2.30	0.47
1:G:107:PHE:HB3	1:G:117:VAL:HG11	1.96	0.47
1:D:95:SER:N	1:D:118:ARG:O	2.40	0.47
2:D:401:MES:H81	2:D:401:MES:H31	1.46	0.47
1:H:132:LEU:O	1:H:165:ARG:NE	2.35	0.47
1:B:144:THR:OG1	6:B:528:HOH:O	2.20	0.47
1:B:178:PRO:HD3	1:B:193:TYR:CE1	2.50	0.47
1:C:9:ARG:HB2	6:C:529:HOH:O	2.14	0.47
1:G:111:ALA:HA	1:G:115:VAL:O	2.15	0.47
1:B:96:THR:HG22	1:B:120:ALA:O	2.14	0.47
1:B:19:ALA:CA	6:B:680:HOH:O	2.60	0.47
1:B:337:MSE:H	1:B:340:ARG:HB2	1.79	0.47
1:C:213:ARG:NH1	6:C:644:HOH:O	2.37	0.47
1:C:253:ARG:HG2	1:C:363:ILE:HG22	1.96	0.47
1:E:92:CYS:HA	1:E:116:ARG:O	2.14	0.47
1:A:267:ALA:O	6:A:501:HOH:O	2.20	0.47
1:G:163:HIS:HE1	1:G:187:GLY:O	1.97	0.47
1:A:334:PRO:HD2	1:A:356:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:HD22	1:B:137:LEU:HD21	1.95	0.47
1:A:27:PRO:HB2	1:C:27:PRO:HB2	1.97	0.47
1:C:334:PRO:HD2	1:C:356:LEU:O	2.14	0.47
1:D:177:SER:OG	1:D:179:VAL:HG23	2.14	0.47
1:F:213:ARG:HB3	1:F:213:ARG:CZ	2.45	0.47
1:H:132:LEU:HD22	1:H:137:LEU:HD21	1.97	0.47
1:B:259:ARG:HG2	1:B:259:ARG:NH1	2.26	0.47
1:D:253:ARG:HA	1:D:253:ARG:CZ	2.45	0.47
1:G:334:PRO:HA	1:G:337:MSE:HB2	1.97	0.47
1:B:6:PHE:HB2	1:B:9:ARG:HH11	1.80	0.47
1:C:277:PRO:HA	1:C:282:HIS:CD2	2.49	0.47
1:G:94:VAL:HG11	1:G:131:ALA:HB1	1.97	0.47
1:A:358:ARG:NH1	2:A:401:MES:O3S	2.46	0.47
1:B:111:ALA:HA	1:B:115:VAL:O	2.14	0.47
1:D:88:ARG:HB2	1:D:91:GLN:HG3	1.97	0.47
1:A:108:ASP:OD1	6:A:606:HOH:O	2.20	0.47
1:C:179:VAL:HG12	1:C:180:LEU:HD23	1.97	0.47
1:C:292:MSE:HE1	6:C:519:HOH:O	2.15	0.47
1:D:292:MSE:SE	1:D:294:ALA:H	2.48	0.47
1:G:18:SER:HB3	1:G:22:GLY:CA	2.45	0.47
1:A:36:ARG:NH2	1:A:45:PHE:CD1	2.83	0.47
1:C:332:GLU:OE2	1:C:337:MSE:HG3	2.15	0.47
1:D:96:THR:HA	1:D:120:ALA:O	2.14	0.47
1:F:321:GLY:CA	1:F:337:MSE:HE1	2.45	0.47
1:H:150:LEU:HD22	1:H:175:PHE:CE2	2.49	0.47
1:E:242:ARG:HB3	1:H:242:ARG:HH12	1.80	0.47
1:A:261:LEU:O	1:A:264:ARG:HB3	2.15	0.47
1:A:291:GLN:C	1:A:292:MSE:HG2	2.35	0.47
1:C:347:ARG:HA	1:C:350:ARG:HG2	1.96	0.47
1:E:68:PRO:O	6:E:596:HOH:O	2.20	0.47
1:D:338:THR:HG22	1:D:339:HIS:ND1	2.30	0.47
1:E:157:GLU:O	1:E:161:ARG:HB2	2.14	0.47
1:E:184:LEU:HB3	1:E:213:ARG:HH11	1.80	0.47
1:E:98:ASP:N	1:E:98:ASP:OD2	2.48	0.47
1:F:3:GLY:O	1:F:4:MSE:HB2	2.15	0.47
1:B:332:GLU:OE1	1:B:358:ARG:NH2	2.48	0.47
1:D:98:ASP:HB2	1:D:146:THR:HB	1.96	0.47
1:E:39:GLN:HE22	1:E:43:ARG:H	1.58	0.47
1:F:122:LEU:N	6:F:666:HOH:O	2.03	0.47
1:A:152:VAL:O	1:A:284:GLN:NE2	2.48	0.47
1:E:173:ASN:HB3	1:E:193:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:PRO:HG2	1:F:292:MSE:HE2	1.97	0.47
1:F:51:ASN:HB3	1:F:54:ARG:NH1	2.30	0.47
1:G:282:HIS:CG	1:G:283:PRO:HD2	2.50	0.47
1:B:15:ARG:O	1:B:16:ARG:HG2	2.15	0.46
1:D:264:ARG:HD2	1:D:374:SER:OG	2.15	0.46
1:F:248:SER:O	1:F:252:HIS:HD2	1.99	0.46
1:H:110:ALA:HB1	1:H:115:VAL:HG21	1.96	0.46
1:E:176:ALA:HB1	1:E:180:LEU:HB2	1.97	0.46
1:A:173:ASN:HB3	1:A:193:TYR:CE1	2.49	0.46
1:A:36:ARG:NH1	1:A:45:PHE:CE1	2.83	0.46
1:D:84:LEU:HD13	6:D:580:HOH:O	2.14	0.46
1:E:333:CYS:HB3	1:E:336:LEU:HD12	1.97	0.46
1:H:109:LEU:O	1:H:113:GLN:N	2.47	0.46
1:H:161:ARG:HD3	1:H:161:ARG:HA	1.69	0.46
1:H:18:SER:OG	1:H:27:PRO:HD3	2.16	0.46
1:B:17:PRO:HA	6:B:674:HOH:O	2.14	0.46
1:F:98:ASP:HB2	6:F:659:HOH:O	2.15	0.46
1:H:168:ARG:HH22	3:H:404:GOL:H32	1.80	0.46
1:H:6:PHE:HA	1:H:9:ARG:NH2	2.30	0.46
1:D:332:GLU:OE1	1:D:338:THR:OG1	2.30	0.46
1:D:65:GLU:O	1:D:66:ARG:HG2	2.14	0.46
1:G:282:HIS:C	1:G:284:GLN:H	2.18	0.46
1:C:126:GLU:O	1:C:130:ALA:N	2.45	0.46
1:C:180:LEU:HA	1:C:293:SER:OG	2.15	0.46
1:H:264:ARG:NH2	1:H:374:SER:OG	2.48	0.46
1:A:95:SER:OG	1:A:96:THR:N	2.48	0.46
1:A:113:GLN:HB3	1:B:113:GLN:HE22	1.79	0.46
1:B:132:LEU:CD1	1:B:161:ARG:HB3	2.44	0.46
1:B:282:HIS:HE1	1:B:284:GLN:NE2	2.12	0.46
1:B:197:LLP:NZ	2:B:401:MES:O1S	2.49	0.46
1:C:107:PHE:HB3	1:C:117:VAL:HG21	1.96	0.46
1:D:175:PHE:C	1:D:175:PHE:CD1	2.89	0.46
1:C:252:HIS:HE1	6:C:632:HOH:O	1.98	0.46
1:D:126:GLU:O	1:D:130:ALA:N	2.46	0.46
1:E:176:ALA:HB1	1:E:180:LEU:HB2	1.96	0.46
1:F:213:ARG:NH1	3:F:405:GOL:O2	2.45	0.46
1:G:337:MSE:HB3	1:G:338:THR:H	1.47	0.46
1:B:118:ARG:NE	1:B:131:ALA:HB2	2.29	0.46
1:H:173:ASN:HB3	1:H:193:TYR:CE1	2.50	0.46
1:A:339:HIS:HD2	1:A:342:LEU:HD22	1.79	0.46
1:D:45:PHE:HB2	6:D:677:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:276:TYR:HD2	1:H:278:GLY:O	1.98	0.46
1:C:16:ARG:HD2	6:C:604:HOH:O	2.16	0.46
1:C:327:VAL:HG12	1:C:328:HIS:CE1	2.50	0.46
1:C:213:ARG:NH2	3:C:403:GOL:H31	2.30	0.46
1:D:124:THR:O	1:D:126:GLU:N	2.48	0.46
1:E:5:ARG:O	1:E:9:ARG:HD3	2.15	0.46
1:H:173:ASN:HB3	1:H:193:TYR:CE1	2.50	0.46
1:A:146:THR:O	1:A:150:LEU:HA	2.13	0.46
1:E:323:SER:HA	2:E:401:MES:O3S	2.15	0.46
1:F:321:GLY:C	1:F:337:MSE:HE1	2.34	0.46
1:F:34:TYR:OH	1:F:51:ASN:HA	2.15	0.46
1:A:6:PHE:CE2	1:A:179:VAL:HB	2.51	0.46
1:C:143:GLU:HG3	1:C:172:ASP:HB3	1.97	0.46
1:C:39:GLN:HE21	1:C:39:GLN:HB3	1.56	0.46
1:E:214:ASP:OD2	6:E:627:HOH:O	2.21	0.46
1:H:36:ARG:O	1:H:38:ALA:N	2.48	0.46
2:C:401:MES:H61	1:D:46:TYR:CD1	2.51	0.46
2:C:401:MES:O3S	6:C:635:HOH:O	2.20	0.46
1:D:323:SER:HA	2:D:401:MES:O1S	2.15	0.46
1:F:343:SER:C	1:F:345:GLU:H	2.17	0.46
1:G:163:HIS:HE2	1:G:189:ASP:CG	2.19	0.46
1:A:347:ARG:HB3	1:A:352:ILE:O	2.15	0.46
1:C:186:LEU:HD11	1:C:291:GLN:HB2	1.96	0.46
1:E:345:GLU:HA	1:E:348:ALA:HB3	1.98	0.46
1:B:121:ASP:OD2	1:B:124:THR:OG1	2.28	0.46
1:B:98:ASP:HB3	6:B:602:HOH:O	2.15	0.46
1:D:288:VAL:HG12	1:D:289:LYS:N	2.30	0.46
1:D:213:ARG:HG3	1:D:213:ARG:H	1.56	0.46
1:G:268:SER:O	6:G:568:HOH:O	2.21	0.46
1:A:345:GLU:O	1:A:349:ARG:HG2	2.15	0.46
1:D:332:GLU:OE1	1:D:337:MSE:HB3	2.15	0.46
1:F:222:ARG:NH2	5:F:407:FMT:O1	2.49	0.46
1:G:107:PHE:O	1:G:111:ALA:N	2.47	0.46
1:B:15:ARG:HH11	1:B:24:VAL:HA	1.80	0.46
1:C:147:ASN:ND2	1:C:358:ARG:HH11	2.13	0.46
1:D:334:PRO:O	1:D:339:HIS:HB2	2.15	0.46
1:F:197:LLP:HE3	2:F:401:MES:H81	1.96	0.46
1:B:347:ARG:HB3	1:B:352:ILE:HB	1.97	0.46
1:C:292:MSE:HE1	1:C:295:PRO:HA	1.95	0.46
1:C:113:GLN:NE2	1:D:113:GLN:HG2	2.23	0.46
1:A:214:ASP:HB2	1:A:217:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:HG3	1:A:37:ARG:H	1.80	0.46
1:B:333:CYS:O	1:B:336:LEU:N	2.47	0.46
1:C:43:ARG:HG3	1:C:44:TYR:CD1	2.50	0.46
1:C:310:ARG:O	1:C:314:ARG:HG3	2.14	0.46
1:E:263:GLU:OE1	1:E:266:ARG:NH1	2.49	0.46
1:F:180:LEU:HD22	1:F:294:ALA:HB3	1.97	0.46
1:F:43:ARG:HD3	1:F:44:TYR:CD2	2.50	0.46
1:H:197:LLP:NZ	1:H:197:LLP:O3	2.35	0.46
1:A:197:LLP:H6	6:A:586:HOH:O	2.15	0.46
1:E:11:VAL:HA	1:E:245:HIS:ND1	2.30	0.46
1:E:320:CYS:HB2	1:F:37:ARG:HD2	1.96	0.46
1:B:132:LEU:HA	1:B:137:LEU:HD22	1.95	0.46
1:B:216:ASP:HB2	6:B:605:HOH:O	2.14	0.46
1:B:345:GLU:N	1:B:345:GLU:OE2	2.48	0.46
1:A:29:HIS:ND1	1:C:23:ASP:OD2	2.39	0.46
1:E:100:TYR:CE1	2:E:401:MES:H81	2.51	0.46
1:D:15:ARG:O	1:D:17:PRO:HD3	2.16	0.46
1:H:88:ARG:NH1	6:H:505:HOH:O	2.49	0.46
1:A:214:ASP:HB3	1:A:217:LEU:HB3	1.98	0.46
1:D:160:ARG:HB2	1:D:161:ARG:HH11	1.80	0.46
1:F:282:HIS:CG	1:F:283:PRO:HD2	2.50	0.46
1:B:36:ARG:HA	1:B:36:ARG:HD3	1.73	0.46
1:C:173:ASN:HB3	1:C:193:TYR:CE1	2.50	0.46
1:E:4:MSE:CB	1:E:8:THR:HB	2.31	0.46
1:E:100:TYR:HE1	2:E:401:MES:H81	1.81	0.46
1:F:178:PRO:HD3	1:F:193:TYR:CE1	2.49	0.46
1:C:145:PRO:HD2	1:C:175:PHE:CD1	2.50	0.46
1:E:112:ARG:NH1	6:E:577:HOH:O	2.49	0.46
1:B:266:ARG:HH11	1:B:279:LEU:HD22	1.81	0.46
1:C:100:TYR:O	1:C:103:THR:N	2.44	0.46
1:D:281:GLU:CD	1:D:281:GLU:H	2.18	0.46
1:G:39:GLN:OE1	1:G:42:PRO:HA	2.15	0.46
1:C:48:ARG:O	1:C:226:THR:HG23	2.15	0.46
1:B:287:VAL:O	1:B:291:GLN:HG2	2.15	0.46
1:C:339:HIS:CG	1:C:352:ILE:HD13	2.50	0.46
1:E:46:TYR:CG	2:F:401:MES:H61	2.50	0.46
1:A:16:ARG:HG2	1:A:17:PRO:HD2	1.98	0.46
1:C:160:ARG:C	1:C:161:ARG:HE	2.18	0.46
6:E:646:HOH:O	1:F:337:MSE:HE3	2.16	0.46
2:E:401:MES:H52	1:F:46:TYR:CE2	2.50	0.46
1:H:285:HIS:HD2	1:H:286:ALA:N	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:HH22	3:A:402:GOL:H11	1.80	0.46
1:B:178:PRO:HD3	1:B:193:TYR:CE1	2.50	0.46
1:B:36:ARG:NH1	1:B:45:PHE:HD1	2.06	0.46
1:D:276:TYR:CD1	1:D:299:VAL:HG22	2.51	0.46
1:E:175:PHE:C	1:E:175:PHE:CD1	2.89	0.46
1:F:168:ARG:NH2	3:F:403:GOL:O3	2.45	0.46
1:A:173:ASN:HB3	1:A:193:TYR:CE1	2.50	0.46
1:C:264:ARG:NE	6:C:648:HOH:O	2.48	0.46
1:F:180:LEU:HA	1:F:293:SER:OG	2.16	0.46
1:G:152:VAL:H	1:G:284:GLN:NE2	2.14	0.46
1:A:236:ASP:OD2	6:A:683:HOH:O	2.20	0.46
1:B:132:LEU:HD12	1:B:161:ARG:HB3	1.98	0.46
1:B:337:MSE:O	1:B:340:ARG:N	2.46	0.46
1:F:124:THR:HB	1:F:126:GLU:HG3	1.97	0.46
1:G:342:LEU:HD12	1:G:347:ARG:HG3	1.97	0.46
1:C:112:ARG:HB3	1:D:88:ARG:NH1	2.29	0.46
1:D:220:ALA:HB2	3:D:404:GOL:H11	1.97	0.46
1:G:276:TYR:HB3	1:G:279:LEU:HG	1.98	0.46
1:G:113:GLN:NE2	1:H:113:GLN:OE1	2.40	0.46
1:B:124:THR:OG1	1:B:127:GLY:N	2.43	0.46
1:B:96:THR:HG21	1:B:153:VAL:HG21	1.97	0.46
1:G:280:PRO:HG2	6:G:677:HOH:O	2.14	0.46
1:E:5:ARG:O	1:E:9:ARG:NH1	2.48	0.46
6:G:693:HOH:O	1:H:112:ARG:HD3	2.14	0.46
1:H:35:GLU:HG3	1:H:37:ARG:H	1.80	0.46
1:A:97:ASP:O	1:A:350:ARG:NH1	2.48	0.46
1:E:35:GLU:OE2	1:E:37:ARG:NE	2.42	0.46
1:F:323:SER:O	1:F:330:LEU:HD12	2.16	0.46
1:G:137:LEU:H	1:G:165:ARG:HH22	1.62	0.46
1:A:96:THR:HG22	1:A:120:ALA:O	2.15	0.46
1:C:184:LEU:HB3	1:C:213:ARG:NH2	2.30	0.46
1:C:23:ASP:OD1	1:C:23:ASP:N	2.48	0.46
1:E:175:PHE:C	1:E:175:PHE:CD1	2.89	0.46
1:C:197:LLP:NZ	1:C:197:LLP:O3	2.38	0.46
1:D:201:GLY:O	1:D:327:VAL:HG13	2.16	0.46
1:E:345:GLU:O	1:E:349:ARG:HG3	2.16	0.46
1:H:277:PRO:HA	1:H:282:HIS:CD2	2.50	0.46
1:C:39:GLN:HE22	1:C:43:ARG:H	1.61	0.46
1:E:324:LEU:HD23	2:E:401:MES:O3S	2.15	0.46
1:A:343:SER:O	1:A:347:ARG:N	2.30	0.46
1:B:124:THR:O	1:B:128:ILE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HD23	1:B:72:VAL:HG11	1.97	0.46
1:C:11:VAL:HA	1:C:245:HIS:ND1	2.31	0.46
1:D:339:HIS:CD2	1:D:352:ILE:HD13	2.50	0.46
1:F:120:ALA:CB	1:F:131:ALA:HB2	2.45	0.46
1:F:101:ALA:HA	1:F:104:ASP:HB2	1.96	0.46
1:A:112:ARG:O	1:B:88:ARG:NH1	2.48	0.46
1:G:123:THR:HB	1:G:284:GLN:HE21	1.81	0.46
1:G:292:MSE:O	3:G:404:GOL:O1	2.19	0.46
1:B:9:ARG:CD	1:B:64:LEU:HA	2.45	0.46
1:F:185:ALA:HA	3:F:405:GOL:H32	1.97	0.46
1:G:289:LYS:HD2	6:G:656:HOH:O	2.15	0.46
1:A:222:ARG:O	1:A:226:THR:OG1	2.32	0.46
1:C:337:MSE:HG2	1:D:36:ARG:NE	2.30	0.46
2:D:401:MES:H82	2:D:401:MES:H32	1.39	0.46
6:G:663:HOH:O	1:H:235:LEU:HB2	2.15	0.46
1:F:124:THR:O	1:F:128:ILE:N	2.46	0.46
1:G:292:MSE:SE	1:G:295:PRO:CA	3.13	0.46
1:F:254:GLN:HB3	1:F:297:ALA:CB	2.46	0.46
1:B:197:LLP:HG2	1:B:324:LEU:HG	1.97	0.46
1:F:91:GLN:HA	1:F:136:ASP:HB3	1.96	0.46
1:D:173:ASN:HB3	1:D:193:TYR:CE1	2.50	0.46
1:F:37:ARG:NH2	6:F:663:HOH:O	2.49	0.46
1:H:94:VAL:HG23	1:H:137:LEU:HD13	1.98	0.46
1:G:323:SER:HA	2:G:401:MES:S	2.56	0.46
1:D:322:VAL:CG1	1:D:337:MSE:SE	3.01	0.46
1:E:150:LEU:HD22	1:E:175:PHE:HZ	1.80	0.46
1:A:175:PHE:C	1:A:175:PHE:CD1	2.89	0.46
1:A:6:PHE:CE2	1:A:179:VAL:HG12	2.50	0.46
1:B:178:PRO:HD3	1:B:193:TYR:CE1	2.51	0.46
1:C:42:PRO:HB3	1:C:45:PHE:HE1	1.81	0.46
1:G:334:PRO:O	1:G:339:HIS:N	2.48	0.46
1:F:6:PHE:CE2	1:F:179:VAL:HG22	2.51	0.46
1:F:350:ARG:O	1:F:352:ILE:HG13	2.16	0.46
1:G:281:GLU:N	6:G:677:HOH:O	2.48	0.46
1:H:173:ASN:HB3	1:H:193:TYR:CE1	2.50	0.46
1:C:336:LEU:O	1:C:340:ARG:HD2	2.16	0.46
1:D:281:GLU:HG3	6:D:676:HOH:O	2.15	0.46
1:D:180:LEU:HD22	1:D:294:ALA:HB3	1.97	0.46
1:D:335:ALA:CB	1:D:354:GLU:HA	2.45	0.46
1:G:120:ALA:O	1:G:122:LEU:HG	2.15	0.46
1:H:43:ARG:NH1	1:H:44:TYR:OH	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:401:MES:H82	2:E:401:MES:H32	1.74	0.46
1:F:375:ARG:HB3	6:F:625:HOH:O	2.15	0.46
1:C:347:ARG:HB3	1:C:352:ILE:O	2.16	0.46
1:A:16:ARG:HA	1:A:17:PRO:HD2	1.85	0.46
1:D:139:LEU:HD12	1:D:168:ARG:O	2.16	0.46
1:E:161:ARG:HD3	1:E:164:GLU:OE1	2.16	0.46
1:G:97:ASP:OD1	1:G:98:ASP:N	2.49	0.46
1:A:213:ARG:NH2	6:A:611:HOH:O	2.46	0.46
1:B:94:VAL:HG21	1:B:131:ALA:O	2.16	0.46
1:C:347:ARG:NH1	6:C:658:HOH:O	2.49	0.46
1:G:348:ALA:O	1:G:350:ARG:N	2.43	0.46
1:H:199:ILE:HG23	1:H:244:LEU:HG	1.97	0.46
1:H:39:GLN:OE1	1:H:43:ARG:N	2.49	0.46
1:A:112:ARG:HD2	6:A:584:HOH:O	2.15	0.46
1:A:40:ASP:HB3	1:A:41:GLU:H	1.49	0.46
1:A:368:ASP:OD2	1:D:5:ARG:HB2	2.16	0.46
1:B:43:ARG:HH22	1:B:55:GLU:CD	2.19	0.46
1:C:100:TYR:CE1	2:C:401:MES:H82	2.51	0.46
1:C:98:ASP:OD1	1:C:98:ASP:N	2.46	0.46
1:D:173:ASN:HB3	1:D:193:TYR:CE1	2.50	0.46
1:G:96:THR:HG22	1:G:121:ASP:HA	1.98	0.46
1:G:338:THR:HG1	1:G:339:HIS:CE1	2.27	0.46
1:C:20:GLY:O	1:C:21:THR:OG1	2.24	0.46
1:F:291:GLN:HG3	1:F:292:MSE:HG2	1.96	0.46
1:F:342:LEU:HD13	1:F:346:ALA:HB1	1.98	0.46
1:G:132:LEU:O	1:G:165:ARG:NH1	2.42	0.46
1:H:93:VAL:HG12	1:H:139:LEU:HB3	1.97	0.46
1:H:35:GLU:CD	1:H:37:ARG:HH21	2.18	0.46
1:B:321:GLY:CA	1:B:337:MSE:HE1	2.45	0.46
6:A:630:HOH:O	1:B:33:THR:HB	2.15	0.46
1:D:334:PRO:HD2	1:D:356:LEU:O	2.16	0.46
1:F:180:LEU:HD21	1:F:252:HIS:CE1	2.51	0.46
1:F:282:HIS:CD2	1:F:283:PRO:HD2	2.51	0.46
1:H:281:GLU:CG	6:H:661:HOH:O	2.64	0.46
1:F:175:PHE:C	1:F:175:PHE:CD1	2.89	0.46
1:G:36:ARG:CZ	4:H:407:CL:CL	3.01	0.46
1:D:160:ARG:HG2	1:D:161:ARG:HH11	1.81	0.46
1:A:9:ARG:HH12	1:A:66:ARG:NH2	2.13	0.46
1:D:276:TYR:CD1	1:D:299:VAL:HG22	2.50	0.46
1:E:175:PHE:HZ	6:E:536:HOH:O	1.98	0.46
1:E:309:GLU:HG2	1:E:309:GLU:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLU:HG3	1:B:38:ALA:HB2	1.98	0.46
1:B:254:GLN:HG2	1:B:361:VAL:O	2.16	0.46
1:F:308:ALA:O	1:F:312:LEU:HG	2.16	0.46
1:E:6:PHE:HE2	1:E:179:VAL:HG22	1.80	0.46
1:F:263:GLU:HG3	6:F:650:HOH:O	2.14	0.46
1:F:253:ARG:NH1	3:G:404:GOL:H12	2.31	0.46
1:E:8:THR:HG23	1:H:364:GLU:CB	2.46	0.46
1:C:150:LEU:HD22	1:C:175:PHE:CE2	2.51	0.46
1:D:18:SER:O	1:D:20:GLY:N	2.49	0.46
1:D:147:ASN:ND2	1:D:358:ARG:HH11	2.14	0.46
1:E:213:ARG:HH11	3:E:402:GOL:H11	1.79	0.46
1:F:249:LEU:HD23	3:F:403:GOL:H2	1.98	0.46
1:G:259:ARG:HB2	6:G:558:HOH:O	2.16	0.46
1:B:334:PRO:HB3	1:B:339:HIS:HD2	1.81	0.46
1:E:9:ARG:HB3	6:E:654:HOH:O	2.15	0.46
1:G:111:ALA:HB3	1:G:112:ARG:HH12	1.81	0.46
1:E:16:ARG:NH1	1:E:16:ARG:HB3	2.31	0.46
1:E:334:PRO:HA	1:E:338:THR:OG1	2.14	0.46
1:H:147:ASN:HD22	1:H:148:PRO:CA	2.29	0.46
1:C:16:ARG:HD2	1:C:56:GLU:HG2	1.97	0.46
1:F:4:MSE:HE1	1:F:12:HIS:C	2.36	0.46
1:F:368:ASP:OD1	1:G:4:MSE:N	2.49	0.46
1:C:16:ARG:HA	6:C:666:HOH:O	2.15	0.46
1:F:173:ASN:HB3	1:F:193:TYR:CE1	2.51	0.46
1:A:36:ARG:CZ	1:B:337:MSE:HE3	2.46	0.46
1:A:27:PRO:HB2	1:C:27:PRO:HB2	1.98	0.46
1:C:197:LLP:HB2	1:C:324:LEU:HD12	1.98	0.46
1:E:175:PHE:CZ	1:E:298:ILE:HB	2.51	0.46
1:G:108:ASP:O	1:G:112:ARG:NH1	2.46	0.46
1:H:9:ARG:HB3	1:H:64:LEU:HD23	1.97	0.46
1:D:121:ASP:OD2	1:D:123:THR:HG22	2.15	0.46
1:E:110:ALA:HB1	1:E:115:VAL:HB	1.98	0.46
1:B:321:GLY:O	1:B:332:GLU:HB3	2.16	0.46
1:C:288:VAL:O	1:C:289:LYS:HB3	2.16	0.46
1:E:263:GLU:OE2	1:E:266:ARG:NH1	2.49	0.46
1:E:292:MSE:HE3	6:E:573:HOH:O	2.16	0.46
1:B:368:ASP:OD2	1:C:5:ARG:HB2	2.16	0.46
1:B:51:ASN:HA	1:B:52:PRO:HD3	1.86	0.46
1:D:35:GLU:HG3	1:D:38:ALA:H	1.80	0.46
1:A:17:PRO:HA	6:A:662:HOH:O	2.15	0.46
1:B:6:PHE:HA	1:B:9:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:ARG:O	1:F:9:ARG:HG3	2.16	0.46
1:B:371:GLU:O	1:B:375:ARG:HB2	2.14	0.46
1:C:124:THR:CB	6:C:660:HOH:O	2.63	0.46
1:D:333:CYS:H	1:D:337:MSE:HE2	1.80	0.46
1:F:368:ASP:OD2	1:G:5:ARG:N	2.40	0.46
1:G:146:THR:OG1	1:G:151:THR:OG1	2.19	0.46
1:E:322:VAL:HG22	6:F:517:HOH:O	2.15	0.46
1:E:346:ALA:HB1	1:E:350:ARG:HD2	1.97	0.46
1:B:96:THR:C	1:B:98:ASP:H	2.18	0.46
1:E:199:ILE:HD12	6:E:556:HOH:O	2.16	0.46
1:F:178:PRO:HD3	1:F:193:TYR:CE1	2.51	0.46
1:A:97:ASP:OD2	1:A:98:ASP:N	2.49	0.45
1:C:347:ARG:HD2	1:C:352:ILE:O	2.16	0.45
1:F:253:ARG:HD2	3:F:405:GOL:H11	1.97	0.45
1:H:35:GLU:OE2	1:H:37:ARG:HB2	2.16	0.45
1:G:183:PRO:HA	1:G:186:LEU:HD12	1.98	0.45
1:G:4:MSE:O	1:G:9:ARG:HG3	2.16	0.45
1:B:335:ALA:O	1:B:340:ARG:HB2	2.15	0.45
1:B:178:PRO:HD3	1:B:193:TYR:CE1	2.51	0.45
1:B:264:ARG:CZ	1:B:370:ALA:HB1	2.46	0.45
1:D:347:ARG:CD	6:D:672:HOH:O	2.62	0.45
1:A:334:PRO:HD2	1:A:356:LEU:O	2.16	0.45
1:B:6:PHE:CE2	1:B:179:VAL:HG22	2.52	0.45
1:C:319:THR:HB	1:C:330:LEU:HD23	1.98	0.45
1:D:5:ARG:O	1:D:9:ARG:HG3	2.16	0.45
1:F:159:SER:HA	1:F:169:VAL:HG21	1.98	0.45
1:A:112:ARG:CZ	1:E:135:PRO:HG3	2.46	0.45
1:A:6:PHE:CE2	1:A:179:VAL:HG12	2.50	0.45
1:B:177:SER:HB2	1:B:178:PRO:HD2	1.97	0.45
1:F:16:ARG:HB3	1:F:17:PRO:HD2	1.97	0.45
1:A:36:ARG:CZ	1:B:337:MSE:HE3	2.46	0.45
1:B:338:THR:OG1	1:B:339:HIS:N	2.49	0.45
1:B:4:MSE:HG3	1:B:9:ARG:HG2	1.97	0.45
1:C:347:ARG:HB3	1:C:352:ILE:O	2.16	0.45
1:D:145:PRO:HD2	1:D:175:PHE:CD1	2.51	0.45
1:E:277:PRO:O	1:E:285:HIS:ND1	2.49	0.45
1:C:92:CYS:HA	1:C:116:ARG:O	2.15	0.45
1:G:276:TYR:OH	1:G:295:PRO:HB2	2.17	0.45
1:B:100:TYR:HB3	1:B:103:THR:OG1	2.16	0.45
1:B:142:ILE:HD11	1:B:158:VAL:HG11	1.97	0.45
1:C:310:ARG:O	1:C:314:ARG:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ARG:NE	1:D:320:CYS:SG	2.89	0.45
1:G:273:ALA:HB3	1:G:302:ASP:OD2	2.16	0.45
1:G:46:TYR:OH	1:H:196:THR:HG21	2.16	0.45
1:A:116:ARG:NH2	1:A:135:PRO:HG2	2.32	0.45
1:A:41:GLU:O	1:A:43:ARG:N	2.49	0.45
1:B:124:THR:OG1	1:B:127:GLY:N	2.37	0.45
1:B:88:ARG:NE	1:E:136:ASP:OD1	2.49	0.45
1:E:88:ARG:HD2	6:E:676:HOH:O	2.17	0.45
1:C:16:ARG:NH2	1:C:55:GLU:HB3	2.31	0.45
1:C:104:ASP:CG	1:C:119:TYR:HH	2.18	0.45
1:C:4:MSE:HG3	1:C:9:ARG:HG2	1.98	0.45
1:E:113:GLN:HB3	1:F:113:GLN:OE1	2.16	0.45
1:G:343:SER:HB2	1:G:344:ALA:H	1.60	0.45
1:A:227:THR:HA	4:A:405:GOL:C3	2.44	0.45
1:A:233:GLY:O	1:A:236:ASP:HB2	2.17	0.45
1:B:107:PHE:HB3	1:B:117:VAL:HG11	1.97	0.45
1:C:96:THR:HG21	1:C:143:GLU:H	1.81	0.45
1:G:84:LEU:HD13	1:G:110:ALA:HB2	1.97	0.45
1:H:43:ARG:HB3	1:H:43:ARG:HH21	1.80	0.45
1:A:132:LEU:HD12	1:A:137:LEU:HD21	1.97	0.45
1:E:180:LEU:HD22	1:E:294:ALA:HB3	1.97	0.45
1:G:121:ASP:HB3	1:G:127:GLY:HA3	1.97	0.45
1:G:347:ARG:HB3	1:G:352:ILE:O	2.15	0.45
1:D:214:ASP:OD2	1:D:217:LEU:N	2.22	0.45
1:A:17:PRO:HG2	6:A:679:HOH:O	2.14	0.45
2:C:401:MES:H61	1:D:46:TYR:CG	2.50	0.45
1:E:124:THR:O	1:E:126:GLU:N	2.48	0.45
1:F:94:VAL:HG21	1:F:131:ALA:O	2.16	0.45
1:A:4:MSE:HE3	1:A:4:MSE:HB3	1.72	0.45
1:B:4:MSE:HE2	1:B:8:THR:CG2	2.46	0.45
1:C:121:ASP:OD1	1:C:123:THR:OG1	2.18	0.45
1:C:309:GLU:HB3	1:C:310:ARG:CZ	2.46	0.45
1:F:147:ASN:ND2	1:F:358:ARG:HH11	2.15	0.45
1:F:332:GLU:HG2	1:F:358:ARG:HH21	1.81	0.45
1:A:372:ASP:OD2	1:A:375:ARG:NH1	2.47	0.45
1:C:253:ARG:HG3	1:C:253:ARG:HH11	1.81	0.45
1:E:92:CYS:SG	1:E:116:ARG:HD2	2.56	0.45
1:H:116:ARG:HH21	1:H:134:GLU:HG2	1.81	0.45
1:H:251:VAL:HA	1:H:254:GLN:HE21	1.81	0.45
1:A:107:PHE:O	1:A:111:ALA:N	2.42	0.45
1:D:91:GLN:O	1:D:116:ARG:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:HIS:HD2	1:E:342:LEU:CD1	2.29	0.45
1:G:19:ALA:C	1:G:21:THR:H	2.20	0.45
1:G:332:GLU:OE2	1:G:358:ARG:CZ	2.64	0.45
1:D:122:LEU:HA	1:D:128:ILE:HG13	1.99	0.45
1:H:96:THR:O	1:H:98:ASP:N	2.49	0.45
1:A:4:MSE:HB2	1:A:8:THR:HB	1.97	0.45
1:C:134:GLU:HG3	1:C:135:PRO:HD2	1.98	0.45
1:E:160:ARG:O	1:E:164:GLU:HG3	2.15	0.45
1:A:96:THR:O	1:A:119:TYR:HB3	2.16	0.45
1:B:128:ILE:O	1:B:132:LEU:HG	2.16	0.45
1:C:100:TYR:HE1	2:C:401:MES:H31	1.81	0.45
1:D:168:ARG:NH2	3:D:403:GOL:H2	2.18	0.45
1:E:130:ALA:HA	6:E:690:HOH:O	2.17	0.45
1:F:146:THR:HG21	6:F:659:HOH:O	2.15	0.45
1:H:173:ASN:HB3	1:H:193:TYR:CE1	2.51	0.45
1:A:337:MSE:HE3	6:A:577:HOH:O	2.15	0.45
1:E:347:ARG:NE	1:E:354:GLU:OE1	2.50	0.45
1:A:292:MSE:SE	1:A:295:PRO:C	3.04	0.45
1:D:168:ARG:CZ	4:D:405:CL:CL	3.01	0.45
1:G:99:VAL:HG13	1:G:100:TYR:O	2.17	0.45
1:H:173:ASN:HB3	1:H:193:TYR:CE1	2.52	0.45
1:G:116:ARG:NH1	1:G:134:GLU:HG2	2.30	0.45
1:G:292:MSE:HE3	1:G:295:PRO:HA	1.99	0.45
1:G:3:GLY:N	6:G:1441:HOH:O	2.50	0.45
1:G:93:VAL:HG22	1:G:139:LEU:HB3	1.98	0.45
1:A:112:ARG:HE	1:E:135:PRO:CG	2.29	0.45
1:A:37:ARG:HH11	1:B:313:ASP:HA	1.81	0.45
1:B:97:ASP:HB3	1:B:119:TYR:HB3	1.97	0.45
1:A:319:THR:HG23	1:B:35:GLU:OE1	2.17	0.45
1:G:334:PRO:O	1:G:339:HIS:N	2.49	0.45
1:A:173:ASN:HB3	1:A:193:TYR:CE1	2.51	0.45
1:B:358:ARG:NH1	2:B:401:MES:O3S	2.47	0.45
1:C:337:MSE:CE	1:D:36:ARG:HD2	2.47	0.45
1:H:289:LYS:HB3	6:H:576:HOH:O	2.15	0.45
1:G:337:MSE:HE2	1:G:337:MSE:HB2	1.67	0.45
1:D:156:ALA:O	1:D:160:ARG:NE	2.45	0.45
2:E:401:MES:H62	4:E:404:GOL:H11	1.99	0.45
1:F:322:VAL:HB	2:F:401:MES:H72	1.98	0.45
1:F:38:ALA:C	1:F:39:GLN:HG2	2.35	0.45
1:H:53:THR:HA	1:H:56:GLU:OE1	2.16	0.45
1:E:15:ARG:HG2	1:E:16:ARG:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:PRO:HA	1:E:282:HIS:CD2	2.51	0.45
1:E:112:ARG:CZ	6:E:668:HOH:O	2.63	0.45
1:D:277:PRO:HA	1:D:282:HIS:CD2	2.51	0.45
1:F:7:GLY:HA2	1:F:10:LEU:HD12	1.99	0.45
1:A:137:LEU:HG	1:A:167:ALA:HB2	1.97	0.45
1:B:149:LEU:HD11	1:B:350:ARG:O	2.15	0.45
1:B:4:MSE:O	1:B:66:ARG:NH1	2.49	0.45
1:B:9:ARG:HD3	1:B:63:GLY:O	2.17	0.45
1:C:112:ARG:NH1	6:C:503:HOH:O	2.50	0.45
1:H:37:ARG:C	1:H:39:GLN:H	2.20	0.45
1:A:99:VAL:HG13	1:A:103:THR:HB	1.97	0.45
1:C:145:PRO:HB2	1:C:175:PHE:CE1	2.52	0.45
1:D:277:PRO:HA	1:D:282:HIS:CD2	2.51	0.45
1:H:116:ARG:NH2	1:H:135:PRO:O	2.49	0.45
1:D:292:MSE:HE3	1:D:295:PRO:HA	1.93	0.45
1:H:102:GLY:HA2	3:H:403:GOL:H31	1.97	0.45
1:D:367:GLN:CD	6:D:671:HOH:O	2.55	0.45
1:H:350:ARG:HG3	6:H:668:HOH:O	2.16	0.45
1:B:179:VAL:CG1	1:B:252:HIS:HE1	2.29	0.45
1:F:127:GLY:O	1:F:131:ALA:N	2.35	0.45
1:G:180:LEU:HD22	1:G:294:ALA:HB3	1.99	0.45
1:A:277:PRO:HA	1:A:282:HIS:CD2	2.52	0.45
1:B:23:ASP:OD2	1:D:29:HIS:ND1	2.49	0.45
1:B:50:GLU:HA	6:B:605:HOH:O	2.17	0.45
1:D:197:LLP:H4'1	2:D:401:MES:H81	1.98	0.45
1:F:180:LEU:HD22	1:F:294:ALA:HB3	1.99	0.45
1:H:37:ARG:H	1:H:37:ARG:HG3	1.61	0.45
1:B:93:VAL:HG22	1:B:139:LEU:HB3	1.99	0.45
1:F:109:LEU:HD23	1:F:112:ARG:HH21	1.81	0.45
1:F:173:ASN:HB3	1:F:193:TYR:CE1	2.51	0.45
1:F:288:VAL:HG13	1:F:292:MSE:SE	2.65	0.45
1:A:179:VAL:CG2	1:A:251:VAL:HG11	2.47	0.45
1:D:98:ASP:HB2	1:D:146:THR:CB	2.46	0.45
1:D:252:HIS:CD2	6:D:667:HOH:O	2.69	0.45
1:E:276:TYR:OH	1:E:296:GLY:O	2.25	0.45
1:C:314:ARG:HD3	6:C:628:HOH:O	2.16	0.45
1:D:150:LEU:HD22	1:D:175:PHE:HZ	1.81	0.45
1:H:184:LEU:HB3	1:H:213:ARG:HH11	1.81	0.45
1:F:314:ARG:NH2	1:F:376:ALA:O	2.43	0.45
1:A:90:GLY:HA3	1:F:89:PRO:HG2	1.98	0.45
1:G:225:ARG:HD2	1:G:231:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:HB3	3:B:404:GOL:O2	2.16	0.45
1:E:315:PHE:HB2	1:F:37:ARG:HH22	1.80	0.45
1:E:289:LYS:HE3	1:E:289:LYS:HB3	1.84	0.45
1:G:344:ALA:HA	1:G:347:ARG:NH2	2.32	0.45
1:H:333:CYS:O	1:H:337:MSE:HB2	2.17	0.45
1:A:173:ASN:HB3	1:A:193:TYR:CE1	2.52	0.45
1:C:121:ASP:O	1:C:127:GLY:HA3	2.16	0.45
1:D:95:SER:O	1:D:120:ALA:N	2.41	0.45
1:H:350:ARG:O	1:H:352:ILE:HG13	2.17	0.45
1:D:41:GLU:HA	6:D:642:HOH:O	2.17	0.45
1:B:14:GLY:O	1:B:16:ARG:N	2.49	0.45
1:A:337:MSE:HE1	1:B:36:ARG:NH2	2.32	0.45
1:E:275:HIS:HB2	1:E:300:SER:OG	2.17	0.45
1:G:192:LEU:HD12	1:G:193:TYR:N	2.32	0.45
1:A:39:GLN:HB2	1:A:42:PRO:HA	1.98	0.45
1:H:149:LEU:HD23	1:H:149:LEU:HA	1.88	0.45
1:H:89:PRO:HG2	6:H:501:HOH:O	2.17	0.45
1:C:337:MSE:HE2	1:D:36:ARG:HD2	1.98	0.45
1:F:105:GLY:O	1:F:109:LEU:N	2.39	0.45
1:G:108:ASP:HB3	1:G:112:ARG:HH12	1.80	0.45
1:G:84:LEU:HG	1:G:141:TRP:HZ3	1.82	0.45
1:B:3:GLY:HA2	1:B:66:ARG:NH2	2.31	0.45
3:F:404:GOL:H12	1:G:253:ARG:HH11	1.82	0.45
2:B:401:MES:H82	2:B:401:MES:H31	1.74	0.45
1:C:322:VAL:HG12	2:C:401:MES:H72	1.98	0.45
1:D:337:MSE:HB2	1:D:337:MSE:HE2	1.77	0.45
1:E:23:ASP:OD2	1:G:29:HIS:ND1	2.39	0.45
1:G:337:MSE:C	1:G:337:MSE:SE	2.93	0.45
1:H:174:THR:O	6:H:594:HOH:O	2.21	0.45
1:H:334:PRO:HD2	1:H:356:LEU:O	2.17	0.45
1:H:168:ARG:NH2	3:H:404:GOL:H32	2.27	0.45
1:A:16:ARG:HA	1:A:17:PRO:HD3	1.63	0.45
1:C:338:THR:O	1:C:341:PRO:HD2	2.17	0.45
1:C:339:HIS:CG	6:C:657:HOH:O	2.68	0.45
1:E:41:GLU:HA	6:E:673:HOH:O	2.15	0.45
1:F:147:ASN:HD21	1:F:358:ARG:HH11	1.64	0.45
1:G:176:ALA:HB1	1:G:180:LEU:HB2	1.99	0.45
1:G:36:ARG:NH1	1:H:337:MSE:HG2	2.31	0.45
1:B:96:THR:O	1:B:99:VAL:HG13	2.17	0.45
1:C:43:ARG:NH2	1:C:55:GLU:OE2	2.47	0.45
1:E:178:PRO:HG3	1:E:193:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLY:HA2	1:A:59:GLU:CD	2.37	0.45
1:B:337:MSE:O	1:B:340:ARG:HB2	2.17	0.45
1:C:37:ARG:NH2	1:D:320:CYS:SG	2.89	0.45
1:D:350:ARG:HB3	1:D:352:ILE:HG13	1.99	0.45
1:F:308:ALA:O	1:F:312:LEU:HG	2.17	0.45
1:B:175:PHE:CZ	1:B:298:ILE:HB	2.52	0.45
1:D:160:ARG:HD3	6:D:573:HOH:O	2.16	0.45
1:E:273:ALA:HB3	1:E:302:ASP:OD1	2.17	0.45
1:G:100:TYR:CE1	2:G:401:MES:H81	2.51	0.45
1:H:161:ARG:HA	1:H:161:ARG:HD3	1.68	0.45
1:C:124:THR:HG23	1:C:127:GLY:HA3	1.99	0.45
1:C:149:LEU:HD22	1:C:275:HIS:CE1	2.52	0.45
1:D:77:GLN:OE1	1:D:102:GLY:HA3	2.17	0.45
1:D:88:ARG:HG2	1:D:91:GLN:NE2	2.32	0.45
1:F:124:THR:HA	1:F:125:PRO:HD2	1.60	0.45
1:F:94:VAL:HA	1:F:118:ARG:O	2.17	0.45
1:C:289:LYS:HB3	6:C:596:HOH:O	2.15	0.45
1:C:83:LEU:HD22	1:C:210:LEU:HD22	1.98	0.45
1:E:16:ARG:HB2	1:E:56:GLU:OE1	2.17	0.45
1:E:95:SER:OG	1:E:99:VAL:HG11	2.17	0.45
1:F:14:GLY:HA2	1:F:59:GLU:OE2	2.16	0.45
1:A:88:ARG:HG2	1:A:89:PRO:HD2	1.98	0.45
1:F:109:LEU:HD23	1:F:112:ARG:NH2	2.31	0.45
1:F:39:GLN:HG3	1:F:40:ASP:N	2.31	0.45
1:B:4:MSE:HG3	1:B:8:THR:HG21	1.98	0.45
1:H:303:TYR:CD1	1:H:311:LEU:HD22	2.51	0.45
1:C:84:LEU:HD21	1:C:107:PHE:CD1	2.51	0.45
1:E:39:GLN:OE1	6:E:600:HOH:O	2.21	0.45
1:F:175:PHE:C	1:F:175:PHE:CD1	2.90	0.45
1:F:175:PHE:C	1:F:175:PHE:HD1	2.20	0.45
1:F:205:VAL:HG23	1:F:236:ASP:OD1	2.16	0.45
1:F:254:GLN:HB3	1:F:297:ALA:HB2	1.98	0.45
1:F:69:PHE:HA	5:F:407:FMT:O1	2.17	0.45
1:C:92:CYS:HB2	1:C:116:ARG:HH21	1.81	0.45
1:D:95:SER:OG	1:D:96:THR:N	2.49	0.45
1:E:310:ARG:HD3	6:E:629:HOH:O	2.17	0.45
1:E:338:THR:O	1:E:341:PRO:HD2	2.17	0.45
1:F:345:GLU:CB	6:F:639:HOH:O	2.64	0.45
1:A:197:LLP:H4'1	1:A:197:LLP:OP3	2.16	0.45
1:B:321:GLY:HA2	1:B:337:MSE:HE1	1.97	0.45
1:B:3:GLY:CA	1:B:66:ARG:HH22	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:ARG:HD3	6:E:513:HOH:O	2.15	0.45
1:E:346:ALA:HA	1:E:349:ARG:NH1	2.32	0.45
1:G:337:MSE:HG2	1:G:337:MSE:H	1.53	0.45
1:A:118:ARG:HE	1:A:120:ALA:HB2	1.82	0.45
1:A:29:HIS:O	1:A:51:ASN:ND2	2.49	0.45
1:B:259:ARG:HE	1:B:295:PRO:HG2	1.81	0.45
1:E:44:TYR:CE2	1:G:21:THR:HG22	2.52	0.45
1:D:335:ALA:O	1:D:347:ARG:NH1	2.50	0.45
1:E:4:MSE:O	1:E:9:ARG:HD2	2.16	0.45
1:G:347:ARG:HB3	1:G:352:ILE:O	2.17	0.45
1:H:257:THR:HG21	1:H:369:LEU:HD12	1.98	0.45
1:D:100:TYR:CE1	2:D:401:MES:H82	2.52	0.45
1:D:137:LEU:HD23	1:D:167:ALA:HB2	1.98	0.45
1:D:173:ASN:HB3	1:D:193:TYR:CE1	2.51	0.45
1:F:197:LLP:HB2	1:F:324:LEU:HD12	1.99	0.45
1:G:83:LEU:HG	1:G:210:LEU:HD13	1.99	0.45
1:A:179:VAL:HG23	1:A:180:LEU:HG	1.98	0.45
1:E:378:ALA:HB1	6:E:667:HOH:O	2.16	0.45
1:F:58:GLU:OE2	1:F:72:VAL:HG22	2.17	0.45
1:G:5:ARG:O	1:G:9:ARG:HG3	2.16	0.45
1:H:214:ASP:OD2	6:H:586:HOH:O	2.21	0.45
1:H:332:GLU:HA	1:H:337:MSE:SE	2.66	0.45
1:H:7:GLY:HA2	1:H:10:LEU:HD12	1.98	0.45
1:E:175:PHE:CZ	1:E:298:ILE:HG21	2.52	0.45
1:F:54:ARG:HG3	1:F:237:CYS:SG	2.57	0.45
1:G:303:TYR:CG	1:G:311:LEU:HD22	2.52	0.45
1:A:41:GLU:HA	1:A:42:PRO:HD3	1.83	0.45
1:C:343:SER:OG	1:C:344:ALA:N	2.49	0.45
1:E:37:ARG:NE	6:E:621:HOH:O	2.50	0.45
1:F:361:VAL:O	6:F:541:HOH:O	2.21	0.45
1:H:285:HIS:HE1	6:H:659:HOH:O	1.97	0.45
1:H:323:SER:N	2:H:401:MES:O2S	2.50	0.45
1:H:41:GLU:HA	1:H:42:PRO:HD2	1.79	0.45
1:H:43:ARG:HB3	1:H:43:ARG:NH2	2.32	0.45
1:B:374:SER:HB2	6:B:608:HOH:O	2.17	0.45
1:A:342:LEU:HD13	1:A:343:SER:O	2.16	0.45
1:B:338:THR:HG22	2:B:401:MES:H32	1.98	0.45
1:D:94:VAL:HG11	1:D:131:ALA:HB1	1.98	0.45
1:E:98:ASP:HB2	1:E:146:THR:HB	1.98	0.45
1:G:322:VAL:O	1:H:33:THR:HG21	2.17	0.45
1:H:347:ARG:HB3	1:H:352:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLY:O	1:B:56:GLU:HB3	2.17	0.45
1:F:102:GLY:CA	3:F:402:GOL:H11	2.47	0.45
1:D:168:ARG:HH12	3:D:404:GOL:H32	1.82	0.45
1:E:332:GLU:HB2	1:E:337:MSE:HE1	1.98	0.45
1:H:107:PHE:HB3	1:H:117:VAL:HG11	1.99	0.45
1:A:118:ARG:HD2	1:A:134:GLU:HG3	1.99	0.45
1:A:143:GLU:O	1:A:146:THR:HG22	2.17	0.45
1:E:110:ALA:HB1	1:E:115:VAL:HB	1.99	0.45
1:F:264:ARG:HD3	1:F:264:ARG:HA	1.86	0.45
1:F:281:GLU:HA	6:F:505:HOH:O	2.17	0.45
1:F:292:MSE:HE2	6:F:562:HOH:O	2.16	0.45
1:D:344:ALA:O	1:D:348:ALA:N	2.42	0.45
1:E:97:ASP:OD2	1:E:98:ASP:N	2.50	0.45
1:F:175:PHE:HB2	6:F:583:HOH:O	2.17	0.45
1:E:16:ARG:HA	1:E:17:PRO:HD3	1.71	0.45
1:A:163:HIS:O	1:A:166:GLY:N	2.48	0.45
1:C:291:GLN:HG3	1:C:292:MSE:HG2	1.99	0.45
1:E:143:GLU:HG3	1:E:172:ASP:HB3	1.99	0.45
1:F:248:SER:O	1:F:252:HIS:HD2	2.00	0.45
1:C:173:ASN:HB3	1:C:193:TYR:CE1	2.52	0.45
1:H:92:CYS:HB3	1:H:137:LEU:HA	1.99	0.45
1:B:9:ARG:NH2	1:B:66:ARG:HE	2.15	0.45
1:E:161:ARG:HA	1:E:161:ARG:HD3	1.63	0.45
1:H:259:ARG:NE	6:H:665:HOH:O	2.50	0.45
1:A:126:GLU:CD	1:A:126:GLU:H	2.19	0.45
1:D:252:HIS:HD2	6:D:616:HOH:O	2.00	0.45
1:H:100:TYR:HE1	2:H:401:MES:H82	1.82	0.45
1:H:6:PHE:HA	1:H:9:ARG:HE	1.82	0.45
1:B:98:ASP:HB2	1:B:146:THR:HB	1.99	0.45
1:D:279:LEU:HA	1:D:280:PRO:HD3	1.83	0.45
1:F:342:LEU:HD12	1:F:342:LEU:H	1.81	0.45
1:G:332:GLU:OE1	1:G:334:PRO:HG3	2.16	0.45
1:A:337:MSE:HG2	1:B:36:ARG:NH2	2.32	0.45
1:E:84:LEU:HD12	1:E:106:LEU:HB3	1.99	0.45
1:G:161:ARG:NH1	1:G:164:GLU:OE2	2.50	0.45
1:H:71:THR:OG1	1:H:212:TYR:OH	2.32	0.45
1:C:214:ASP:OD2	1:C:216:ASP:HB2	2.17	0.45
1:H:96:THR:HB	6:H:647:HOH:O	2.16	0.45
1:B:18:SER:N	6:B:636:HOH:O	2.37	0.45
1:B:251:VAL:O	1:B:255:VAL:HG23	2.16	0.45
1:E:319:THR:HG23	1:F:35:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:ARG:HH21	1:G:9:ARG:CG	2.30	0.45
1:D:214:ASP:OD2	1:D:217:LEU:HB2	2.16	0.45
2:E:401:MES:H62	1:F:48:ARG:HH12	1.81	0.45
1:B:364:GLU:HB2	1:B:369:LEU:HD11	1.98	0.45
1:C:116:ARG:HH12	1:C:134:GLU:CD	2.19	0.45
1:G:175:PHE:CZ	1:G:298:ILE:HB	2.52	0.45
1:C:310:ARG:HA	1:C:310:ARG:NE	2.31	0.45
1:E:321:GLY:CA	1:E:337:MSE:HE1	2.46	0.45
1:G:95:SER:HB2	1:G:141:TRP:HB3	1.99	0.45
1:H:86:LEU:HB3	3:H:404:GOL:H31	1.99	0.45
1:B:29:HIS:ND1	1:D:23:ASP:OD2	2.39	0.45
1:G:333:CYS:CA	1:G:337:MSE:HE3	2.44	0.45
1:H:143:GLU:HG3	1:H:172:ASP:HB3	1.99	0.45
1:B:368:ASP:OD2	1:C:4:MSE:HA	2.17	0.45
1:D:283:PRO:HB2	1:D:284:GLN:NE2	2.31	0.45
1:G:111:ALA:HB3	1:G:112:ARG:NH1	2.32	0.45
1:A:174:THR:CG2	1:A:197:LLP:HG2	2.47	0.45
1:B:14:GLY:HA2	1:B:59:GLU:OE2	2.17	0.45
1:D:335:ALA:HA	1:D:347:ARG:NH1	2.31	0.45
1:E:109:LEU:HD12	1:E:112:ARG:HD2	1.99	0.45
1:B:180:LEU:HA	1:B:293:SER:OG	2.17	0.45
1:F:365:ASP:OD1	1:G:5:ARG:HD3	2.17	0.45
1:G:100:TYR:O	1:G:104:ASP:HB2	2.16	0.45
1:H:281:GLU:HG3	6:H:661:HOH:O	2.16	0.45
1:B:108:ASP:O	1:B:111:ALA:HB3	2.17	0.45
1:B:343:SER:O	1:B:346:ALA:HB3	2.16	0.44
1:A:96:THR:OG1	1:A:99:VAL:HG23	2.17	0.44
1:C:332:GLU:HB2	1:C:337:MSE:SE	2.68	0.44
1:F:100:TYR:OH	2:F:401:MES:H62	2.17	0.44
1:H:9:ARG:HH11	1:H:66:ARG:CD	2.30	0.44
1:H:9:ARG:CB	1:H:9:ARG:HH21	2.31	0.44
1:B:29:HIS:CD2	1:B:52:PRO:HB2	2.52	0.44
1:C:156:ALA:HA	1:C:186:LEU:O	2.17	0.44
1:D:122:LEU:HA	1:D:122:LEU:HD23	1.67	0.44
1:G:300:SER:HB2	1:G:356:LEU:HD11	1.98	0.44
2:G:401:MES:H52	1:H:46:TYR:CE2	2.52	0.44
1:C:236:ASP:CG	6:C:671:HOH:O	2.56	0.44
1:D:251:VAL:O	1:D:255:VAL:HG23	2.17	0.44
1:E:161:ARG:HA	1:E:161:ARG:HD3	1.56	0.44
1:G:92:CYS:SG	1:G:134:GLU:HG2	2.57	0.44
1:G:322:VAL:HB	2:G:401:MES:H72	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ARG:HD2	6:A:535:HOH:O	2.16	0.44
1:C:9:ARG:NH2	1:C:66:ARG:HD2	2.32	0.44
1:H:84:LEU:HD12	1:H:106:LEU:HB3	1.98	0.44
1:B:149:LEU:HD11	1:B:350:ARG:C	2.37	0.44
1:G:147:ASN:ND2	1:G:358:ARG:HH11	2.11	0.44
1:H:245:HIS:HE1	6:H:536:HOH:O	1.99	0.44
1:A:59:GLU:HG3	6:A:663:HOH:O	2.16	0.44
1:B:147:ASN:N	6:B:685:HOH:O	1.97	0.44
1:B:147:ASN:HA	1:B:148:PRO:HA	1.75	0.44
1:C:276:TYR:OH	1:C:295:PRO:HG2	2.16	0.44
1:D:38:ALA:HB2	6:D:634:HOH:O	2.17	0.44
1:G:347:ARG:NH1	1:G:354:GLU:OE2	2.50	0.44
1:A:16:ARG:NH1	1:A:59:GLU:OE1	2.50	0.44
1:E:84:LEU:HD11	1:E:107:PHE:CD1	2.49	0.44
1:F:282:HIS:CG	1:F:283:PRO:HD2	2.52	0.44
1:G:173:ASN:HB3	1:G:193:TYR:CE1	2.52	0.44
1:H:137:LEU:HG	1:H:167:ALA:HB2	2.00	0.44
1:C:4:MSE:O	1:C:9:ARG:NE	2.51	0.44
1:D:6:PHE:HA	6:D:613:HOH:O	2.17	0.44
1:E:187:GLY:HA3	6:E:542:HOH:O	2.17	0.44
1:F:150:LEU:HD22	1:F:175:PHE:CZ	2.44	0.44
1:H:4:MSE:HB3	1:H:9:ARG:HD2	1.98	0.44
1:G:148:PRO:HD3	1:G:339:HIS:CE1	2.52	0.44
1:H:245:HIS:HE1	6:H:537:HOH:O	1.99	0.44
1:A:339:HIS:HE1	6:A:552:HOH:O	1.99	0.44
1:B:29:HIS:CD2	3:B:404:GOL:HO3	2.35	0.44
1:E:277:PRO:HA	1:E:282:HIS:CD2	2.51	0.44
1:F:43:ARG:HG2	6:F:624:HOH:O	2.17	0.44
1:H:16:ARG:HD3	1:H:17:PRO:CD	2.47	0.44
1:H:168:ARG:HH12	3:H:404:GOL:H32	1.83	0.44
1:A:337:MSE:HB2	1:A:337:MSE:HE2	1.69	0.44
1:B:344:ALA:HB2	1:B:347:ARG:HH21	1.81	0.44
1:E:150:LEU:HD22	1:E:175:PHE:HZ	1.82	0.44
1:B:245:HIS:HB3	1:C:327:VAL:HG11	1.99	0.44
1:D:109:LEU:O	1:D:113:GLN:HG2	2.17	0.44
1:E:150:LEU:HD22	1:E:175:PHE:CE2	2.52	0.44
1:G:285:HIS:CG	1:G:286:ALA:N	2.86	0.44
1:A:160:ARG:NH2	6:A:635:HOH:O	2.51	0.44
3:B:407:GOL:O1	3:B:407:GOL:O3	2.29	0.44
1:C:352:ILE:HG23	1:C:356:LEU:HD23	1.99	0.44
1:E:347:ARG:CB	1:E:352:ILE:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:ARG:HH21	1:F:213:ARG:HB2	1.82	0.44
1:F:342:LEU:HD11	6:F:670:HOH:O	2.17	0.44
1:C:150:LEU:HD23	1:C:150:LEU:N	2.33	0.44
1:D:338:THR:HG1	1:D:339:HIS:N	2.15	0.44
1:F:118:ARG:HG2	6:F:662:HOH:O	2.16	0.44
1:H:100:TYR:OH	2:H:401:MES:H62	2.17	0.44
1:B:250:ARG:O	1:B:254:GLN:HG3	2.17	0.44
1:B:276:TYR:OH	1:B:295:PRO:HB2	2.17	0.44
1:G:149:LEU:HD11	1:G:351:GLY:HA3	2.00	0.44
1:F:364:GLU:HG2	1:G:8:THR:HG23	1.99	0.44
1:F:42:PRO:HB3	1:F:45:PHE:CZ	2.53	0.44
1:A:307:PRO:HB3	1:A:309:GLU:OE2	2.17	0.44
1:A:94:VAL:HG11	1:A:131:ALA:HB1	1.99	0.44
1:B:16:ARG:HA	1:B:17:PRO:HD2	1.71	0.44
1:D:108:ASP:O	1:D:112:ARG:N	2.50	0.44
1:D:157:GLU:O	1:D:161:ARG:HG2	2.17	0.44
1:D:5:ARG:O	1:D:7:GLY:N	2.50	0.44
1:F:182:GLN:OE1	6:F:602:HOH:O	2.21	0.44
1:F:337:MSE:HB2	1:F:338:THR:H	1.58	0.44
1:B:109:LEU:HA	1:B:109:LEU:HD12	1.69	0.44
1:B:110:ALA:O	1:B:115:VAL:HB	2.18	0.44
1:B:118:ARG:O	1:B:118:ARG:HG3	2.16	0.44
1:B:320:CYS:HA	1:B:331:VAL:O	2.16	0.44
1:B:343:SER:C	1:B:345:GLU:N	2.65	0.44
1:F:338:THR:HG22	2:F:401:MES:H32	1.99	0.44
1:H:34:TYR:CE1	1:H:44:TYR:HB3	2.52	0.44
1:A:17:PRO:HA	6:A:652:HOH:O	2.17	0.44
1:A:199:ILE:HG23	1:A:244:LEU:HD11	1.99	0.44
1:D:292:MSE:SE	1:D:294:ALA:O	2.86	0.44
1:E:126:GLU:HG2	1:E:126:GLU:H	1.51	0.44
1:E:96:THR:O	1:E:98:ASP:N	2.50	0.44
1:F:321:GLY:HA2	1:F:337:MSE:HE1	1.98	0.44
1:B:132:LEU:HD13	1:B:161:ARG:HB3	1.99	0.44
1:C:257:THR:HG21	1:C:369:LEU:HD12	2.00	0.44
1:D:6:PHE:O	1:D:10:LEU:HG	2.18	0.44
1:H:276:TYR:CZ	1:H:295:PRO:HB2	2.52	0.44
1:A:131:ALA:O	1:A:133:ALA:N	2.51	0.44
6:E:619:HOH:O	1:H:3:GLY:HA3	2.17	0.44
1:C:339:HIS:CG	1:C:342:LEU:HD23	2.52	0.44
1:E:175:PHE:CZ	1:E:298:ILE:HB	2.52	0.44
1:G:284:GLN:HB3	1:G:287:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ALA:CB	1:C:131:ALA:HB2	2.46	0.44
1:F:16:ARG:HA	1:F:17:PRO:HD2	1.79	0.44
1:F:311:LEU:HG	1:F:315:PHE:HE2	1.83	0.44
1:F:375:ARG:O	1:F:379:GLY:HA2	2.17	0.44
1:F:54:ARG:HG3	1:F:72:VAL:CG2	2.46	0.44
1:H:100:TYR:CE1	2:H:401:MES:H82	2.53	0.44
1:D:324:LEU:HD22	2:D:401:MES:O2S	2.18	0.44
1:C:107:PHE:HB3	1:C:117:VAL:HG11	1.99	0.44
1:C:149:LEU:HD23	1:C:149:LEU:HA	1.84	0.44
1:C:347:ARG:CB	1:C:352:ILE:HB	2.48	0.44
1:E:244:LEU:HD23	1:E:244:LEU:HA	1.59	0.44
2:H:401:MES:H82	2:H:401:MES:H31	1.78	0.44
1:D:197:LLP:HG3	1:D:197:LLP:H	1.57	0.44
1:E:62:ALA:HB1	1:E:67:ALA:O	2.17	0.44
1:F:145:PRO:HD3	1:F:292:MSE:CE	2.48	0.44
1:F:44:TYR:OH	1:F:55:GLU:OE1	2.18	0.44
1:H:41:GLU:O	1:H:43:ARG:HG3	2.17	0.44
1:B:14:GLY:HA2	1:B:59:GLU:OE2	2.18	0.44
1:E:160:ARG:HB2	1:E:160:ARG:CZ	2.48	0.44
1:G:213:ARG:HH21	3:G:402:GOL:C2	2.30	0.44
1:B:134:GLU:HB2	1:B:137:LEU:HB2	1.98	0.44
3:B:402:GOL:H12	1:C:248:SER:OG	2.17	0.44
1:D:106:LEU:O	1:D:110:ALA:N	2.46	0.44
1:D:175:PHE:CD1	1:D:175:PHE:C	2.90	0.44
1:E:278:GLY:HA2	1:E:285:HIS:HE1	1.83	0.44
1:H:26:PRO:HB2	6:H:666:HOH:O	2.16	0.44
1:B:346:ALA:HA	1:B:349:ARG:HB2	1.98	0.44
1:D:288:VAL:HA	1:D:292:MSE:HE3	1.99	0.44
1:A:282:HIS:CG	1:A:283:PRO:HD2	2.53	0.44
1:B:343:SER:OG	1:B:345:GLU:HB2	2.17	0.44
1:C:39:GLN:HB3	6:C:673:HOH:O	2.17	0.44
1:D:145:PRO:HD3	1:D:292:MSE:HE1	1.99	0.44
1:D:163:HIS:HE1	1:D:187:GLY:O	2.00	0.44
1:D:39:GLN:OE1	1:D:43:ARG:HB2	2.17	0.44
1:E:254:GLN:HG2	1:E:361:VAL:O	2.17	0.44
1:A:173:ASN:HB3	1:A:193:TYR:CE1	2.52	0.44
1:B:180:LEU:HD22	1:B:294:ALA:HB3	1.98	0.44
1:C:289:LYS:HG2	6:C:663:HOH:O	2.17	0.44
1:D:144:THR:OG1	1:D:152:VAL:HG23	2.16	0.44
1:F:335:ALA:HA	1:F:347:ARG:CD	2.47	0.44
1:F:374:SER:O	6:F:545:HOH:O	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:PRO:HA	6:H:658:HOH:O	2.16	0.44
1:D:339:HIS:CD2	1:D:342:LEU:HD12	2.52	0.44
1:D:96:THR:O	1:D:99:VAL:HB	2.18	0.44
1:E:33:THR:HG23	1:F:203:ALA:HB1	1.99	0.44
1:C:148:PRO:HD3	1:C:339:HIS:CE1	2.53	0.44
1:C:107:PHE:CG	1:C:117:VAL:HG11	2.53	0.44
1:D:314:ARG:CD	1:D:379:GLY:HA3	2.45	0.44
1:H:88:ARG:O	1:H:91:GLN:HB2	2.18	0.44
1:B:100:TYR:HA	6:B:669:HOH:O	2.17	0.44
1:E:11:VAL:HA	1:E:245:HIS:ND1	2.33	0.44
1:C:163:HIS:NE2	1:C:189:ASP:OD2	2.44	0.44
1:C:4:MSE:HB2	1:C:4:MSE:HE2	1.77	0.44
1:C:95:SER:HB2	1:C:141:TRP:HB3	1.99	0.44
1:C:5:ARG:O	1:C:9:ARG:HG3	2.17	0.44
1:F:125:PRO:HB3	6:F:663:HOH:O	2.16	0.44
1:G:367:GLN:O	1:G:371:GLU:HG2	2.18	0.44
1:F:39:GLN:NE2	1:H:21:THR:O	2.51	0.44
1:B:340:ARG:N	1:B:341:PRO:CD	2.81	0.44
1:D:180:LEU:HD22	1:D:294:ALA:HB3	1.98	0.44
1:G:96:THR:HG23	6:G:663:HOH:O	2.18	0.44
1:A:263:GLU:OE1	6:A:501:HOH:O	2.21	0.44
1:A:168:ARG:NH2	3:A:402:GOL:O3	2.48	0.44
1:B:156:ALA:O	1:B:160:ARG:HG3	2.17	0.44
1:B:4:MSE:O	1:B:9:ARG:NE	2.50	0.44
1:C:18:SER:N	6:C:619:HOH:O	2.41	0.44
1:D:11:VAL:HA	1:D:245:HIS:ND1	2.33	0.44
1:F:96:THR:C	1:F:98:ASP:N	2.70	0.44
1:D:16:ARG:O	6:D:657:HOH:O	2.21	0.44
1:D:121:ASP:N	6:D:671:HOH:O	2.50	0.44
1:D:40:ASP:CB	6:D:656:HOH:O	2.66	0.44
1:F:96:THR:O	1:F:99:VAL:HG13	2.16	0.44
1:F:96:THR:O	1:F:98:ASP:N	2.50	0.44
1:D:163:HIS:HE1	1:D:187:GLY:O	2.00	0.44
1:E:124:THR:HG1	1:E:127:GLY:H	1.56	0.44
1:G:317:LEU:HD11	1:G:364:GLU:HG2	2.00	0.44
1:G:96:THR:HB	1:G:98:ASP:OD1	2.18	0.44
1:H:365:ASP:HB3	1:H:368:ASP:OD2	2.18	0.44
1:A:252:HIS:CE1	6:A:675:HOH:O	2.70	0.44
1:A:367:GLN:NE2	6:A:584:HOH:O	2.47	0.44
1:F:163:HIS:HE1	1:F:187:GLY:O	2.01	0.44
1:F:175:PHE:HD1	1:F:175:PHE:C	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:H	1:A:36:ARG:HG2	1.55	0.44
1:B:294:ALA:HB1	1:B:295:PRO:HD2	2.00	0.44
1:E:343:SER:HB3	1:E:344:ALA:H	1.66	0.44
1:F:175:PHE:CD1	1:F:175:PHE:C	2.91	0.44
1:F:285:HIS:CD2	1:F:285:HIS:O	2.71	0.44
1:G:152:VAL:HG21	1:G:288:VAL:HG22	2.00	0.44
1:G:4:MSE:HG2	1:G:8:THR:CG2	2.48	0.44
1:H:36:ARG:O	1:H:39:GLN:HB2	2.17	0.44
1:B:104:ASP:OD1	1:B:119:TYR:OH	2.26	0.44
1:E:68:PRO:HG2	1:E:213:ARG:HA	2.00	0.44
1:E:112:ARG:HB3	1:F:88:ARG:HH12	1.83	0.44
1:H:277:PRO:HA	1:H:282:HIS:CD2	2.53	0.44
1:H:333:CYS:O	1:H:336:LEU:N	2.33	0.44
1:C:285:HIS:HE1	6:C:652:HOH:O	1.96	0.44
1:F:54:ARG:NH1	6:F:662:HOH:O	2.50	0.44
1:C:143:GLU:HG3	1:C:172:ASP:HB3	2.00	0.44
1:C:148:PRO:HD3	1:C:339:HIS:CE1	2.53	0.44
1:E:84:LEU:HD23	1:E:84:LEU:HA	1.82	0.44
1:E:96:THR:O	1:E:99:VAL:N	2.51	0.44
1:A:39:GLN:HG3	1:A:39:GLN:H	1.55	0.44
1:A:43:ARG:CD	6:A:664:HOH:O	2.66	0.44
1:B:253:ARG:NH2	1:B:257:THR:OG1	2.50	0.44
1:B:84:LEU:HD13	1:B:106:LEU:HB3	2.00	0.44
1:C:375:ARG:NH1	6:C:576:HOH:O	2.34	0.44
1:C:6:PHE:C	1:C:8:THR:H	2.20	0.44
1:E:96:THR:OG1	1:E:97:ASP:N	2.47	0.44
1:A:198:SER:HB3	6:A:580:HOH:O	2.18	0.44
1:E:285:HIS:HD2	1:E:289:LYS:HG3	1.83	0.44
1:E:339:HIS:O	1:E:347:ARG:NH1	2.50	0.44
1:G:100:TYR:HB2	6:G:585:HOH:O	2.17	0.44
1:H:165:ARG:HA	1:H:165:ARG:HD2	1.72	0.44
1:C:253:ARG:NH2	6:C:641:HOH:O	2.34	0.44
1:D:275:HIS:HA	6:D:575:HOH:O	2.18	0.44
1:E:124:THR:CB	1:E:126:GLU:HG2	2.46	0.44
1:B:15:ARG:HA	6:B:623:HOH:O	2.17	0.44
1:B:32:THR:OG1	1:B:33:THR:HG22	2.18	0.44
1:E:14:GLY:HA2	1:E:59:GLU:CD	2.38	0.44
1:F:213:ARG:NH2	6:F:574:HOH:O	2.49	0.44
1:H:52:PRO:HA	1:H:55:GLU:OE2	2.17	0.44
1:C:179:VAL:HG12	1:C:180:LEU:HD23	2.00	0.44
1:C:320:CYS:HA	1:C:331:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:ASP:HB3	1:E:119:TYR:HB3	2.00	0.44
1:F:9:ARG:HB2	6:F:528:HOH:O	2.18	0.44
1:H:137:LEU:H	1:H:165:ARG:NH1	2.15	0.44
1:B:154:ASP:OD2	6:B:538:HOH:O	2.21	0.44
1:F:152:VAL:HG13	6:F:550:HOH:O	2.18	0.44
1:D:4:MSE:O	1:D:9:ARG:NE	2.51	0.44
1:E:309:GLU:H	1:E:309:GLU:CD	2.21	0.44
2:F:401:MES:H22	6:F:658:HOH:O	2.17	0.44
1:G:264:ARG:NE	1:G:370:ALA:HB1	2.32	0.44
1:A:6:PHE:HE2	1:A:179:VAL:HB	1.83	0.44
1:D:189:ASP:OD1	6:D:668:HOH:O	2.20	0.44
1:E:338:THR:OG1	1:E:339:HIS:CD2	2.71	0.44
1:B:175:PHE:CZ	1:B:298:ILE:HB	2.53	0.44
1:B:97:ASP:HB2	1:B:119:TYR:CD2	2.53	0.44
1:D:124:THR:OG1	1:D:126:GLU:OE1	2.36	0.44
1:E:368:ASP:OD2	1:H:5:ARG:N	2.32	0.44
1:A:147:ASN:C	1:A:149:LEU:H	2.20	0.44
1:D:288:VAL:HG13	1:D:292:MSE:HE3	1.99	0.44
1:G:294:ALA:HA	1:G:295:PRO:HD3	1.68	0.44
1:E:337:MSE:SE	6:E:673:HOH:O	2.85	0.44
1:G:33:THR:HG22	1:H:203:ALA:HB1	1.99	0.44
1:C:98:ASP:HA	1:C:350:ARG:HE	1.83	0.44
1:F:352:ILE:HG23	1:F:356:LEU:HD23	1.99	0.44
1:G:149:LEU:HD21	1:G:351:GLY:O	2.18	0.44
1:A:17:PRO:O	1:A:18:SER:C	2.55	0.44
1:A:18:SER:CB	3:A:403:GOL:H31	2.48	0.44
1:B:288:VAL:HG22	1:B:292:MSE:HE3	1.99	0.44
1:E:332:GLU:O	1:E:332:GLU:HG3	2.17	0.44
1:H:178:PRO:HD3	1:H:193:TYR:CE1	2.53	0.44
1:A:29:HIS:HB3	6:A:574:HOH:O	2.18	0.44
1:D:281:GLU:HB2	6:D:683:HOH:O	2.17	0.44
1:F:94:VAL:HG22	1:F:118:ARG:HB3	2.00	0.44
1:G:300:SER:HA	1:G:357:ILE:O	2.18	0.44
1:H:93:VAL:HG22	1:H:139:LEU:HB3	2.00	0.44
1:C:199:ILE:HG23	1:C:244:LEU:CD1	2.45	0.44
1:D:163:HIS:HE1	1:D:187:GLY:O	2.01	0.44
1:G:93:VAL:HB	1:G:117:VAL:HG13	1.99	0.44
1:B:11:VAL:HG13	1:C:327:VAL:HG13	1.99	0.44
1:E:313:ASP:HA	1:F:37:ARG:HH21	1.83	0.44
1:G:214:ASP:OD1	1:G:216:ASP:N	2.51	0.44
1:E:213:ARG:HH11	3:E:402:GOL:H2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:GLN:O	1:E:288:VAL:HG23	2.18	0.44
1:A:195:THR:HA	1:A:199:ILE:HB	1.98	0.44
1:A:277:PRO:O	1:A:288:VAL:HG11	2.17	0.44
1:E:149:LEU:HB2	6:E:656:HOH:O	2.17	0.44
1:E:285:HIS:HB2	6:E:643:HOH:O	2.17	0.44
1:E:345:GLU:OE2	1:E:349:ARG:NH2	2.51	0.44
1:B:322:VAL:O	1:B:322:VAL:HG23	2.17	0.44
1:D:358:ARG:NH2	2:D:401:MES:O1S	2.46	0.44
1:E:315:PHE:CE2	1:E:331:VAL:HG21	2.53	0.44
1:C:277:PRO:HB3	1:C:292:MSE:HE1	1.99	0.44
1:E:108:ASP:HB3	1:E:112:ARG:NH2	2.32	0.44
1:A:16:ARG:CD	1:A:17:PRO:HD2	2.44	0.44
1:D:43:ARG:HB3	1:D:44:TYR:CE2	2.53	0.44
1:E:84:LEU:HA	1:E:84:LEU:HD23	1.77	0.44
1:C:132:LEU:HD23	1:C:132:LEU:HA	1.79	0.44
1:C:159:SER:HA	1:C:169:VAL:HG21	2.00	0.44
1:D:253:ARG:NH1	1:D:366:PRO:HD3	2.33	0.44
1:D:320:CYS:CB	6:D:648:HOH:O	2.63	0.44
1:D:347:ARG:NH2	1:D:354:GLU:OE2	2.43	0.44
1:E:72:VAL:HG23	1:E:232:PRO:HG3	1.99	0.44
1:F:97:ASP:HB2	1:F:119:TYR:HB3	1.99	0.44
1:G:196:THR:HG21	1:H:46:TYR:OH	2.17	0.44
1:G:348:ALA:O	1:G:350:ARG:N	2.51	0.44
1:H:343:SER:O	1:H:347:ARG:HB2	2.18	0.44
1:B:14:GLY:HA2	1:B:59:GLU:CD	2.38	0.44
1:B:305:GLY:O	6:B:501:HOH:O	2.21	0.44
1:C:112:ARG:NE	6:C:576:HOH:O	2.51	0.44
1:D:251:VAL:O	1:D:255:VAL:HG23	2.17	0.44
1:E:125:PRO:HD2	1:E:126:GLU:OE1	2.17	0.44
1:E:291:GLN:HG3	1:E:292:MSE:CG	2.47	0.44
1:G:276:TYR:CZ	1:G:295:PRO:HB2	2.52	0.44
2:H:401:MES:H51	2:H:401:MES:H81	1.48	0.44
1:A:5:ARG:O	1:A:9:ARG:HG3	2.17	0.44
1:E:259:ARG:HH12	1:E:295:PRO:CG	2.31	0.44
1:G:173:ASN:HB3	1:G:193:TYR:CE1	2.53	0.44
1:H:342:LEU:HG	1:H:342:LEU:H	1.53	0.44
1:H:371:GLU:HB2	6:H:615:HOH:O	2.17	0.44
1:A:35:GLU:OE2	1:A:37:ARG:HG2	2.18	0.44
1:B:98:ASP:HB3	1:B:146:THR:HB	2.00	0.44
1:C:183:PRO:HA	1:C:186:LEU:HD12	2.00	0.44
1:F:338:THR:HG23	6:F:646:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:44:TYR:OH	1:F:55:GLU:OE1	2.16	0.44
1:G:150:LEU:HD22	1:G:175:PHE:HE2	1.82	0.44
1:B:14:GLY:O	1:B:56:GLU:HG2	2.18	0.44
1:C:16:ARG:HB3	6:C:658:HOH:O	2.17	0.44
1:D:121:ASP:OD2	1:D:123:THR:HB	2.18	0.44
1:G:93:VAL:HG22	1:G:139:LEU:HB3	2.00	0.44
1:A:88:ARG:NH2	6:A:636:HOH:O	2.51	0.44
1:C:282:HIS:HA	1:C:283:PRO:HD3	1.93	0.44
1:C:248:SER:OG	5:C:404:GOL:H11	2.18	0.44
1:D:132:LEU:HA	1:D:137:LEU:HD22	2.00	0.44
1:D:132:LEU:HD12	1:D:161:ARG:HB2	2.00	0.44
1:E:46:TYR:OH	1:F:196:THR:HG21	2.18	0.44
1:F:34:TYR:CE2	1:F:44:TYR:HB3	2.53	0.44
1:H:184:LEU:HB3	3:H:402:GOL:O2	2.18	0.44
1:A:173:ASN:HB3	1:A:193:TYR:CE1	2.52	0.44
1:E:150:LEU:HD22	1:E:175:PHE:CZ	2.52	0.44
1:F:303:TYR:CZ	1:F:305:GLY:HA3	2.52	0.44
1:G:147:ASN:HA	1:G:148:PRO:HA	1.87	0.44
1:G:36:ARG:HD2	6:G:663:HOH:O	2.18	0.44
1:H:137:LEU:HD12	1:H:137:LEU:HA	1.80	0.44
1:A:6:PHE:HA	1:A:9:ARG:HH12	1.82	0.44
1:B:344:ALA:HB3	1:B:345:GLU:OE2	2.17	0.44
1:E:46:TYR:OH	1:F:196:THR:HG21	2.18	0.44
1:F:214:ASP:HB3	1:F:217:LEU:HB3	1.99	0.44
1:B:4:MSE:H	1:B:66:ARG:NH1	2.16	0.44
1:F:337:MSE:HE2	6:F:597:HOH:O	2.18	0.44
1:F:43:ARG:HD2	1:F:44:TYR:CE2	2.53	0.44
1:H:253:ARG:NH1	6:H:624:HOH:O	2.50	0.44
1:A:322:VAL:HB	2:A:401:MES:H72	1.98	0.44
1:C:36:ARG:HD3	1:D:320:CYS:SG	2.58	0.44
1:F:165:ARG:HB3	1:F:165:ARG:NH2	2.33	0.44
1:B:197:LLP:H4'1	2:B:401:MES:H81	1.99	0.44
1:B:97:ASP:C	1:B:99:VAL:N	2.70	0.44
1:F:23:ASP:OD2	1:H:29:HIS:ND1	2.30	0.44
1:H:118:ARG:NH2	1:H:120:ALA:HB2	2.32	0.44
1:B:118:ARG:CZ	1:B:120:ALA:HB2	2.47	0.44
1:C:103:THR:HG22	1:C:107:PHE:CZ	2.53	0.44
1:C:314:ARG:CZ	1:C:379:GLY:HA3	2.47	0.44
1:H:259:ARG:O	1:H:263:GLU:HG2	2.18	0.44
1:H:95:SER:OG	1:H:96:THR:N	2.50	0.44
1:B:335:ALA:HA	1:B:347:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ARG:H	1:C:16:ARG:HG3	1.39	0.43
1:E:184:LEU:HD11	1:E:211:VAL:HG12	1.99	0.43
1:F:350:ARG:NE	6:F:645:HOH:O	2.31	0.43
1:G:180:LEU:HD22	1:G:294:ALA:HB3	1.99	0.43
1:G:44:TYR:HA	1:G:50:GLU:OE1	2.18	0.43
1:H:104:ASP:HB3	6:H:650:HOH:O	2.16	0.43
1:C:231:VAL:HG12	1:C:232:PRO:HD2	1.98	0.43
1:D:124:THR:C	1:D:126:GLU:N	2.71	0.43
1:H:213:ARG:HH11	3:H:402:GOL:C2	2.27	0.43
1:B:16:ARG:HH11	3:B:405:GOL:H32	1.82	0.43
1:D:339:HIS:CD2	1:D:352:ILE:HD13	2.52	0.43
1:E:264:ARG:NH1	1:E:370:ALA:HB1	2.33	0.43
1:F:254:GLN:HB3	1:F:297:ALA:HB2	1.99	0.43
1:B:95:SER:CB	1:B:141:TRP:HB3	2.48	0.43
1:F:10:LEU:O	1:F:241:ARG:NH1	2.51	0.43
1:A:235:LEU:HG	6:A:695:HOH:O	2.17	0.43
1:B:160:ARG:O	1:B:164:GLU:HG3	2.18	0.43
1:B:33:THR:HG23	1:D:24:VAL:HB	1.99	0.43
1:C:180:LEU:HD22	1:C:294:ALA:HB3	2.00	0.43
1:E:176:ALA:HB1	1:E:180:LEU:HB2	1.99	0.43
1:F:29:HIS:CD2	1:F:52:PRO:HB2	2.52	0.43
1:G:336:LEU:HB2	1:G:337:MSE:CE	2.42	0.43
1:F:34:TYR:CE2	1:H:23:ASP:HA	2.51	0.43
1:C:92:CYS:SG	1:C:134:GLU:HG2	2.58	0.43
1:D:121:ASP:O	1:D:127:GLY:HA3	2.18	0.43
1:D:9:ARG:NH1	1:D:64:LEU:O	2.51	0.43
1:E:51:ASN:O	1:E:55:GLU:HG3	2.18	0.43
1:F:66:ARG:NH1	6:F:628:HOH:O	2.51	0.43
1:B:118:ARG:HD3	1:B:134:GLU:OE1	2.18	0.43
1:B:264:ARG:HB2	1:B:264:ARG:HE	1.17	0.43
1:D:44:TYR:OH	1:D:55:GLU:OE2	2.35	0.43
1:E:39:GLN:NE2	1:E:44:TYR:HB2	2.32	0.43
1:F:266:ARG:HD2	1:F:279:LEU:HD21	1.99	0.43
1:G:192:LEU:HD12	1:G:193:TYR:N	2.33	0.43
1:C:43:ARG:HB2	1:C:44:TYR:CD1	2.53	0.43
1:E:145:PRO:HG2	1:E:175:PHE:CE1	2.53	0.43
1:F:277:PRO:O	1:F:288:VAL:HG11	2.18	0.43
1:F:92:CYS:SG	1:F:93:VAL:N	2.90	0.43
1:C:99:VAL:HA	6:C:654:HOH:O	2.16	0.43
1:F:173:ASN:HB3	1:F:193:TYR:CE1	2.54	0.43
1:A:340:ARG:C	1:A:342:LEU:H	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:PHE:CE1	1:A:64:LEU:HB3	2.52	0.43
1:C:184:LEU:HB3	1:C:213:ARG:NH2	2.33	0.43
1:D:309:GLU:HA	1:D:312:LEU:HD12	2.00	0.43
1:F:303:TYR:CZ	1:F:305:GLY:HA3	2.53	0.43
1:G:292:MSE:HB2	1:G:292:MSE:HE2	1.94	0.43
1:A:94:VAL:HG11	1:A:131:ALA:HB1	1.99	0.43
1:F:323:SER:HA	2:F:401:MES:O3S	2.18	0.43
1:G:332:GLU:HG2	1:G:358:ARG:HB3	2.00	0.43
1:A:145:PRO:HD2	1:A:175:PHE:CG	2.54	0.43
1:A:55:GLU:O	1:A:59:GLU:HG3	2.18	0.43
1:E:96:THR:O	1:E:98:ASP:N	2.51	0.43
1:H:124:THR:CG2	1:H:127:GLY:H	2.31	0.43
1:A:94:VAL:HG22	1:A:118:ARG:HB3	2.00	0.43
1:E:175:PHE:C	1:E:175:PHE:HD1	2.20	0.43
1:F:178:PRO:HD3	1:F:193:TYR:CE1	2.53	0.43
1:F:285:HIS:O	1:F:285:HIS:HD2	2.00	0.43
1:A:322:VAL:HG13	1:A:337:MSE:SE	2.68	0.43
1:D:344:ALA:O	1:D:348:ALA:N	2.42	0.43
1:D:88:ARG:NH2	4:D:405:CL:CL	2.88	0.43
1:D:214:ASP:HB3	1:D:217:LEU:HB3	2.00	0.43
1:F:254:GLN:HB3	1:F:297:ALA:CB	2.47	0.43
1:A:199:ILE:HG23	1:A:244:LEU:CD1	2.48	0.43
1:C:343:SER:OG	1:C:344:ALA:N	2.48	0.43
1:D:68:PRO:HG2	1:D:213:ARG:HA	2.01	0.43
1:B:243:GLY:O	1:B:250:ARG:NH2	2.46	0.43
1:B:368:ASP:OD2	1:C:5:ARG:N	2.48	0.43
1:C:97:ASP:HA	1:C:119:TYR:HB3	1.99	0.43
1:C:132:LEU:HD13	1:C:161:ARG:O	2.17	0.43
1:F:147:ASN:HD21	1:F:358:ARG:HH11	1.66	0.43
1:F:180:LEU:HD13	1:F:294:ALA:O	2.18	0.43
1:H:4:MSE:HB3	1:H:9:ARG:HE	1.83	0.43
1:C:322:VAL:HG13	1:C:337:MSE:SE	2.68	0.43
1:C:43:ARG:NH1	1:C:55:GLU:OE2	2.51	0.43
1:A:332:GLU:HB2	1:A:337:MSE:HE1	2.00	0.43
1:A:347:ARG:O	1:A:352:ILE:N	2.47	0.43
1:A:36:ARG:HD3	1:A:36:ARG:HA	1.70	0.43
1:E:168:ARG:NE	4:E:406:CL:CL	2.88	0.43
1:G:337:MSE:O	6:G:662:HOH:O	2.21	0.43
1:G:149:LEU:HD11	1:G:351:GLY:HA3	2.00	0.43
1:H:192:LEU:HD12	1:H:210:LEU:HD21	2.00	0.43
6:G:697:HOH:O	1:H:337:MSE:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:PRO:HG3	6:B:649:HOH:O	2.18	0.43
1:C:4:MSE:HE3	6:C:596:HOH:O	2.17	0.43
1:F:345:GLU:CB	6:F:653:HOH:O	2.66	0.43
1:G:109:LEU:O	1:G:113:GLN:HG2	2.18	0.43
1:G:334:PRO:HA	1:G:338:THR:OG1	2.16	0.43
1:G:62:ALA:HB1	1:G:67:ALA:O	2.18	0.43
1:H:149:LEU:HA	1:H:149:LEU:HD23	1.81	0.43
1:A:334:PRO:HD2	1:A:356:LEU:O	2.18	0.43
1:B:281:GLU:N	6:B:638:HOH:O	2.51	0.43
1:B:5:ARG:HB3	1:C:368:ASP:OD2	2.17	0.43
1:D:291:GLN:O	1:D:292:MSE:HB3	2.18	0.43
1:F:152:VAL:HG21	1:F:288:VAL:HG22	2.00	0.43
1:F:333:CYS:HB3	1:F:336:LEU:HB2	2.00	0.43
1:G:319:THR:HB	1:G:330:LEU:HD23	2.00	0.43
1:G:97:ASP:N	1:G:97:ASP:OD1	2.51	0.43
1:B:254:GLN:HB3	1:B:297:ALA:CB	2.49	0.43
1:D:145:PRO:HD2	1:D:175:PHE:CD1	2.53	0.43
1:H:287:VAL:O	1:H:292:MSE:SE	2.86	0.43
1:H:84:LEU:HD23	1:H:84:LEU:HA	1.88	0.43
1:H:121:ASP:O	1:H:127:GLY:HA3	2.18	0.43
1:A:168:ARG:NH2	3:A:402:GOL:H31	2.33	0.43
1:E:126:GLU:HA	1:E:129:ALA:HB3	1.99	0.43
1:G:256:ALA:O	1:G:260:VAL:HG23	2.19	0.43
1:G:277:PRO:HA	1:G:282:HIS:CD2	2.53	0.43
1:H:36:ARG:CZ	6:H:677:HOH:O	2.66	0.43
1:A:144:THR:HA	1:A:145:PRO:C	2.39	0.43
1:C:303:TYR:O	1:C:355:SER:OG	2.36	0.43
1:E:102:GLY:HA2	3:E:405:GOL:O3	2.17	0.43
1:F:33:THR:HG22	1:F:34:TYR:N	2.32	0.43
1:G:235:LEU:O	1:G:238:PHE:HB3	2.18	0.43
1:G:96:THR:C	1:G:98:ASP:H	2.20	0.43
1:G:173:ASN:HB3	1:G:193:TYR:CE1	2.52	0.43
1:G:36:ARG:HD2	1:G:45:PHE:CD1	2.52	0.43
1:A:266:ARG:HB3	1:A:266:ARG:HH11	1.82	0.43
1:B:180:LEU:CD2	1:B:294:ALA:HB3	2.44	0.43
1:B:334:PRO:HA	1:B:338:THR:OG1	2.17	0.43
1:E:112:ARG:HB3	1:F:88:ARG:NH1	2.32	0.43
1:G:109:LEU:HD12	6:G:1471:HOH:O	2.19	0.43
1:G:92:CYS:N	1:G:136:ASP:O	2.37	0.43
1:G:51:ASN:HA	1:G:52:PRO:HD3	1.92	0.43
1:A:43:ARG:CB	1:A:43:ARG:HH11	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:THR:O	1:G:150:LEU:HA	2.19	0.43
1:C:147:ASN:HD22	1:C:175:PHE:HE2	1.63	0.43
1:C:310:ARG:O	1:C:314:ARG:HG3	2.17	0.43
1:G:100:TYR:CE2	1:G:102:GLY:N	2.86	0.43
1:C:101:ALA:HA	1:C:104:ASP:HB2	2.00	0.43
1:F:174:THR:HB	1:F:197:LLP:H2'2	1.99	0.43
1:G:112:ARG:HD2	6:G:666:HOH:O	2.18	0.43
1:G:29:HIS:CD2	1:G:52:PRO:HB2	2.54	0.43
1:D:180:LEU:O	1:D:292:MSE:HB2	2.19	0.43
1:F:6:PHE:N	6:F:678:HOH:O	2.44	0.43
1:B:284:GLN:O	1:B:288:VAL:HG23	2.17	0.43
1:D:97:ASP:CA	1:D:119:TYR:HB3	2.47	0.43
1:F:23:ASP:OD2	1:H:29:HIS:ND1	2.41	0.43
1:F:36:ARG:O	1:F:37:ARG:HG2	2.16	0.43
1:B:16:ARG:NH1	1:B:52:PRO:HB3	2.33	0.43
1:B:264:ARG:HD3	1:B:264:ARG:HA	1.88	0.43
1:B:338:THR:HB	1:B:339:HIS:ND1	2.34	0.43
1:G:16:ARG:HA	1:G:17:PRO:HD3	1.77	0.43
1:A:9:ARG:HH22	1:A:66:ARG:NH2	2.16	0.43
1:C:334:PRO:HD2	1:C:356:LEU:O	2.18	0.43
1:E:18:SER:O	1:E:19:ALA:O	2.36	0.43
1:E:198:SER:HA	1:E:325:GLY:O	2.18	0.43
1:F:160:ARG:NH1	6:F:560:HOH:O	2.48	0.43
1:G:367:GLN:O	1:G:371:GLU:HG3	2.19	0.43
1:C:222:ARG:HD2	6:C:594:HOH:O	2.18	0.43
1:G:178:PRO:HD3	1:G:193:TYR:CE1	2.54	0.43
1:G:319:THR:HB	1:G:330:LEU:HD23	1.99	0.43
1:B:12:HIS:O	1:B:15:ARG:HB2	2.18	0.43
1:G:345:GLU:O	1:G:349:ARG:N	2.27	0.43
1:G:41:GLU:HA	1:G:42:PRO:HD2	1.74	0.43
1:F:109:LEU:O	1:F:113:GLN:HG2	2.18	0.43
1:B:6:PHE:CA	1:B:9:ARG:HE	2.10	0.43
1:D:338:THR:HG22	1:D:339:HIS:CE1	2.53	0.43
1:D:339:HIS:ND1	1:D:339:HIS:N	2.66	0.43
1:F:276:TYR:CD1	1:F:299:VAL:HG22	2.54	0.43
1:F:372:ASP:OD1	1:F:375:ARG:NH1	2.47	0.43
1:H:41:GLU:HA	1:H:42:PRO:HD3	1.67	0.43
1:A:91:GLN:HB3	1:A:138:ALA:HB2	2.01	0.43
1:D:248:SER:O	1:D:252:HIS:CD2	2.68	0.43
1:F:152:VAL:HG21	1:F:288:VAL:HG22	2.00	0.43
1:C:9:ARG:HB3	6:C:530:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:PRO:O	1:D:288:VAL:HG11	2.18	0.43
1:G:259:ARG:HH21	1:G:295:PRO:CD	2.31	0.43
1:A:319:THR:HG23	1:B:35:GLU:OE1	2.18	0.43
1:D:349:ARG:C	1:D:351:GLY:H	2.21	0.43
1:E:336:LEU:O	1:E:338:THR:N	2.47	0.43
1:E:338:THR:C	1:E:340:ARG:H	2.20	0.43
1:G:299:VAL:O	1:G:359:LEU:N	2.36	0.43
1:G:301:PHE:N	1:G:357:ILE:O	2.48	0.43
1:A:178:PRO:HD3	1:A:193:TYR:CE1	2.53	0.43
1:B:108:ASP:O	1:B:112:ARG:HG2	2.18	0.43
1:A:65:GLU:O	6:A:558:HOH:O	2.21	0.43
1:A:92:CYS:SG	1:A:93:VAL:N	2.92	0.43
1:B:84:LEU:HD23	1:B:106:LEU:HB3	2.00	0.43
1:C:313:ASP:HA	1:D:37:ARG:CD	2.48	0.43
1:F:310:ARG:HG2	1:F:314:ARG:HH12	1.83	0.43
1:F:41:GLU:HA	1:F:42:PRO:HD2	1.63	0.43
1:A:157:GLU:OE2	1:A:161:ARG:NE	2.51	0.43
1:A:276:TYR:HB3	1:A:279:LEU:HG	2.00	0.43
1:E:17:PRO:HA	6:E:567:HOH:O	2.19	0.43
1:G:173:ASN:HB3	1:G:193:TYR:CE1	2.52	0.43
1:B:7:GLY:HA3	6:C:661:HOH:O	2.17	0.43
1:B:88:ARG:NH1	1:E:136:ASP:OD2	2.52	0.43
1:D:322:VAL:O	2:D:401:MES:H82	2.18	0.43
1:F:134:GLU:HA	1:F:135:PRO:HD3	1.89	0.43
1:F:365:ASP:H	1:G:8:THR:CG2	2.31	0.43
1:H:181:GLN:HG3	1:H:291:GLN:O	2.18	0.43
1:E:84:LEU:HA	1:E:84:LEU:HD23	1.90	0.43
1:A:84:LEU:HD13	1:A:110:ALA:HB2	1.99	0.43
1:A:54:ARG:HG3	1:A:237:CYS:SG	2.58	0.43
1:B:335:ALA:O	1:B:340:ARG:HB3	2.18	0.43
1:B:338:THR:CG2	2:B:401:MES:H71	2.48	0.43
1:C:84:LEU:HD21	1:C:107:PHE:HD1	1.84	0.43
1:E:292:MSE:SE	1:E:295:PRO:HA	2.68	0.43
1:E:242:ARG:HH11	1:H:242:ARG:HD3	1.83	0.43
1:F:365:ASP:OD1	6:F:632:HOH:O	2.21	0.43
1:B:66:ARG:HG2	1:B:66:ARG:NH2	2.29	0.43
1:F:197:LLP:HB2	1:F:324:LEU:HD12	2.01	0.43
1:H:340:ARG:N	1:H:341:PRO:HD2	2.33	0.43
1:D:286:ALA:HB3	6:D:609:HOH:O	2.18	0.43
1:F:147:ASN:HD21	1:F:358:ARG:HD3	1.84	0.43
1:C:142:ILE:O	1:C:171:VAL:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LLP:HD3	1:D:324:LEU:CD2	2.44	0.43
1:D:248:SER:O	1:D:252:HIS:ND1	2.51	0.43
1:H:188:ALA:O	1:H:213:ARG:NH1	2.51	0.43
1:E:21:THR:HG22	1:G:44:TYR:CE2	2.53	0.43
1:A:292:MSE:HE2	1:A:295:PRO:HA	2.00	0.43
1:C:73:PHE:HA	1:C:232:PRO:HD3	2.01	0.43
1:D:335:ALA:N	6:D:562:HOH:O	2.24	0.43
1:A:116:ARG:NE	1:E:112:ARG:HA	2.33	0.43
1:G:282:HIS:CE1	1:G:284:GLN:HG2	2.52	0.43
1:H:147:ASN:ND2	2:H:401:MES:O1S	2.52	0.43
1:B:347:ARG:HB2	1:B:352:ILE:HB	1.99	0.43
1:F:254:GLN:HG2	1:F:361:VAL:O	2.19	0.43
1:F:96:THR:C	1:F:98:ASP:H	2.20	0.43
1:G:342:LEU:HG	1:G:342:LEU:H	1.54	0.43
1:G:39:GLN:HB2	6:G:582:HOH:O	2.18	0.43
1:H:116:ARG:HH21	1:H:134:GLU:HG3	1.84	0.43
1:H:161:ARG:HA	1:H:161:ARG:HD3	1.63	0.43
1:A:336:LEU:C	1:A:337:MSE:SE	3.07	0.43
1:B:36:ARG:HB2	1:B:36:ARG:NH2	2.34	0.43
1:B:5:ARG:NH1	1:C:368:ASP:OD1	2.49	0.43
1:C:95:SER:OG	1:C:96:THR:N	2.52	0.43
1:B:36:ARG:NH1	4:B:409:CL:CL	2.88	0.43
1:D:61:LEU:HD21	1:D:244:LEU:HD11	2.00	0.43
1:C:37:ARG:HD3	1:D:313:ASP:HA	2.00	0.43
1:E:148:PRO:HD3	1:E:339:HIS:CE1	2.53	0.43
1:F:321:GLY:C	1:F:337:MSE:HE1	2.38	0.43
1:H:285:HIS:CD2	1:H:286:ALA:N	2.87	0.43
1:A:159:SER:HA	1:A:169:VAL:HG21	2.01	0.43
1:F:331:VAL:HG23	1:F:359:LEU:HD23	1.99	0.43
1:H:173:ASN:HB3	1:H:193:TYR:CE1	2.54	0.43
1:A:112:ARG:O	1:B:88:ARG:NH1	2.48	0.43
1:B:176:ALA:HB2	1:B:292:MSE:HE3	2.01	0.43
1:C:156:ALA:HA	1:C:186:LEU:O	2.19	0.43
1:A:112:ARG:NE	1:E:135:PRO:HG2	2.32	0.43
1:E:213:ARG:NH1	3:E:402:GOL:H2	2.33	0.43
1:F:96:THR:CG2	6:F:659:HOH:O	2.64	0.43
1:G:49:GLY:C	1:G:54:ARG:HH22	2.22	0.43
1:C:147:ASN:ND2	1:C:175:PHE:CE2	2.80	0.43
1:A:27:PRO:HB2	1:C:27:PRO:HB2	2.01	0.43
1:D:268:SER:HA	1:D:269:PRO:HD3	1.93	0.43
1:E:236:ASP:OD2	1:F:233:GLY:HA3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:VAL:HG22	1:F:232:PRO:HD2	2.00	0.43
1:B:350:ARG:HD3	6:B:602:HOH:O	2.18	0.43
1:C:124:THR:O	1:C:128:ILE:HG13	2.19	0.43
1:C:222:ARG:HD3	1:C:222:ARG:HA	1.84	0.43
1:E:332:GLU:CG	1:E:358:ARG:HB3	2.49	0.43
1:H:96:THR:O	1:H:99:VAL:HG13	2.18	0.43
1:B:292:MSE:HE1	1:B:295:PRO:HA	1.99	0.43
1:C:147:ASN:CG	1:C:148:PRO:HA	2.39	0.43
1:D:332:GLU:CD	1:D:338:THR:OG1	2.57	0.43
1:E:339:HIS:HD2	1:E:342:LEU:HD12	1.83	0.43
1:E:346:ALA:O	1:E:349:ARG:HB2	2.19	0.43
1:D:175:PHE:HB3	6:D:521:HOH:O	2.18	0.43
1:D:224:TYR:HA	1:D:227:THR:HG22	2.00	0.43
1:F:161:ARG:O	6:F:593:HOH:O	2.21	0.43
1:G:51:ASN:HA	1:G:52:PRO:HD3	1.93	0.43
1:B:341:PRO:HB2	6:B:664:HOH:O	2.18	0.43
1:C:9:ARG:NH1	1:C:66:ARG:HH11	2.17	0.43
2:E:401:MES:H51	2:E:401:MES:H81	1.89	0.43
1:H:287:VAL:HG23	6:H:533:HOH:O	2.18	0.43
1:A:109:LEU:HD13	1:B:227:THR:HG21	2.01	0.43
1:C:43:ARG:HA	1:C:45:PHE:CE2	2.54	0.43
1:C:98:ASP:HB3	1:C:146:THR:HB	2.01	0.43
1:E:276:TYR:HA	1:E:277:PRO:HD3	1.89	0.43
1:E:303:TYR:OH	1:E:310:ARG:HD2	2.19	0.43
1:F:346:ALA:HB2	6:F:669:HOH:O	2.18	0.43
1:G:36:ARG:HH21	1:H:322:VAL:HG22	1.82	0.43
1:B:16:ARG:HA	6:B:652:HOH:O	2.18	0.43
1:B:343:SER:OG	1:B:346:ALA:N	2.50	0.43
1:E:320:CYS:SG	1:E:337:MSE:HE3	2.59	0.43
1:C:197:LLP:HD3	1:C:324:LEU:HG	2.00	0.43
1:C:303:TYR:CZ	1:C:305:GLY:HA3	2.53	0.43
1:A:100:TYR:CE2	1:A:102:GLY:HA3	2.54	0.43
1:B:195:THR:HA	1:B:199:ILE:HB	1.99	0.43
1:F:175:PHE:CD1	1:F:175:PHE:C	2.92	0.43
1:F:29:HIS:CD2	1:F:52:PRO:HB2	2.53	0.43
1:H:126:GLU:HG2	1:H:127:GLY:N	2.34	0.43
1:A:33:THR:OG1	1:C:24:VAL:HB	2.19	0.43
1:C:175:PHE:HB2	6:C:552:HOH:O	2.18	0.43
1:C:375:ARG:HD2	6:C:651:HOH:O	2.18	0.43
1:H:346:ALA:O	1:H:350:ARG:HG3	2.19	0.43
1:B:107:PHE:CD2	1:B:117:VAL:HG11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:GLY:HA2	1:C:337:MSE:HE3	2.00	0.43
1:E:332:GLU:HG2	1:E:358:ARG:HB3	1.99	0.43
1:G:143:GLU:HG3	1:G:172:ASP:HB3	2.01	0.43
1:B:173:ASN:HB3	1:B:193:TYR:CE1	2.54	0.43
1:D:132:LEU:CD1	1:D:161:ARG:HB2	2.48	0.43
1:D:165:ARG:HB3	1:D:165:ARG:CZ	2.48	0.43
1:E:8:THR:HG23	1:H:364:GLU:HB3	2.00	0.43
1:F:332:GLU:OE2	1:F:338:THR:HB	2.18	0.43
1:A:36:ARG:H	1:A:36:ARG:HG2	1.24	0.43
1:B:202:HIS:HB3	6:B:542:HOH:O	2.19	0.43
1:C:178:PRO:HD3	1:C:193:TYR:CE1	2.53	0.43
1:B:10:LEU:O	1:B:241:ARG:NH2	2.47	0.43
1:C:303:TYR:HE2	6:C:668:HOH:O	2.02	0.43
1:C:334:PRO:HB3	1:C:339:HIS:CE1	2.54	0.43
1:D:5:ARG:O	1:D:9:ARG:HG3	2.19	0.43
1:F:214:ASP:OD2	1:F:215:ALA:N	2.52	0.43
1:A:273:ALA:HB1	1:A:275:HIS:CE1	2.54	0.43
1:A:6:PHE:HA	1:A:9:ARG:NE	2.34	0.43
1:E:112:ARG:HB3	1:F:88:ARG:NH1	2.33	0.43
1:H:162:ALA:HB1	1:H:167:ALA:HB3	2.01	0.43
1:H:16:ARG:HA	1:H:16:ARG:HD3	1.29	0.43
1:H:264:ARG:CD	1:H:370:ALA:HB1	2.45	0.43
1:H:6:PHE:O	1:H:9:ARG:HB2	2.18	0.43
1:E:9:ARG:HD3	1:E:63:GLY:O	2.19	0.43
1:F:337:MSE:O	1:F:338:THR:C	2.57	0.43
1:H:109:LEU:O	1:H:112:ARG:HB2	2.19	0.43
1:E:199:ILE:HG23	1:E:244:LEU:HD21	2.01	0.43
1:A:97:ASP:HB3	1:A:119:TYR:CG	2.53	0.43
1:F:282:HIS:O	1:F:285:HIS:HB2	2.19	0.43
1:F:350:ARG:HH21	1:F:350:ARG:HD3	1.70	0.43
1:B:161:ARG:NH2	6:B:683:HOH:O	2.06	0.43
1:B:277:PRO:O	1:B:288:VAL:HG21	2.18	0.43
1:B:254:GLN:HB3	1:B:297:ALA:CB	2.49	0.43
1:B:334:PRO:HD2	1:B:356:LEU:O	2.18	0.43
1:E:16:ARG:CB	1:E:16:ARG:HH11	2.32	0.43
1:F:192:LEU:HD12	1:F:193:TYR:N	2.33	0.43
1:F:242:ARG:NH1	6:F:536:HOH:O	2.52	0.43
1:F:4:MSE:C	1:F:4:MSE:SE	3.04	0.43
1:F:235:LEU:O	1:F:238:PHE:HB3	2.19	0.43
1:G:36:ARG:NH2	6:G:697:HOH:O	2.51	0.43
1:A:364:GLU:HB2	1:A:369:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLU:OE1	3:B:404:GOL:O2	2.30	0.43
1:A:161:ARG:HA	1:A:161:ARG:HD3	1.80	0.43
1:B:274:VAL:O	3:B:406:GOL:H32	2.19	0.43
1:C:100:TYR:O	1:C:103:THR:HB	2.19	0.43
1:E:6:PHE:CE2	1:E:179:VAL:HG22	2.53	0.43
1:F:201:GLY:O	1:F:327:VAL:HG13	2.19	0.43
1:B:104:ASP:HB2	1:B:119:TYR:OH	2.18	0.43
1:B:380:GLY:CA	6:B:512:HOH:O	2.66	0.43
1:D:320:CYS:SG	1:D:337:MSE:CE	3.04	0.43
1:B:88:ARG:HH11	1:E:136:ASP:CG	2.22	0.43
1:C:309:GLU:HB2	6:C:650:HOH:O	2.18	0.43
1:F:276:TYR:OH	1:F:295:PRO:HG2	2.19	0.43
1:A:322:VAL:HG11	4:A:406:CL:CL	2.56	0.43
1:C:142:ILE:O	1:C:171:VAL:HA	2.19	0.43
1:F:178:PRO:HD3	1:F:193:TYR:CE1	2.53	0.43
1:A:333:CYS:H	1:A:337:MSE:CE	2.31	0.43
1:B:346:ALA:HB1	1:B:350:ARG:NE	2.33	0.43
1:C:148:PRO:HG2	1:C:356:LEU:HD21	2.01	0.43
1:C:375:ARG:HB2	6:C:582:HOH:O	2.18	0.43
1:F:339:HIS:CD2	1:F:352:ILE:HD13	2.53	0.43
1:A:197:LLP:O3	1:A:197:LLP:NZ	2.35	0.43
1:A:88:ARG:HH21	1:A:88:ARG:HB3	1.83	0.43
1:B:152:VAL:HG22	1:B:284:GLN:HE21	1.84	0.43
1:C:137:LEU:HG	1:C:167:ALA:HB2	2.01	0.43
1:C:263:GLU:HG3	6:C:668:HOH:O	2.18	0.43
1:G:277:PRO:HA	1:G:282:HIS:CD2	2.54	0.43
1:B:41:GLU:HA	1:B:42:PRO:HD2	1.90	0.43
1:E:4:MSE:O	1:E:9:ARG:HD3	2.19	0.43
1:G:15:ARG:O	1:G:17:PRO:CD	2.66	0.43
1:A:124:THR:O	1:A:128:ILE:N	2.46	0.43
1:A:160:ARG:HG2	1:A:161:ARG:CZ	2.49	0.43
1:B:214:ASP:OD2	6:B:664:HOH:O	2.21	0.43
1:C:116:ARG:HH22	1:C:134:GLU:HG2	1.84	0.43
1:D:343:SER:O	1:D:346:ALA:HB3	2.19	0.43
1:E:308:ALA:HB3	1:E:336:LEU:HD12	2.00	0.43
1:H:44:TYR:CD1	1:H:50:GLU:HB3	2.53	0.43
1:D:252:HIS:CG	6:D:660:HOH:O	2.66	0.43
1:D:339:HIS:HB3	1:D:342:LEU:HD12	2.00	0.43
1:G:198:SER:OG	6:G:528:HOH:O	2.21	0.43
1:B:292:MSE:HE2	6:B:562:HOH:O	2.18	0.43
1:C:180:LEU:HA	1:C:293:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:ALA:HA	1:D:259:ARG:HD2	2.01	0.43
1:F:323:SER:N	2:F:401:MES:O2S	2.45	0.43
1:G:51:ASN:HA	1:G:52:PRO:HD3	1.89	0.43
1:H:152:VAL:HG21	1:H:288:VAL:HG22	2.01	0.43
1:H:97:ASP:C	1:H:99:VAL:N	2.71	0.43
1:E:365:ASP:CG	1:H:5:ARG:HB2	2.39	0.43
1:A:225:ARG:HG2	1:A:231:VAL:HG13	2.01	0.43
1:C:100:TYR:CE1	2:C:401:MES:H82	2.52	0.43
1:G:150:LEU:HD22	1:G:175:PHE:CE2	2.54	0.43
1:H:147:ASN:HD22	1:H:147:ASN:C	2.22	0.43
1:E:368:ASP:OD2	1:H:5:ARG:N	2.40	0.43
1:F:277:PRO:HA	1:F:282:HIS:CD2	2.53	0.43
1:F:84:LEU:HA	1:F:84:LEU:HD23	1.84	0.43
1:G:96:THR:O	1:G:99:VAL:HB	2.19	0.43
1:H:176:ALA:HB1	1:H:292:MSE:HE3	2.01	0.43
1:C:3:GLY:O	1:C:8:THR:OG1	2.14	0.43
1:D:122:LEU:HA	1:D:128:ILE:HG13	2.01	0.43
1:D:64:LEU:HD11	1:D:244:LEU:HD21	2.00	0.43
1:G:180:LEU:HB3	1:G:292:MSE:HE2	2.01	0.43
1:G:4:MSE:HB3	1:G:9:ARG:CG	2.49	0.43
1:H:116:ARG:NH2	1:H:135:PRO:HG2	2.34	0.43
1:H:9:ARG:HG3	6:H:620:HOH:O	2.19	0.43
1:C:330:LEU:HB2	1:C:360:SER:HB3	2.00	0.43
1:D:95:SER:O	1:D:119:TYR:HA	2.19	0.43
1:E:144:THR:HA	1:E:145:PRO:C	2.39	0.43
1:A:189:ASP:HA	1:A:213:ARG:HH22	1.84	0.43
1:B:105:GLY:O	1:B:109:LEU:HD13	2.19	0.43
1:H:275:HIS:HE1	6:H:581:HOH:O	2.02	0.43
1:B:315:PHE:CD1	1:B:318:PHE:HB2	2.54	0.43
1:D:175:PHE:CZ	1:D:298:ILE:HB	2.53	0.43
1:E:214:ASP:OD2	6:E:623:HOH:O	2.20	0.43
1:F:259:ARG:HH12	1:F:295:PRO:CG	2.31	0.43
1:F:180:LEU:HD22	1:F:294:ALA:HB3	2.00	0.43
1:G:332:GLU:OE1	1:G:338:THR:HG23	2.18	0.43
1:A:4:MSE:HE2	1:A:4:MSE:HA	2.00	0.43
1:E:371:GLU:O	1:E:375:ARG:HB2	2.17	0.43
1:F:84:LEU:CD1	1:F:110:ALA:HB2	2.49	0.43
1:G:16:ARG:HD2	1:G:59:GLU:OE2	2.18	0.43
1:B:364:GLU:HB2	1:B:369:LEU:HD11	2.01	0.43
1:C:36:ARG:HG2	1:C:37:ARG:HG3	2.01	0.43
1:C:337:MSE:HE2	1:D:36:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:MSE:SE	1:F:8:THR:O	2.86	0.43
1:G:92:CYS:SG	1:G:134:GLU:HG2	2.59	0.43
1:H:118:ARG:HD3	1:H:134:GLU:OE2	2.19	0.43
1:C:347:ARG:CB	1:C:347:ARG:HH21	2.32	0.43
1:D:100:TYR:HB2	6:D:605:HOH:O	2.19	0.43
1:F:314:ARG:NH1	1:F:379:GLY:O	2.52	0.43
1:C:314:ARG:NH1	6:C:503:HOH:O	2.32	0.42
1:E:334:PRO:O	1:E:339:HIS:N	2.51	0.42
1:F:92:CYS:SG	1:F:116:ARG:NH1	2.91	0.42
1:F:322:VAL:HB	2:F:401:MES:H72	2.00	0.42
1:H:149:LEU:HD23	1:H:149:LEU:HA	1.82	0.42
1:B:254:GLN:HB3	1:B:297:ALA:HB2	2.01	0.42
1:G:84:LEU:HG	1:G:141:TRP:CZ3	2.54	0.42
1:H:375:ARG:HG2	6:H:673:HOH:O	2.19	0.42
1:B:3:GLY:HA2	1:B:66:ARG:HH12	1.84	0.42
1:F:11:VAL:HA	1:F:245:HIS:ND1	2.34	0.42
1:A:84:LEU:HG	1:A:141:TRP:CZ3	2.53	0.42
1:B:148:PRO:HD2	1:B:352:ILE:HD12	2.00	0.42
1:E:347:ARG:HB3	1:E:352:ILE:O	2.19	0.42
1:H:259:ARG:O	1:H:263:GLU:HG2	2.18	0.42
1:A:37:ARG:NH1	6:A:673:HOH:O	2.52	0.42
1:G:337:MSE:O	1:G:340:ARG:N	2.41	0.42
1:H:84:LEU:HD12	1:H:106:LEU:HB3	2.01	0.42
1:C:342:LEU:HA	1:C:342:LEU:HD13	1.86	0.42
1:C:4:MSE:HE2	6:C:657:HOH:O	2.17	0.42
1:E:213:ARG:NE	3:E:402:GOL:O2	2.51	0.42
1:C:287:VAL:O	1:C:291:GLN:HG2	2.19	0.42
1:D:84:LEU:HA	1:D:84:LEU:HD22	1.87	0.42
1:F:150:LEU:HD22	1:F:175:PHE:CE2	2.53	0.42
1:F:4:MSE:CB	1:F:9:ARG:HG2	2.27	0.42
1:C:96:THR:C	1:C:98:ASP:N	2.72	0.42
1:E:111:ALA:O	1:E:114:GLY:N	2.36	0.42
1:G:99:VAL:HG13	1:G:103:THR:HB	2.01	0.42
1:G:88:ARG:HG3	1:G:91:GLN:OE1	2.18	0.42
1:D:14:GLY:C	1:D:16:ARG:H	2.23	0.42
1:G:46:TYR:CG	2:H:401:MES:H61	2.54	0.42
1:E:339:HIS:CD2	1:E:342:LEU:HD12	2.54	0.42
1:H:84:LEU:HD13	1:H:110:ALA:HB2	2.00	0.42
1:H:157:GLU:O	1:H:161:ARG:HG2	2.18	0.42
1:B:84:LEU:HD12	1:B:84:LEU:HA	1.86	0.42
1:A:109:LEU:HB3	6:A:568:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:ARG:HD2	1:H:365:ASP:OD1	2.19	0.42
1:H:4:MSE:HB2	1:H:4:MSE:HE2	1.86	0.42
1:H:4:MSE:O	1:H:9:ARG:CZ	2.67	0.42
1:D:68:PRO:HG2	1:D:213:ARG:HA	2.00	0.42
1:G:18:SER:HA	6:G:664:HOH:O	2.19	0.42
1:G:259:ARG:NH2	1:G:295:PRO:HD3	2.35	0.42
1:H:257:THR:OG1	6:H:664:HOH:O	2.21	0.42
6:G:620:HOH:O	1:H:33:THR:HG23	2.18	0.42
1:A:224:TYR:OH	6:A:607:HOH:O	2.13	0.42
1:B:343:SER:O	1:B:346:ALA:N	2.52	0.42
1:C:181:GLN:HE21	1:C:181:GLN:HB3	1.58	0.42
1:C:47:GLY:HA2	6:C:665:HOH:O	2.19	0.42
1:D:311:LEU:HA	1:D:311:LEU:HD12	1.90	0.42
1:E:35:GLU:HG3	1:E:35:GLU:O	2.18	0.42
1:F:11:VAL:HA	1:F:245:HIS:ND1	2.35	0.42
1:G:336:LEU:C	1:G:337:MSE:HG3	2.40	0.42
2:G:401:MES:H82	2:G:401:MES:H32	1.21	0.42
1:E:116:ARG:HG3	6:E:633:HOH:O	2.18	0.42
1:F:175:PHE:CZ	1:F:298:ILE:HB	2.54	0.42
1:A:4:MSE:HB3	1:A:8:THR:CG2	2.48	0.42
1:B:32:THR:OG1	1:B:33:THR:HG22	2.19	0.42
1:D:7:GLY:HA2	1:D:10:LEU:HD12	2.02	0.42
1:F:97:ASP:N	1:F:119:TYR:HB3	2.34	0.42
1:B:132:LEU:HD13	1:B:161:ARG:HB3	2.01	0.42
1:B:100:TYR:CE1	2:B:401:MES:H81	2.54	0.42
1:D:146:THR:O	1:D:150:LEU:HA	2.19	0.42
1:H:178:PRO:HD3	1:H:193:TYR:CE1	2.54	0.42
1:D:161:ARG:NH1	1:D:164:GLU:OE2	2.31	0.42
1:D:352:ILE:H	1:D:352:ILE:HG13	1.53	0.42
1:E:289:LYS:HE2	6:E:661:HOH:O	2.18	0.42
1:G:319:THR:HB	1:G:330:LEU:HD23	2.00	0.42
1:D:339:HIS:HB3	1:D:342:LEU:HD12	2.01	0.42
1:D:364:GLU:HB2	1:D:369:LEU:HD11	2.00	0.42
1:E:161:ARG:NH1	1:E:164:GLU:OE2	2.52	0.42
1:F:179:VAL:CG2	1:F:247:LEU:HG	2.49	0.42
1:F:324:LEU:HG	2:F:401:MES:O3S	2.19	0.42
1:G:273:ALA:HB3	1:G:302:ASP:OD1	2.19	0.42
1:A:323:SER:OG	1:B:46:TYR:HE1	2.01	0.42
1:B:11:VAL:HA	1:B:245:HIS:ND1	2.35	0.42
1:B:275:HIS:ND1	3:B:406:GOL:H2	2.35	0.42
1:C:54:ARG:NH1	6:C:674:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:MES:H82	2:D:401:MES:H32	1.41	0.42
1:E:34:TYR:CG	1:E:44:TYR:HB3	2.53	0.42
1:F:36:ARG:O	1:F:38:ALA:N	2.42	0.42
1:H:142:ILE:O	1:H:171:VAL:HA	2.20	0.42
1:D:332:GLU:HB2	1:D:337:MSE:HG2	2.01	0.42
1:C:14:GLY:HA2	1:C:59:GLU:HG2	2.01	0.42
1:C:14:GLY:O	1:C:56:GLU:HB3	2.20	0.42
1:E:123:THR:HG23	1:E:124:THR:HG23	2.02	0.42
1:H:318:PHE:HD1	1:H:372:ASP:OD2	2.01	0.42
1:H:3:GLY:HA2	6:H:657:HOH:O	2.19	0.42
1:A:157:GLU:O	1:A:161:ARG:HG2	2.19	0.42
1:A:42:PRO:HB3	1:A:45:PHE:CE1	2.54	0.42
1:F:175:PHE:HB3	6:F:532:HOH:O	2.19	0.42
2:G:401:MES:H82	2:G:401:MES:H31	1.78	0.42
1:H:98:ASP:N	1:H:350:ARG:HH22	2.17	0.42
1:H:88:ARG:CZ	1:H:89:PRO:HD2	2.49	0.42
1:A:129:ALA:C	1:A:131:ALA:H	2.22	0.42
1:E:93:VAL:HG13	1:E:139:LEU:HB3	2.01	0.42
1:E:320:CYS:C	1:E:337:MSE:HE1	2.39	0.42
1:E:345:GLU:HG2	1:E:349:ARG:CZ	2.49	0.42
1:H:96:THR:OG1	1:H:98:ASP:OD1	2.36	0.42
1:B:173:ASN:HB3	1:B:193:TYR:CE1	2.53	0.42
1:A:8:THR:HG23	1:D:364:GLU:CG	2.46	0.42
1:D:48:ARG:HG3	1:D:231:VAL:HG21	2.00	0.42
1:F:14:GLY:CA	1:F:59:GLU:HG2	2.49	0.42
1:H:41:GLU:HA	1:H:42:PRO:HD2	1.81	0.42
1:A:174:THR:HB	1:A:197:LLP:H2'2	2.01	0.42
1:A:336:LEU:O	1:A:340:ARG:HD2	2.19	0.42
1:E:96:THR:HA	1:E:120:ALA:O	2.20	0.42
1:G:157:GLU:OE1	1:G:161:ARG:HD3	2.18	0.42
1:H:280:PRO:HB2	1:H:281:GLU:OE2	2.20	0.42
1:E:6:PHE:HD1	1:E:9:ARG:HH11	1.66	0.42
1:F:145:PRO:HD2	1:F:175:PHE:CD1	2.54	0.42
1:F:289:LYS:CB	6:F:508:HOH:O	2.67	0.42
1:F:6:PHE:CE1	1:F:64:LEU:HD22	2.55	0.42
1:A:16:ARG:HH11	1:A:16:ARG:HD2	1.72	0.42
1:B:337:MSE:O	1:B:339:HIS:N	2.52	0.42
1:B:36:ARG:NH2	1:B:45:PHE:CD1	2.88	0.42
1:A:196:THR:HG21	1:B:46:TYR:OH	2.19	0.42
1:D:264:ARG:CZ	1:D:370:ALA:HB1	2.49	0.42
1:F:18:SER:CB	1:F:27:PRO:HD3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:ARG:HD2	1:F:56:GLU:HG2	2.01	0.42
1:H:9:ARG:HH12	1:H:66:ARG:NH2	2.17	0.42
1:B:253:ARG:HD3	3:B:402:GOL:H12	2.01	0.42
1:C:96:THR:HG23	1:C:120:ALA:O	2.19	0.42
1:E:253:ARG:NH2	1:E:257:THR:OG1	2.49	0.42
1:B:6:PHE:HA	1:B:9:ARG:NE	2.35	0.42
1:G:6:PHE:O	1:G:9:ARG:HB2	2.18	0.42
1:C:5:ARG:O	1:C:9:ARG:N	2.50	0.42
1:E:213:ARG:HE	3:E:402:GOL:H2	1.84	0.42
1:H:262:VAL:O	1:H:266:ARG:HG3	2.19	0.42
1:A:39:GLN:NE2	1:A:44:TYR:O	2.21	0.42
1:F:197:LLP:HB2	1:F:324:LEU:HD12	2.01	0.42
1:H:6:PHE:CD1	1:H:9:ARG:NH2	2.87	0.42
1:H:132:LEU:C	1:H:134:GLU:H	2.22	0.42
1:H:5:ARG:O	1:H:8:THR:N	2.41	0.42
1:A:214:ASP:HB3	1:A:217:LEU:HB3	2.00	0.42
1:E:16:ARG:HD2	1:E:17:PRO:HD2	2.00	0.42
1:F:16:ARG:HG2	1:F:56:GLU:HG2	2.02	0.42
1:A:163:HIS:HE1	1:A:187:GLY:O	2.02	0.42
1:A:371:GLU:O	1:A:375:ARG:HG3	2.19	0.42
1:B:16:ARG:NH2	6:B:677:HOH:O	2.42	0.42
1:C:285:HIS:O	1:C:288:VAL:HB	2.20	0.42
1:D:100:TYR:CE2	1:D:102:GLY:HA3	2.54	0.42
1:G:36:ARG:O	1:G:38:ALA:N	2.52	0.42
1:H:84:LEU:HD11	1:H:107:PHE:HD1	1.84	0.42
1:A:332:GLU:HG2	1:A:358:ARG:HH21	1.84	0.42
1:F:157:GLU:OE1	1:F:161:ARG:NH1	2.52	0.42
1:F:175:PHE:CZ	1:F:298:ILE:HB	2.55	0.42
1:G:93:VAL:HG22	1:G:139:LEU:HB3	2.02	0.42
1:H:89:PRO:HB2	6:H:507:HOH:O	2.19	0.42
1:A:345:GLU:O	1:A:349:ARG:HG3	2.19	0.42
1:C:175:PHE:CD1	1:C:175:PHE:C	2.92	0.42
1:C:35:GLU:HG3	1:C:37:ARG:H	1.85	0.42
1:B:132:LEU:CD1	1:B:161:ARG:HB3	2.49	0.42
1:E:93:VAL:HA	1:E:139:LEU:O	2.20	0.42
1:F:336:LEU:HD23	1:F:336:LEU:HA	1.59	0.42
1:F:253:ARG:HD2	3:F:405:GOL:C1	2.50	0.42
1:F:39:GLN:CD	1:F:42:PRO:HA	2.40	0.42
1:H:147:ASN:C	1:H:147:ASN:HD22	2.23	0.42
1:B:6:PHE:HB2	1:B:9:ARG:NH1	2.35	0.42
1:D:175:PHE:C	1:D:175:PHE:CD1	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:PHE:HB3	6:F:532:HOH:O	2.20	0.42
1:H:104:ASP:HA	1:H:107:PHE:CD2	2.54	0.42
1:A:4:MSE:HE2	1:A:4:MSE:HB3	1.67	0.42
1:D:18:SER:O	1:D:20:GLY:N	2.53	0.42
1:G:132:LEU:O	1:G:165:ARG:NH1	2.52	0.42
1:H:92:CYS:HB2	1:H:116:ARG:HB3	2.01	0.42
1:C:184:LEU:HB3	1:C:213:ARG:NH2	2.33	0.42
1:E:92:CYS:SG	1:E:93:VAL:N	2.92	0.42
1:G:94:VAL:HA	1:G:118:ARG:O	2.19	0.42
1:C:175:PHE:C	1:C:175:PHE:CD1	2.92	0.42
1:D:108:ASP:O	1:D:112:ARG:HB2	2.18	0.42
1:D:161:ARG:HH11	1:D:164:GLU:CD	2.22	0.42
1:G:83:LEU:HD23	1:G:83:LEU:HA	1.81	0.42
1:A:348:ALA:HA	1:A:351:GLY:O	2.19	0.42
1:A:51:ASN:HA	1:A:52:PRO:HD3	1.89	0.42
1:F:16:ARG:HD2	1:F:17:PRO:HD3	2.01	0.42
1:G:288:VAL:O	1:G:292:MSE:HG3	2.19	0.42
1:G:4:MSE:SE	6:G:604:HOH:O	2.86	0.42
1:G:45:PHE:HB2	1:G:50:GLU:OE2	2.19	0.42
1:A:320:CYS:HB3	1:B:35:GLU:OE2	2.20	0.42
1:C:314:ARG:HD3	1:C:380:GLY:HA3	2.02	0.42
1:D:350:ARG:HG3	1:D:350:ARG:H	1.57	0.42
1:A:5:ARG:HB2	1:D:365:ASP:CG	2.39	0.42
1:E:95:SER:OG	1:E:99:VAL:HG11	2.19	0.42
1:H:205:VAL:HG23	1:H:236:ASP:OD2	2.20	0.42
1:H:92:CYS:SG	1:H:134:GLU:HG2	2.59	0.42
1:A:101:ALA:O	1:A:105:GLY:N	2.44	0.42
1:D:86:LEU:HB3	3:D:404:GOL:H31	2.01	0.42
1:G:41:GLU:HA	1:G:42:PRO:HD2	1.85	0.42
1:H:3:GLY:N	6:H:535:HOH:O	2.52	0.42
1:B:202:HIS:NE2	6:B:521:HOH:O	2.36	0.42
1:D:375:ARG:HB2	1:D:375:ARG:HE	1.68	0.42
1:E:145:PRO:HA	1:E:151:THR:O	2.19	0.42
1:E:197:LLP:NZ	1:E:197:LLP:O3	2.49	0.42
1:D:144:THR:HA	1:D:145:PRO:C	2.40	0.42
1:F:252:HIS:CE1	3:F:404:GOL:H32	2.54	0.42
1:F:47:GLY:HA2	1:F:50:GLU:O	2.20	0.42
1:B:213:ARG:NE	3:B:402:GOL:O3	2.41	0.42
1:B:43:ARG:HD3	6:B:639:HOH:O	2.18	0.42
1:F:145:PRO:HB2	1:F:175:PHE:CE1	2.54	0.42
1:G:358:ARG:O	6:G:527:HOH:O	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:VAL:HG21	1:A:251:VAL:HG11	2.02	0.42
1:A:199:ILE:HB	6:A:548:HOH:O	2.19	0.42
1:C:108:ASP:O	1:C:112:ARG:HG2	2.20	0.42
1:C:199:ILE:CG2	1:C:244:LEU:HD21	2.45	0.42
1:C:96:THR:C	1:C:98:ASP:H	2.21	0.42
1:E:150:LEU:HD22	1:E:175:PHE:HE2	1.83	0.42
1:F:319:THR:HB	1:F:330:LEU:HD23	2.02	0.42
1:H:343:SER:OG	1:H:344:ALA:N	2.53	0.42
1:A:118:ARG:HD2	1:A:118:ARG:C	2.39	0.42
1:C:54:ARG:HD2	1:C:225:ARG:NH1	2.34	0.42
1:E:160:ARG:HB3	1:E:161:ARG:HH11	1.83	0.42
1:G:11:VAL:HA	1:G:245:HIS:ND1	2.34	0.42
1:A:27:PRO:HD2	3:A:403:GOL:O1	2.20	0.42
1:A:336:LEU:HB2	1:A:337:MSE:SE	2.70	0.42
1:A:39:GLN:CB	1:A:42:PRO:HA	2.50	0.42
1:B:368:ASP:CG	1:C:4:MSE:HG3	2.40	0.42
1:C:16:ARG:NE	1:C:59:GLU:OE1	2.52	0.42
1:F:147:ASN:HA	1:F:148:PRO:HA	1.77	0.42
1:F:307:PRO:HB3	1:F:309:GLU:OE2	2.20	0.42
1:G:316:THR:OG1	1:G:375:ARG:NH1	2.45	0.42
1:A:139:LEU:HD11	1:A:170:VAL:HG12	2.00	0.42
1:A:197:LLP:HG2	1:A:324:LEU:O	2.19	0.42
1:E:88:ARG:HH21	1:E:88:ARG:CG	2.25	0.42
1:H:335:ALA:CB	1:H:354:GLU:HA	2.50	0.42
1:A:254:GLN:HG2	1:A:361:VAL:O	2.19	0.42
1:B:163:HIS:NE2	1:B:189:ASP:OD2	2.50	0.42
1:B:9:ARG:CZ	1:B:66:ARG:HH11	2.33	0.42
1:C:347:ARG:HB3	1:C:352:ILE:HB	2.00	0.42
1:F:342:LEU:HD23	6:F:661:HOH:O	2.19	0.42
3:F:405:GOL:HO3	1:G:252:HIS:HD1	1.66	0.42
1:A:28:ILE:HG21	1:A:235:LEU:HD23	2.01	0.42
1:B:343:SER:HB2	1:B:345:GLU:OE1	2.20	0.42
1:B:343:SER:O	1:B:347:ARG:HG3	2.20	0.42
1:C:326:GLY:HA3	6:C:543:HOH:O	2.19	0.42
1:D:122:LEU:HA	1:D:128:ILE:HG13	2.01	0.42
1:B:43:ARG:CD	6:B:672:HOH:O	2.68	0.42
1:C:337:MSE:HE2	1:D:36:ARG:NH2	2.34	0.42
1:F:98:ASP:N	1:F:98:ASP:OD1	2.50	0.42
1:G:242:ARG:HA	1:G:245:HIS:HD2	1.84	0.42
1:D:367:GLN:OE1	6:D:671:HOH:O	2.21	0.42
1:E:337:MSE:HE1	1:F:36:ARG:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:PRO:HG2	1:F:213:ARG:HA	2.00	0.42
1:H:245:HIS:HE1	6:H:538:HOH:O	2.01	0.42
1:B:12:HIS:O	1:B:15:ARG:HB3	2.20	0.42
1:C:15:ARG:HA	6:C:519:HOH:O	2.19	0.42
1:C:322:VAL:HG21	1:D:46:TYR:HB2	2.02	0.42
1:A:36:ARG:HH11	1:A:42:PRO:HB3	1.84	0.42
1:E:46:TYR:CD2	2:F:401:MES:H61	2.55	0.42
1:G:108:ASP:O	1:G:112:ARG:HD2	2.19	0.42
1:G:224:TYR:OH	6:G:649:HOH:O	2.20	0.42
1:H:18:SER:O	1:H:19:ALA:O	2.38	0.42
1:H:6:PHE:O	1:H:9:ARG:HB2	2.20	0.42
1:A:88:ARG:HG2	1:A:88:ARG:H	1.66	0.42
1:B:161:ARG:NH2	6:B:640:HOH:O	2.52	0.42
1:D:292:MSE:HE1	6:D:525:HOH:O	2.18	0.42
1:F:165:ARG:NH2	1:F:165:ARG:HB3	2.35	0.42
1:B:142:ILE:HD11	1:B:158:VAL:HG11	2.00	0.42
1:B:322:VAL:O	1:B:323:SER:O	2.37	0.42
1:B:337:MSE:HA	1:B:340:ARG:HD3	2.01	0.42
1:A:21:THR:HG22	1:C:44:TYR:CD1	2.55	0.42
1:E:333:CYS:O	1:E:337:MSE:HB2	2.19	0.42
1:E:8:THR:HG22	1:E:12:HIS:HD2	1.85	0.42
1:F:236:ASP:OD1	6:F:626:HOH:O	2.22	0.42
1:G:51:ASN:HA	1:G:52:PRO:HD3	1.91	0.42
1:B:43:ARG:HB2	1:B:44:TYR:CE2	2.54	0.42
1:B:124:THR:O	1:B:128:ILE:N	2.53	0.42
1:B:288:VAL:HA	1:B:292:MSE:CE	2.47	0.42
1:C:248:SER:O	1:C:252:HIS:CD2	2.73	0.42
1:E:145:PRO:HD2	1:E:175:PHE:CG	2.55	0.42
1:E:289:LYS:HG2	6:E:561:HOH:O	2.19	0.42
1:F:16:ARG:H	1:F:16:ARG:HG2	1.60	0.42
1:C:13:GLY:HA3	6:C:531:HOH:O	2.19	0.42
1:C:264:ARG:HD2	1:C:374:SER:OG	2.19	0.42
1:D:197:LLP:NZ	2:D:401:MES:O3S	2.52	0.42
1:E:265:LEU:HG	1:E:373:LEU:HD21	2.01	0.42
1:F:111:ALA:C	1:F:114:GLY:H	2.22	0.42
1:C:134:GLU:HA	1:C:135:PRO:HD2	1.86	0.42
1:E:62:ALA:HB1	1:E:67:ALA:O	2.20	0.42
1:F:368:ASP:OD2	1:G:5:ARG:N	2.43	0.42
1:A:4:MSE:CA	1:A:9:ARG:HG3	2.45	0.42
1:D:44:TYR:CD1	1:D:50:GLU:HB3	2.55	0.42
1:A:33:THR:OG1	1:A:34:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASP:O	1:A:42:PRO:HD3	2.20	0.42
1:B:345:GLU:O	1:B:349:ARG:HG3	2.19	0.42
1:D:109:LEU:O	1:D:113:GLN:N	2.53	0.42
1:F:34:TYR:CZ	1:F:44:TYR:HB3	2.53	0.42
1:H:160:ARG:HB3	1:H:161:ARG:NH2	2.35	0.42
1:A:213:ARG:NH1	3:A:404:GOL:O2	2.53	0.42
1:D:334:PRO:HD2	1:D:356:LEU:O	2.20	0.42
1:D:96:THR:O	1:D:98:ASP:N	2.53	0.42
2:E:401:MES:H52	1:F:46:TYR:CD2	2.55	0.42
1:G:319:THR:HG23	1:H:35:GLU:OE1	2.20	0.42
1:A:264:ARG:NH2	6:A:674:HOH:O	2.33	0.42
1:B:132:LEU:HD22	1:B:162:ALA:HA	2.01	0.42
1:B:4:MSE:HG2	6:C:663:HOH:O	2.20	0.42
1:D:347:ARG:O	1:D:349:ARG:N	2.53	0.42
1:D:88:ARG:H	1:D:91:GLN:NE2	2.17	0.42
1:F:303:TYR:O	1:F:355:SER:HB3	2.19	0.42
1:G:100:TYR:O	1:G:103:THR:N	2.47	0.42
1:H:184:LEU:O	3:H:402:GOL:O2	2.38	0.42
1:B:347:ARG:HA	1:B:350:ARG:HB2	2.01	0.42
1:C:381:THR:O	1:C:381:THR:OG1	2.35	0.42
1:A:5:ARG:HD2	1:D:365:ASP:OD2	2.20	0.42
1:G:174:THR:HG21	1:G:194:SER:HB3	2.02	0.42
1:G:213:ARG:HE	3:G:402:GOL:H11	1.85	0.42
1:C:84:LEU:HD21	1:C:110:ALA:HB2	2.02	0.42
1:D:303:TYR:CG	1:D:311:LEU:HD22	2.54	0.42
1:H:259:ARG:NH1	1:H:295:PRO:HD2	2.23	0.42
1:A:36:ARG:O	1:A:37:ARG:HG3	2.20	0.42
1:E:150:LEU:CD1	1:E:277:PRO:HD3	2.50	0.42
1:F:27:PRO:HB2	1:H:27:PRO:HB2	2.01	0.42
1:G:168:ARG:HH22	3:G:404:FMT:H	1.85	0.42
1:H:148:PRO:HD3	1:H:339:HIS:CE1	2.55	0.42
1:A:323:SER:HB2	1:B:46:TYR:CE1	2.55	0.42
1:E:367:GLN:OE1	1:E:367:GLN:HA	2.19	0.42
1:H:282:HIS:HA	1:H:283:PRO:HD3	1.92	0.42
1:B:10:LEU:HB3	1:B:244:LEU:O	2.20	0.42
1:B:165:ARG:NH2	1:B:165:ARG:HB3	2.34	0.42
1:B:339:HIS:ND1	1:B:352:ILE:HD13	2.35	0.42
1:H:321:GLY:O	1:H:330:LEU:HD13	2.20	0.42
1:H:92:CYS:HG	1:H:116:ARG:NH2	2.18	0.42
1:D:94:VAL:HG21	1:D:131:ALA:O	2.20	0.42
1:F:342:LEU:HB3	1:F:346:ALA:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:ASN:HB3	1:G:193:TYR:CE1	2.54	0.42
1:G:347:ARG:HG2	1:G:352:ILE:HB	2.02	0.42
1:A:94:VAL:HG11	1:A:131:ALA:HB1	2.02	0.42
1:B:289:LYS:HB3	1:B:289:LYS:HE2	1.76	0.42
1:C:276:TYR:OH	1:C:295:PRO:HG2	2.18	0.42
1:C:6:PHE:CE1	1:C:10:LEU:HD11	2.54	0.42
1:A:5:ARG:NH1	1:D:368:ASP:OD2	2.50	0.42
1:F:60:CYS:SG	1:F:244:LEU:HD13	2.60	0.42
1:A:6:PHE:HA	1:A:9:ARG:HG3	2.02	0.42
1:B:16:ARG:HH11	1:B:52:PRO:HB3	1.85	0.42
1:B:364:GLU:HG3	1:C:11:VAL:HG21	2.02	0.42
1:C:147:ASN:ND2	1:C:358:ARG:HD2	2.18	0.42
1:D:106:LEU:HD23	1:D:109:LEU:HD12	2.01	0.42
1:F:248:SER:O	1:F:252:HIS:CD2	2.73	0.42
1:F:39:GLN:HG3	1:F:42:PRO:HA	2.02	0.42
1:G:43:ARG:HG3	1:G:44:TYR:N	2.34	0.42
1:A:206:LEU:HD12	1:B:231:VAL:HG21	2.02	0.42
1:D:124:THR:OG1	1:D:127:GLY:N	2.50	0.42
1:D:43:ARG:NH2	1:D:44:TYR:OH	2.53	0.42
1:E:367:GLN:NE2	6:E:692:HOH:O	2.51	0.42
1:D:108:ASP:HB3	1:D:112:ARG:NH1	2.34	0.42
1:E:29:HIS:HB3	6:G:559:HOH:O	2.19	0.42
2:E:401:MES:H22	6:E:664:HOH:O	2.20	0.42
1:E:165:ARG:CD	6:E:666:HOH:O	2.67	0.42
1:H:180:LEU:CB	1:H:292:MSE:HE3	2.48	0.42
1:B:16:ARG:HA	1:B:17:PRO:HD3	1.85	0.42
1:C:51:ASN:HA	1:C:52:PRO:HD3	1.88	0.42
1:C:83:LEU:HD22	1:C:210:LEU:HD22	2.01	0.42
1:D:276:TYR:CD1	1:D:299:VAL:HG22	2.55	0.42
1:E:89:PRO:HB3	1:E:114:GLY:HA3	2.01	0.42
1:A:332:GLU:HG2	1:A:358:ARG:NH2	2.35	0.42
1:C:277:PRO:HA	1:C:282:HIS:CD2	2.55	0.42
1:G:333:CYS:O	1:G:337:MSE:N	2.49	0.42
1:B:39:GLN:HG2	1:B:39:GLN:H	1.58	0.42
1:E:345:GLU:OE1	1:E:349:ARG:NH2	2.51	0.42
1:F:235:LEU:HA	1:F:235:LEU:HD23	1.89	0.42
1:H:157:GLU:OE2	1:H:161:ARG:NH2	2.49	0.42
1:B:98:ASP:OD2	6:B:658:HOH:O	2.22	0.42
6:C:573:HOH:O	1:D:235:LEU:HD12	2.19	0.42
1:F:275:HIS:HB2	1:F:300:SER:OG	2.20	0.42
1:F:6:PHE:N	6:F:657:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HD23	1:B:106:LEU:HB3	2.02	0.42
1:D:108:ASP:HA	1:D:111:ALA:HB3	2.01	0.42
1:D:4:MSE:CG	6:D:670:HOH:O	2.68	0.42
1:E:277:PRO:HA	1:E:282:HIS:CD2	2.55	0.42
1:F:261:LEU:HD13	1:F:359:LEU:HD13	2.02	0.42
1:A:346:ALA:HA	1:A:349:ARG:HG2	2.02	0.42
1:B:149:LEU:HD21	1:B:352:ILE:HG12	2.02	0.42
1:G:92:CYS:HB2	1:G:116:ARG:CZ	2.49	0.42
2:G:401:MES:H31	2:G:401:MES:H82	1.79	0.42
1:D:184:LEU:HB3	1:D:213:ARG:NH2	2.35	0.42
3:C:402:GOL:O3	1:D:227:THR:HG22	2.20	0.42
1:E:160:ARG:HB3	1:E:161:ARG:CZ	2.49	0.42
1:E:337:MSE:SE	6:E:604:HOH:O	2.88	0.42
1:E:372:ASP:HA	1:E:375:ARG:HH11	1.84	0.42
1:F:108:ASP:HB3	1:F:112:ARG:NH2	2.35	0.42
1:F:128:ILE:HG23	1:F:132:LEU:HD22	2.02	0.42
1:H:197:LLP:H4'1	2:H:401:MES:H72	2.02	0.42
1:H:276:TYR:CZ	1:H:295:PRO:HB2	2.55	0.42
1:A:28:ILE:HG21	1:A:235:LEU:HD23	2.00	0.42
1:A:96:THR:HG22	1:A:120:ALA:O	2.20	0.42
1:B:60:CYS:SG	1:B:244:LEU:HD13	2.60	0.42
1:H:36:ARG:O	1:H:42:PRO:HG3	2.20	0.42
1:A:342:LEU:HA	1:A:342:LEU:HD23	1.86	0.42
1:C:241:ARG:NE	6:C:516:HOH:O	2.45	0.42
1:A:112:ARG:HG2	1:A:112:ARG:H	1.70	0.42
1:A:113:GLN:HE21	1:B:113:GLN:HE21	1.68	0.42
1:A:320:CYS:SG	1:A:337:MSE:HE1	2.60	0.42
1:B:14:GLY:O	1:B:16:ARG:N	2.52	0.42
1:C:99:VAL:HG22	1:C:100:TYR:H	1.85	0.42
1:E:339:HIS:HD2	1:E:342:LEU:HD12	1.84	0.42
1:E:213:ARG:NH1	3:E:402:GOL:H2	2.12	0.42
1:D:145:PRO:N	1:D:292:MSE:HE1	2.35	0.42
1:H:97:ASP:HA	1:H:119:TYR:CD2	2.55	0.42
1:D:150:LEU:HD22	1:D:175:PHE:CE2	2.55	0.42
1:D:338:THR:O	1:D:341:PRO:HD2	2.20	0.42
1:G:184:LEU:HD22	1:G:213:ARG:HH12	1.83	0.42
1:H:4:MSE:SE	1:H:8:THR:HG21	2.70	0.42
1:A:199:ILE:HG23	1:A:244:LEU:HD13	2.02	0.41
1:A:281:GLU:CG	6:A:669:HOH:O	2.67	0.41
1:A:6:PHE:HD1	1:A:9:ARG:NH1	2.17	0.41
1:G:83:LEU:HD23	1:G:83:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:ARG:HH22	1:E:136:ASP:HB2	1.83	0.41
1:F:41:GLU:CB	6:F:667:HOH:O	2.68	0.41
1:G:105:GLY:O	1:G:108:ASP:HB2	2.20	0.41
1:A:343:SER:O	1:A:346:ALA:N	2.31	0.41
1:B:201:GLY:HA3	1:B:250:ARG:NH1	2.35	0.41
1:C:199:ILE:HB	6:C:599:HOH:O	2.20	0.41
1:E:131:ALA:O	1:E:134:GLU:HG2	2.19	0.41
1:E:160:ARG:HB3	1:E:161:ARG:HH11	1.84	0.41
1:E:197:LLP:HB2	1:E:324:LEU:HD12	2.01	0.41
1:F:371:GLU:OE2	1:G:5:ARG:NH1	2.43	0.41
1:G:82:THR:HG23	1:G:224:TYR:CD2	2.55	0.41
1:H:323:SER:O	1:H:330:LEU:HD12	2.20	0.41
1:H:334:PRO:HD2	1:H:356:LEU:O	2.18	0.41
1:H:372:ASP:HA	1:H:375:ARG:CZ	2.50	0.41
1:A:338:THR:HG23	2:A:401:MES:H32	2.01	0.41
1:A:83:LEU:HD22	1:A:210:LEU:HD22	2.02	0.41
1:B:277:PRO:HA	1:B:282:HIS:CD2	2.55	0.41
1:C:276:TYR:HA	1:C:277:PRO:HD3	1.96	0.41
1:H:84:LEU:HD12	1:H:110:ALA:HB2	2.02	0.41
1:H:9:ARG:NH2	1:H:64:LEU:HA	2.34	0.41
1:B:145:PRO:HD2	1:B:175:PHE:CD1	2.54	0.41
1:C:132:LEU:HB3	1:C:165:ARG:HG3	2.01	0.41
1:F:178:PRO:HD3	1:F:193:TYR:CE1	2.54	0.41
1:H:4:MSE:HG3	1:H:9:ARG:HD3	2.02	0.41
1:C:213:ARG:NH1	6:C:586:HOH:O	2.51	0.41
1:D:144:THR:HA	1:D:145:PRO:C	2.40	0.41
1:D:168:ARG:NH2	3:D:404:GOL:HO3	2.06	0.41
1:D:54:ARG:HD2	1:D:225:ARG:NH1	2.35	0.41
1:E:282:HIS:CG	1:E:283:PRO:HD2	2.55	0.41
2:H:401:MES:H51	2:H:401:MES:H82	1.80	0.41
1:A:27:PRO:HG2	3:A:403:GOL:H2	2.02	0.41
1:C:43:ARG:NH2	1:C:44:TYR:OH	2.53	0.41
1:D:94:VAL:HG21	1:D:131:ALA:HB1	2.02	0.41
1:E:97:ASP:OD2	1:E:98:ASP:N	2.53	0.41
1:G:113:GLN:HE21	1:H:113:GLN:CD	2.22	0.41
1:H:68:PRO:HG2	1:H:213:ARG:HA	2.02	0.41
1:H:332:GLU:OE1	1:H:358:ARG:CZ	2.68	0.41
1:A:173:ASN:HB3	1:A:193:TYR:CE1	2.55	0.41
1:B:116:ARG:NH2	1:B:134:GLU:HB3	2.29	0.41
1:B:150:LEU:HD13	1:B:277:PRO:HD3	2.01	0.41
6:A:630:HOH:O	1:B:233:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:VAL:HA	1:B:118:ARG:HB3	2.01	0.41
1:C:51:ASN:HA	1:C:52:PRO:HD3	1.92	0.41
1:H:51:ASN:OD1	1:H:53:THR:N	2.53	0.41
1:C:342:LEU:HD22	1:C:342:LEU:H	1.83	0.41
1:A:251:VAL:HG22	6:A:584:HOH:O	2.20	0.41
1:B:66:ARG:NH2	6:B:683:HOH:O	2.53	0.41
1:D:109:LEU:HA	1:D:112:ARG:HB2	2.02	0.41
1:E:132:LEU:O	1:E:165:ARG:HG3	2.20	0.41
1:E:150:LEU:HD22	1:E:175:PHE:CE2	2.55	0.41
1:E:305:GLY:O	1:E:310:ARG:NH2	2.53	0.41
1:E:35:GLU:OE2	1:E:37:ARG:N	2.53	0.41
1:B:90:GLY:HA2	1:E:88:ARG:NH1	2.35	0.41
1:F:69:PHE:HA	5:F:407:FMT:H	2.02	0.41
1:G:18:SER:HB2	1:G:23:ASP:N	2.35	0.41
1:H:110:ALA:O	1:H:115:VAL:HB	2.20	0.41
1:H:257:THR:HG21	1:H:369:LEU:HD12	2.01	0.41
1:E:287:VAL:O	1:E:291:GLN:HG2	2.19	0.41
1:F:310:ARG:HE	1:F:314:ARG:NH1	2.02	0.41
1:F:4:MSE:CB	1:F:9:ARG:HG2	2.51	0.41
1:B:194:SER:HB2	1:B:197:LLP:OP4	2.19	0.41
1:E:107:PHE:HB3	1:E:117:VAL:HG21	2.02	0.41
1:E:324:LEU:HA	1:E:330:LEU:HD12	2.02	0.41
1:E:345:GLU:C	1:E:347:ARG:N	2.73	0.41
6:E:598:HOH:O	1:G:29:HIS:HE1	2.03	0.41
1:G:213:ARG:NH2	3:G:402:GOL:O2	2.38	0.41
1:H:16:ARG:HA	1:H:17:PRO:HD2	1.55	0.41
1:F:21:THR:HG22	1:H:44:TYR:CE2	2.55	0.41
1:A:104:ASP:OD2	1:A:119:TYR:OH	2.38	0.41
1:C:192:LEU:HD12	1:C:193:TYR:N	2.35	0.41
1:F:254:GLN:HB3	1:F:297:ALA:CB	2.50	0.41
1:H:292:MSE:HB3	1:H:294:ALA:O	2.20	0.41
1:A:248:SER:HB2	1:A:252:HIS:CE1	2.55	0.41
1:B:11:VAL:HA	1:B:245:HIS:ND1	2.35	0.41
1:D:254:GLN:HB3	1:D:297:ALA:CB	2.50	0.41
1:D:7:GLY:HA2	1:D:10:LEU:HD12	2.02	0.41
1:G:196:THR:HG21	1:H:46:TYR:OH	2.20	0.41
1:H:245:HIS:HE1	6:H:536:HOH:O	2.03	0.41
1:A:147:ASN:C	1:A:149:LEU:H	2.24	0.41
1:A:213:ARG:HG2	6:A:562:HOH:O	2.20	0.41
1:A:279:LEU:HD12	6:A:561:HOH:O	2.19	0.41
1:B:16:ARG:HA	1:B:17:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:LEU:HD22	1:C:175:PHE:CE2	2.55	0.41
1:C:102:GLY:HA2	3:D:403:GOL:H32	2.02	0.41
1:G:288:VAL:HA	1:G:292:MSE:SE	2.70	0.41
1:G:96:THR:CG2	6:G:663:HOH:O	2.68	0.41
1:C:37:ARG:NE	6:C:674:HOH:O	2.03	0.41
1:C:34:TYR:HD2	1:C:45:PHE:C	2.23	0.41
1:D:254:GLN:HB3	1:D:297:ALA:HB2	2.02	0.41
1:F:358:ARG:NH1	6:F:599:HOH:O	2.53	0.41
1:H:161:ARG:HD3	1:H:161:ARG:HA	1.85	0.41
1:H:57:LEU:O	1:H:60:CYS:HB3	2.20	0.41
1:B:344:ALA:O	1:B:347:ARG:N	2.54	0.41
1:C:314:ARG:NH2	6:C:550:HOH:O	2.49	0.41
1:D:268:SER:HA	1:D:269:PRO:HD3	1.95	0.41
1:E:213:ARG:NE	3:E:402:GOL:H2	2.35	0.41
1:F:106:LEU:HD23	1:F:109:LEU:HD12	2.01	0.41
1:F:11:VAL:HA	1:F:245:HIS:ND1	2.35	0.41
1:H:168:ARG:HH12	3:H:404:GOL:C3	2.34	0.41
1:B:43:ARG:HD3	6:B:672:HOH:O	2.20	0.41
1:C:112:ARG:O	1:D:88:ARG:NH1	2.40	0.41
1:E:197:LLP:O3	1:E:197:LLP:NZ	2.32	0.41
1:E:365:ASP:OD1	1:E:367:GLN:HB2	2.20	0.41
1:F:276:TYR:CD1	1:F:299:VAL:HG22	2.55	0.41
1:F:277:PRO:O	1:F:285:HIS:ND1	2.52	0.41
1:F:84:LEU:HA	1:F:84:LEU:HD23	1.84	0.41
1:G:376:ALA:N	6:G:696:HOH:O	2.52	0.41
1:G:46:TYR:OH	1:H:196:THR:HG21	2.20	0.41
1:E:276:TYR:OH	1:E:295:PRO:HG2	2.19	0.41
1:B:110:ALA:O	1:B:115:VAL:HB	2.19	0.41
1:B:40:ASP:O	1:B:41:GLU:HB2	2.20	0.41
1:D:197:LLP:NZ	1:D:197:LLP:O3	2.50	0.41
1:E:148:PRO:HD3	1:E:339:HIS:CE1	2.55	0.41
1:E:43:ARG:HD2	1:E:43:ARG:HH11	1.74	0.41
1:E:14:GLY:HA2	1:E:59:GLU:OE1	2.20	0.41
1:B:6:PHE:HA	1:B:9:ARG:HB2	2.02	0.41
1:C:51:ASN:HA	1:C:52:PRO:HD3	1.87	0.41
1:F:29:HIS:CD2	1:F:52:PRO:HB2	2.55	0.41
1:A:160:ARG:HB3	1:A:161:ARG:NE	2.35	0.41
1:A:99:VAL:HG22	6:A:543:HOH:O	2.20	0.41
1:D:92:CYS:O	1:D:137:LEU:HD12	2.20	0.41
1:D:9:ARG:HB3	6:D:519:HOH:O	2.20	0.41
1:F:142:ILE:HD11	1:F:158:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:ARG:HD3	1:F:16:ARG:HA	1.55	0.41
1:F:58:GLU:HB3	5:F:407:FMT:H	2.02	0.41
1:H:84:LEU:HD11	1:H:107:PHE:HD1	1.85	0.41
1:H:226:THR:HG23	6:H:653:HOH:O	2.21	0.41
1:H:236:ASP:OD1	6:H:651:HOH:O	2.21	0.41
1:C:147:ASN:HD21	1:C:358:ARG:HH11	1.68	0.41
1:C:178:PRO:HD3	1:C:193:TYR:CE1	2.55	0.41
1:D:277:PRO:HA	1:D:282:HIS:NE2	2.35	0.41
1:D:39:GLN:OE1	1:D:42:PRO:HA	2.20	0.41
1:E:175:PHE:HZ	1:E:298:ILE:HG21	1.85	0.41
1:E:83:LEU:HA	1:E:83:LEU:HD12	1.94	0.41
1:F:254:GLN:HB3	1:F:297:ALA:CB	2.49	0.41
1:H:174:THR:HB	1:H:197:LLP:H2'2	2.01	0.41
1:H:378:ALA:C	1:H:380:GLY:H	2.23	0.41
1:C:347:ARG:HB3	1:C:352:ILE:O	2.20	0.41
1:G:192:LEU:HD12	1:G:193:TYR:N	2.35	0.41
1:G:7:GLY:O	6:G:596:HOH:O	2.21	0.41
1:A:84:LEU:HD11	1:A:107:PHE:HD1	1.85	0.41
1:A:84:LEU:HD23	1:A:84:LEU:HA	1.88	0.41
1:A:113:GLN:HB3	1:B:113:GLN:NE2	2.35	0.41
1:D:33:THR:OG1	1:D:34:TYR:N	2.52	0.41
1:E:147:ASN:HB3	6:E:653:HOH:O	2.19	0.41
1:F:180:LEU:HA	1:F:293:SER:OG	2.20	0.41
1:G:338:THR:O	1:G:341:PRO:HD2	2.20	0.41
1:H:68:PRO:HD2	1:H:213:ARG:HB3	2.01	0.41
1:A:338:THR:HG1	1:A:339:HIS:CE1	2.39	0.41
1:B:39:GLN:OE1	1:B:42:PRO:HA	2.20	0.41
1:B:66:ARG:HH21	1:B:66:ARG:CB	2.33	0.41
1:C:54:ARG:HG3	1:C:237:CYS:SG	2.60	0.41
1:F:134:GLU:HA	1:F:135:PRO:HD3	1.95	0.41
1:E:46:TYR:OH	1:F:196:THR:HG21	2.20	0.41
1:F:278:GLY:HA2	1:F:285:HIS:HE1	1.85	0.41
1:F:342:LEU:CD1	6:F:670:HOH:O	2.67	0.41
1:B:146:THR:O	1:B:150:LEU:HA	2.20	0.41
1:E:322:VAL:HG21	1:F:46:TYR:HB2	2.02	0.41
1:G:97:ASP:HA	1:G:119:TYR:HD1	1.85	0.41
1:G:319:THR:CG2	1:H:35:GLU:HB2	2.50	0.41
1:G:97:ASP:OD1	1:G:121:ASP:N	2.53	0.41
1:B:282:HIS:HA	1:B:283:PRO:HD3	1.87	0.41
1:D:41:GLU:HA	1:D:42:PRO:HD3	1.79	0.41
1:E:5:ARG:NH1	1:H:368:ASP:OD1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:THR:HA	1:A:199:ILE:HB	2.02	0.41
1:B:4:MSE:HB3	1:B:5:ARG:H	1.48	0.41
1:C:146:THR:O	1:C:150:LEU:HA	2.20	0.41
1:C:14:GLY:O	1:C:16:ARG:N	2.54	0.41
1:A:20:GLY:O	1:C:39:GLN:HG2	2.20	0.41
1:D:342:LEU:HG	1:D:342:LEU:H	1.49	0.41
1:F:107:PHE:HD2	1:F:119:TYR:OH	2.01	0.41
1:F:145:PRO:HG3	1:F:152:VAL:HG22	2.00	0.41
1:H:175:PHE:C	1:H:175:PHE:CD1	2.93	0.41
1:B:146:THR:HG1	1:B:151:THR:H	1.68	0.41
1:A:337:MSE:HE3	1:B:36:ARG:NH2	2.36	0.41
1:H:94:VAL:HG23	1:H:137:LEU:HD13	2.02	0.41
1:F:143:GLU:HG3	1:F:172:ASP:HB3	2.01	0.41
1:F:338:THR:HB	1:F:339:HIS:H	1.46	0.41
1:G:292:MSE:HB3	1:G:294:ALA:O	2.20	0.41
1:G:259:ARG:HH21	1:G:295:PRO:HD3	1.85	0.41
1:H:334:PRO:O	1:H:339:HIS:N	2.54	0.41
1:G:309:GLU:H	1:G:309:GLU:HG3	1.70	0.41
1:B:101:ALA:HB2	1:B:339:HIS:HD2	1.85	0.41
1:B:27:PRO:HB2	1:D:27:PRO:HB2	2.01	0.41
1:B:5:ARG:C	1:B:9:ARG:HE	2.22	0.41
1:A:5:ARG:N	1:D:368:ASP:OD1	2.53	0.41
1:G:161:ARG:NH2	1:G:164:GLU:OE2	2.53	0.41
1:G:292:MSE:HE2	1:G:292:MSE:HB2	1.62	0.41
1:G:36:ARG:HG2	1:G:36:ARG:NH1	2.33	0.41
1:H:225:ARG:HD2	1:H:231:VAL:HG13	2.02	0.41
1:H:4:MSE:HE2	1:H:4:MSE:HB2	1.93	0.41
1:A:4:MSE:HA	1:D:368:ASP:OD1	2.20	0.41
1:C:111:ALA:HA	1:C:115:VAL:O	2.20	0.41
1:D:334:PRO:O	1:D:336:LEU:N	2.52	0.41
1:C:36:ARG:CZ	1:D:337:MSE:HE3	2.49	0.41
1:D:355:SER:N	6:D:648:HOH:O	2.29	0.41
1:D:303:TYR:HB3	1:D:355:SER:OG	2.20	0.41
1:H:147:ASN:HD21	1:H:358:ARG:HD3	1.85	0.41
1:C:23:ASP:HB3	1:C:25:VAL:O	2.20	0.41
1:F:314:ARG:NE	1:F:379:GLY:HA2	2.35	0.41
1:G:235:LEU:O	1:G:238:PHE:HB3	2.20	0.41
1:B:96:THR:HG22	1:B:120:ALA:O	2.20	0.41
1:A:135:PRO:HG3	1:E:112:ARG:HH21	1.85	0.41
1:G:128:ILE:O	1:G:132:LEU:HG	2.20	0.41
1:G:161:ARG:HA	1:G:164:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ASN:HA	1:C:148:PRO:HA	1.94	0.41
1:E:196:THR:HG22	6:E:557:HOH:O	2.21	0.41
1:H:118:ARG:NH1	1:H:131:ALA:HA	2.35	0.41
1:A:11:VAL:HA	1:A:245:HIS:ND1	2.35	0.41
1:A:135:PRO:HA	1:A:165:ARG:NH1	2.35	0.41
1:A:364:GLU:HB2	1:A:369:LEU:HD11	2.02	0.41
1:B:132:LEU:HD13	1:B:161:ARG:HB3	2.03	0.41
1:B:310:ARG:HB3	1:B:314:ARG:HH11	1.86	0.41
1:E:309:GLU:O	1:E:313:ASP:HB2	2.20	0.41
1:F:92:CYS:HB3	1:F:136:ASP:O	2.20	0.41
1:F:180:LEU:HA	1:F:293:SER:OG	2.19	0.41
1:G:152:VAL:H	1:G:284:GLN:NE2	2.19	0.41
1:G:174:THR:HB	1:G:197:LLP:H2'2	2.02	0.41
1:H:16:ARG:N	1:H:16:ARG:HH11	2.18	0.41
1:H:197:LLP:HG3	1:H:197:LLP:H	1.56	0.41
1:A:162:ALA:HB1	1:A:167:ALA:HB3	2.03	0.41
1:B:350:ARG:HD3	6:B:614:HOH:O	2.21	0.41
1:C:88:ARG:H	1:C:88:ARG:HG2	1.50	0.41
1:F:364:GLU:HB2	1:F:369:LEU:HD11	2.03	0.41
1:D:99:VAL:HG13	1:D:103:THR:HB	2.01	0.41
1:E:6:PHE:HE1	1:E:64:LEU:O	2.03	0.41
1:G:97:ASP:C	1:G:99:VAL:N	2.74	0.41
1:H:336:LEU:O	1:H:340:ARG:HB2	2.20	0.41
1:H:82:THR:HG21	1:H:221:VAL:HG13	2.02	0.41
1:A:145:PRO:HD2	1:A:175:PHE:CD1	2.56	0.41
1:A:192:LEU:HD12	1:A:193:TYR:N	2.35	0.41
1:E:29:HIS:HB3	6:G:557:HOH:O	2.20	0.41
1:G:132:LEU:HD12	1:G:161:ARG:HB3	2.03	0.41
1:H:122:LEU:O	1:H:128:ILE:HD11	2.20	0.41
1:H:132:LEU:HD22	1:H:137:LEU:HD21	2.02	0.41
1:H:147:ASN:ND2	6:H:574:HOH:O	2.48	0.41
1:A:159:SER:HA	1:A:169:VAL:HG21	2.03	0.41
1:A:341:PRO:HB2	1:A:342:LEU:H	1.53	0.41
1:C:65:GLU:OE1	6:C:583:HOH:O	2.22	0.41
1:D:292:MSE:SE	1:D:295:PRO:CA	3.18	0.41
1:G:132:LEU:O	1:G:134:GLU:N	2.54	0.41
1:A:144:THR:HA	1:A:145:PRO:C	2.40	0.41
1:A:226:THR:CG2	6:A:674:HOH:O	2.67	0.41
1:B:319:THR:HB	1:B:330:LEU:HD23	2.02	0.41
1:C:97:ASP:HB2	1:C:119:TYR:HB3	2.02	0.41
1:D:252:HIS:CG	6:D:638:HOH:O	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ARG:HB3	1:D:36:ARG:HH21	1.85	0.41
1:F:128:ILE:HG23	1:F:132:LEU:HD22	2.02	0.41
1:B:192:LEU:HD12	1:B:210:LEU:HD21	2.02	0.41
1:D:347:ARG:O	1:D:352:ILE:N	2.43	0.41
1:E:40:ASP:HA	6:E:646:HOH:O	2.20	0.41
1:F:175:PHE:CZ	1:F:298:ILE:HB	2.56	0.41
1:F:9:ARG:NH1	1:F:66:ARG:HD3	2.36	0.41
1:G:90:GLY:N	1:G:114:GLY:O	2.41	0.41
1:C:250:ARG:HD2	6:C:551:HOH:O	2.20	0.41
1:G:109:LEU:O	1:G:112:ARG:HB2	2.20	0.41
1:H:37:ARG:C	1:H:39:GLN:N	2.73	0.41
1:A:163:HIS:HE1	1:A:187:GLY:O	2.02	0.41
1:A:354:GLU:HG2	1:A:354:GLU:H	1.65	0.41
1:C:46:TYR:CD2	2:D:401:MES:H61	2.55	0.41
1:D:132:LEU:HD23	1:D:132:LEU:HA	1.81	0.41
1:D:350:ARG:HD2	1:D:352:ILE:HD12	2.03	0.41
1:D:358:ARG:NH1	2:D:401:MES:O2S	2.45	0.41
1:A:175:PHE:CZ	1:A:298:ILE:HB	2.56	0.41
1:A:65:GLU:OE2	1:A:193:TYR:OH	2.33	0.41
1:B:275:HIS:HB2	1:B:300:SER:HB2	2.01	0.41
1:B:319:THR:O	1:B:330:LEU:HD23	2.20	0.41
1:B:68:PRO:HG2	1:B:213:ARG:HA	2.02	0.41
1:B:96:THR:HB	1:B:98:ASP:OD1	2.20	0.41
1:F:95:SER:OG	1:F:96:THR:N	2.54	0.41
1:G:371:GLU:HB3	1:G:375:ARG:HH22	1.84	0.41
1:B:163:HIS:HE1	1:B:187:GLY:O	2.03	0.41
1:B:68:PRO:HG2	1:B:213:ARG:HA	2.01	0.41
1:D:250:ARG:O	1:D:254:GLN:HG3	2.20	0.41
1:E:238:PHE:HA	6:E:656:HOH:O	2.21	0.41
1:E:368:ASP:OD1	1:H:5:ARG:NH1	2.42	0.41
1:H:146:THR:O	1:H:150:LEU:HA	2.21	0.41
1:A:168:ARG:NH1	3:A:402:GOL:O1	2.53	0.41
1:G:43:ARG:NH2	1:G:55:GLU:OE1	2.38	0.41
1:H:144:THR:HA	1:H:145:PRO:C	2.40	0.41
1:H:137:LEU:N	1:H:165:ARG:HH11	2.16	0.41
1:H:375:ARG:CZ	1:H:375:ARG:HB2	2.50	0.41
1:B:253:ARG:HD3	3:B:402:GOL:H11	2.03	0.41
1:E:315:PHE:CD1	1:E:318:PHE:HB2	2.56	0.41
1:G:338:THR:HG21	2:G:401:MES:H82	2.03	0.41
1:B:364:GLU:HB3	1:C:8:THR:HB	2.02	0.41
1:D:160:ARG:CB	1:D:161:ARG:HH11	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:GLU:CD	1:D:37:ARG:HH21	2.20	0.41
1:G:101:ALA:HA	1:G:104:ASP:CB	2.47	0.41
1:H:88:ARG:HA	1:H:88:ARG:HD2	1.82	0.41
1:A:5:ARG:CZ	1:D:367:GLN:HB3	2.51	0.41
1:E:323:SER:HB3	1:F:33:THR:OG1	2.21	0.41
1:G:18:SER:HB2	6:G:657:HOH:O	2.21	0.41
1:H:178:PRO:HD3	1:H:193:TYR:CE1	2.56	0.41
1:B:128:ILE:O	1:B:132:LEU:HG	2.21	0.41
1:C:263:GLU:CB	6:C:668:HOH:O	2.69	0.41
1:C:313:ASP:HA	1:D:37:ARG:HD3	2.03	0.41
1:F:259:ARG:NH2	1:F:295:PRO:HD3	2.33	0.41
1:F:334:PRO:HB2	6:F:680:HOH:O	2.21	0.41
1:H:97:ASP:HA	1:H:119:TYR:HD2	1.86	0.41
1:H:9:ARG:HB3	1:H:64:LEU:HD23	2.02	0.41
1:A:161:ARG:HD2	1:A:161:ARG:HA	1.77	0.41
2:D:401:MES:H82	2:D:401:MES:H32	1.55	0.41
1:E:14:GLY:HA2	1:E:59:GLU:OE1	2.20	0.41
1:H:277:PRO:HA	1:H:282:HIS:CD2	2.55	0.41
1:E:147:ASN:C	1:E:149:LEU:H	2.24	0.41
1:E:347:ARG:HB2	1:E:352:ILE:O	2.21	0.41
1:F:254:GLN:HB3	1:F:297:ALA:CB	2.51	0.41
1:G:99:VAL:HG22	1:G:143:GLU:OE1	2.20	0.41
1:D:279:LEU:HB3	1:D:281:GLU:HG2	2.03	0.41
1:H:40:ASP:O	1:H:42:PRO:HD3	2.20	0.41
1:A:337:MSE:HE3	1:B:36:ARG:HH21	1.86	0.41
1:A:337:MSE:HB3	1:A:338:THR:H	1.51	0.41
1:B:282:HIS:HE1	1:B:284:GLN:HG3	1.85	0.41
1:C:43:ARG:HB3	1:C:44:TYR:CE1	2.55	0.41
1:E:242:ARG:NH1	6:E:517:HOH:O	2.45	0.41
1:E:264:ARG:CZ	1:E:370:ALA:HB1	2.51	0.41
1:F:147:ASN:HA	1:F:148:PRO:HA	1.89	0.41
1:C:122:LEU:HA	1:C:122:LEU:HD23	1.84	0.41
1:E:356:LEU:HG	1:E:357:ILE:N	2.36	0.41
1:E:365:ASP:HB3	1:E:368:ASP:OD2	2.20	0.41
1:F:34:TYR:CE2	1:F:44:TYR:HB3	2.55	0.41
1:G:105:GLY:O	1:G:109:LEU:N	2.44	0.41
1:G:36:ARG:NH1	1:G:36:ARG:HG3	2.29	0.41
1:E:4:MSE:HA	1:H:368:ASP:OD2	2.20	0.41
1:D:305:GLY:O	1:D:310:ARG:NE	2.54	0.41
1:E:102:GLY:HA2	3:E:405:GOL:H11	2.02	0.41
1:F:121:ASP:HA	6:F:628:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:THR:O	1:F:341:PRO:HD2	2.21	0.41
1:F:35:GLU:HG3	1:F:38:ALA:CB	2.50	0.41
1:F:44:TYR:CD1	1:F:50:GLU:HB3	2.56	0.41
1:B:212:TYR:OH	1:B:218:HIS:ND1	2.30	0.41
1:C:175:PHE:CZ	1:C:298:ILE:HB	2.56	0.41
1:D:277:PRO:HB2	1:D:295:PRO:CB	2.51	0.41
1:E:110:ALA:HB1	1:E:115:VAL:HG21	2.03	0.41
1:F:343:SER:HB3	1:F:346:ALA:HB3	2.02	0.41
1:G:333:CYS:HA	1:G:334:PRO:HD3	1.76	0.41
1:H:251:VAL:HA	1:H:254:GLN:NE2	2.33	0.41
1:B:17:PRO:CA	6:B:674:HOH:O	2.69	0.41
1:B:347:ARG:HB2	1:B:352:ILE:O	2.21	0.41
1:C:34:TYR:CE1	6:C:645:HOH:O	2.71	0.41
1:E:147:ASN:HD21	1:E:358:ARG:CD	2.32	0.41
1:E:60:CYS:SG	1:E:244:LEU:HD13	2.61	0.41
1:A:37:ARG:NH2	1:B:319:THR:HA	2.35	0.41
1:C:112:ARG:HG2	4:C:405:CL:CL	2.57	0.41
1:G:148:PRO:HB3	1:G:358:ARG:HD3	2.02	0.41
1:H:113:GLN:NE2	6:H:662:HOH:O	2.54	0.41
1:A:161:ARG:HA	1:A:161:ARG:HD3	1.77	0.41
2:B:401:MES:H82	2:B:401:MES:H32	1.76	0.41
1:D:276:TYR:CE2	1:D:295:PRO:HB2	2.55	0.41
1:F:16:ARG:NE	1:F:59:GLU:OE2	2.53	0.41
1:H:16:ARG:HA	1:H:17:PRO:HD2	1.77	0.41
1:A:39:GLN:HE22	1:A:44:TYR:N	2.19	0.41
1:F:310:ARG:HG3	6:F:672:HOH:O	2.20	0.41
1:A:16:ARG:HG2	1:A:56:GLU:HG2	2.01	0.41
1:C:160:ARG:O	1:C:164:GLU:HG3	2.20	0.41
1:F:97:ASP:HA	1:F:119:TYR:CD2	2.55	0.41
1:G:129:ALA:HB2	6:G:577:HOH:O	2.21	0.41
1:G:259:ARG:HH21	1:G:295:PRO:HD2	1.86	0.41
1:H:93:VAL:HG23	1:H:117:VAL:HG22	2.03	0.41
1:G:233:GLY:HA3	1:H:236:ASP:OD2	2.21	0.41
1:H:341:PRO:HG2	6:H:671:HOH:O	2.21	0.41
1:A:189:ASP:HA	1:A:213:ARG:NH2	2.33	0.41
1:C:350:ARG:NH2	6:C:624:HOH:O	2.36	0.41
1:E:145:PRO:HD3	6:E:555:HOH:O	2.21	0.41
1:A:68:PRO:HG2	1:A:213:ARG:HA	2.02	0.41
1:A:100:TYR:OH	2:A:401:MES:H62	2.20	0.41
1:B:342:LEU:HB2	1:B:347:ARG:HG3	2.02	0.41
1:B:264:ARG:HD2	1:B:374:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ASN:ND2	6:C:588:HOH:O	2.46	0.41
1:D:176:ALA:O	1:D:177:SER:OG	2.21	0.41
1:D:333:CYS:H	1:D:337:MSE:CE	2.34	0.41
1:G:94:VAL:O	1:G:140:VAL:HA	2.21	0.41
1:A:134:GLU:O	1:A:165:ARG:NH1	2.52	0.41
1:C:188:ALA:O	1:C:213:ARG:NH2	2.52	0.41
1:C:113:GLN:HB3	1:D:113:GLN:OE1	2.20	0.41
1:D:259:ARG:NH2	6:D:503:HOH:O	2.34	0.41
1:D:333:CYS:O	1:D:337:MSE:N	2.54	0.41
1:F:35:GLU:CG	1:F:38:ALA:HB2	2.51	0.41
1:G:289:LYS:CE	6:G:653:HOH:O	2.68	0.41
1:G:337:MSE:HB3	1:G:338:THR:H	1.22	0.41
1:H:126:GLU:HG2	1:H:126:GLU:H	1.57	0.41
1:H:178:PRO:HD3	1:H:193:TYR:CZ	2.56	0.41
1:B:179:VAL:CG1	1:B:252:HIS:CE1	3.04	0.41
1:D:347:ARG:HB2	1:D:352:ILE:HB	2.03	0.41
1:E:147:ASN:OD1	1:E:358:ARG:HD2	2.20	0.41
1:F:9:ARG:HG2	1:F:9:ARG:H	1.64	0.41
1:G:259:ARG:HH21	1:G:295:PRO:CD	2.34	0.41
1:H:288:VAL:HG22	1:H:292:MSE:HE1	2.01	0.41
1:A:367:GLN:HG3	6:A:682:HOH:O	2.21	0.41
1:B:146:THR:O	1:B:150:LEU:HA	2.21	0.41
1:C:95:SER:OG	1:C:96:THR:N	2.54	0.41
1:E:149:LEU:HD11	1:E:351:GLY:HA3	2.03	0.41
1:A:163:HIS:HE1	1:A:187:GLY:O	2.03	0.41
1:D:6:PHE:HE1	1:D:182:GLN:NE2	2.18	0.41
1:A:112:ARG:NE	1:E:135:PRO:HG3	2.36	0.41
1:E:214:ASP:HB3	1:E:217:LEU:HB3	2.01	0.41
1:E:61:LEU:HA	1:E:61:LEU:HD23	1.89	0.41
1:F:253:ARG:HD2	3:G:404:GOL:O1	2.21	0.41
1:A:112:ARG:HG3	6:A:679:HOH:O	2.20	0.41
1:A:4:MSE:SE	6:D:602:HOH:O	2.89	0.41
1:C:150:LEU:HD22	1:C:175:PHE:HE2	1.83	0.41
1:C:373:LEU:O	1:C:377:LEU:HG	2.21	0.41
1:D:147:ASN:HA	1:D:148:PRO:HA	1.78	0.41
1:E:84:LEU:HD12	1:E:106:LEU:HB3	2.02	0.41
1:E:124:THR:O	1:E:126:GLU:N	2.54	0.41
1:F:365:ASP:H	1:G:8:THR:HG23	1.86	0.41
1:A:16:ARG:HH21	1:A:59:GLU:CD	2.22	0.41
1:C:277:PRO:O	1:C:288:VAL:HG11	2.21	0.41
1:D:163:HIS:HE2	1:D:189:ASP:CG	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:LEU:HA	1:G:280:PRO:HD3	1.89	0.41
1:H:121:ASP:OD2	1:H:123:THR:N	2.53	0.41
1:C:175:PHE:C	1:C:175:PHE:CD1	2.94	0.41
1:D:332:GLU:OE1	1:D:338:THR:HB	2.21	0.41
1:D:6:PHE:CE1	1:D:10:LEU:HD21	2.55	0.41
1:D:84:LEU:HD23	1:D:141:TRP:CZ3	2.55	0.41
1:F:254:GLN:HB3	1:F:297:ALA:CB	2.51	0.41
1:G:169:VAL:N	1:G:189:ASP:OD2	2.44	0.41
1:G:333:CYS:H	1:G:337:MSE:SE	2.53	0.41
1:G:43:ARG:NH2	1:G:55:GLU:OE1	2.54	0.41
1:B:241:ARG:HA	1:B:244:LEU:HD12	2.02	0.41
1:D:9:ARG:HH12	1:D:66:ARG:NE	2.19	0.41
1:E:109:LEU:O	1:E:113:GLN:HG2	2.20	0.41
1:E:134:GLU:HG3	1:E:135:PRO:HD2	2.02	0.41
1:E:213:ARG:HE	3:E:402:GOL:C2	2.34	0.41
1:F:197:LLP:HG3	1:F:197:LLP:H	1.68	0.41
1:A:342:LEU:HD13	1:A:346:ALA:CB	2.50	0.41
1:B:4:MSE:HE2	1:B:8:THR:HG22	2.02	0.41
1:C:51:ASN:HA	1:C:52:PRO:HD3	1.90	0.41
1:C:66:ARG:CZ	6:C:661:HOH:O	2.68	0.41
1:D:279:LEU:C	1:D:281:GLU:N	2.73	0.41
1:E:111:ALA:HA	1:E:115:VAL:O	2.20	0.41
1:E:146:THR:O	1:E:150:LEU:HA	2.19	0.41
1:E:41:GLU:HA	1:E:42:PRO:HD2	1.84	0.41
1:C:112:ARG:HD3	4:C:406:CL:CL	2.58	0.41
1:D:100:TYR:CG	1:D:101:ALA:N	2.89	0.41
1:D:98:ASP:O	6:D:560:HOH:O	2.22	0.41
1:G:347:ARG:O	1:G:351:GLY:N	2.53	0.41
1:G:96:THR:HA	1:G:120:ALA:O	2.20	0.41
1:E:4:MSE:HG3	1:E:8:THR:HB	2.03	0.41
1:H:276:TYR:CZ	1:H:295:PRO:HB2	2.56	0.41
1:B:336:LEU:C	1:B:337:MSE:SE	3.10	0.41
1:C:150:LEU:HD12	1:C:277:PRO:HD3	2.01	0.41
1:C:97:ASP:O	1:C:350:ARG:CZ	2.69	0.41
1:E:16:ARG:CZ	1:E:59:GLU:OE1	2.68	0.41
1:G:323:SER:H	2:G:401:MES:H82	1.86	0.41
1:A:100:TYR:O	1:A:104:ASP:N	2.51	0.41
1:C:13:GLY:HA3	6:C:536:HOH:O	2.20	0.41
1:C:279:LEU:HA	1:C:279:LEU:HD23	1.90	0.41
1:D:109:LEU:O	1:D:112:ARG:HB2	2.21	0.41
1:E:344:ALA:HA	1:E:347:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLU:HG2	6:B:652:HOH:O	2.21	0.41
1:C:320:CYS:SG	1:C:337:MSE:SE	3.29	0.41
1:E:28:ILE:HB	1:G:28:ILE:HB	2.03	0.41
1:B:371:GLU:HB3	1:B:375:ARG:NH2	2.36	0.41
1:C:203:ALA:HB1	1:D:33:THR:HG23	2.02	0.41
1:E:40:ASP:CB	6:E:666:HOH:O	2.68	0.41
1:G:91:GLN:HA	1:G:136:ASP:HB3	2.01	0.41
1:A:161:ARG:HA	1:A:161:ARG:HD3	1.84	0.41
1:B:279:LEU:O	6:B:556:HOH:O	2.21	0.41
1:F:94:VAL:HG11	1:F:131:ALA:HB1	2.03	0.41
1:G:276:TYR:OH	1:G:295:PRO:HG2	2.21	0.41
1:A:6:PHE:CE2	1:A:179:VAL:HG12	2.55	0.41
1:A:96:THR:HB	1:A:97:ASP:H	1.66	0.41
1:B:9:ARG:HG2	6:B:647:HOH:O	2.20	0.41
1:D:177:SER:HB3	6:D:566:HOH:O	2.21	0.41
1:D:52:PRO:O	1:D:56:GLU:HG3	2.21	0.41
1:E:43:ARG:HB3	1:E:44:TYR:CE2	2.55	0.41
1:G:96:THR:O	1:G:98:ASP:N	2.53	0.41
1:B:54:ARG:HG3	1:B:237:CYS:SG	2.61	0.41
1:E:142:ILE:HD11	1:E:158:VAL:HG11	2.02	0.41
1:F:127:GLY:O	1:F:131:ALA:HB2	2.21	0.41
1:G:4:MSE:HB3	1:G:9:ARG:HG2	2.02	0.41
1:A:145:PRO:HD2	1:A:175:PHE:CD1	2.56	0.41
1:A:282:HIS:HA	1:A:283:PRO:HD2	1.85	0.41
1:C:176:ALA:HB3	1:C:292:MSE:CE	2.51	0.41
1:D:94:VAL:CG2	1:D:134:GLU:HG3	2.50	0.41
1:H:281:GLU:HB2	6:H:652:HOH:O	2.21	0.41
1:C:233:GLY:N	1:C:236:ASP:OD1	2.54	0.41
1:C:284:GLN:O	1:C:288:VAL:HG23	2.21	0.41
1:D:328:HIS:O	1:D:330:LEU:HD13	2.21	0.41
1:E:213:ARG:NE	3:E:402:GOL:H2	2.36	0.41
1:E:54:ARG:HG3	1:E:72:VAL:CG2	2.51	0.41
1:F:6:PHE:HD1	1:F:9:ARG:NH1	2.19	0.41
1:G:235:LEU:HA	1:G:235:LEU:HD23	1.90	0.41
1:H:93:VAL:HG13	1:H:139:LEU:HB3	2.02	0.41
1:A:90:GLY:N	1:A:114:GLY:O	2.32	0.41
1:A:238:PHE:O	1:A:242:ARG:HB2	2.21	0.41
1:C:3:GLY:O	1:C:4:MSE:HG3	2.21	0.41
1:D:268:SER:HA	1:D:269:PRO:HD3	1.92	0.41
6:C:615:HOH:O	1:D:74:SER:HB3	2.21	0.41
1:E:276:TYR:HA	1:E:277:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:VAL:HG13	6:F:571:HOH:O	2.19	0.41
1:F:292:MSE:CE	1:F:295:PRO:HA	2.51	0.41
1:F:323:SER:H	2:F:401:MES:H72	1.86	0.41
1:B:262:VAL:HG12	1:B:266:ARG:HD2	2.03	0.41
1:F:118:ARG:CZ	1:F:134:GLU:OE2	2.68	0.41
1:F:264:ARG:HA	1:F:264:ARG:HD3	1.94	0.41
1:F:310:ARG:HA	1:F:313:ASP:OD1	2.21	0.41
1:F:5:ARG:NH1	1:G:368:ASP:OD1	2.41	0.41
1:A:33:THR:HG23	1:B:203:ALA:HB1	2.03	0.41
1:D:60:CYS:SG	1:D:244:LEU:HD13	2.60	0.41
1:F:254:GLN:HG2	1:F:361:VAL:O	2.21	0.41
1:G:126:GLU:CB	6:G:1482:HOH:O	2.69	0.41
1:G:342:LEU:HD23	1:G:342:LEU:HA	1.83	0.41
1:C:147:ASN:HA	1:C:148:PRO:HA	1.94	0.41
1:D:231:VAL:HG12	1:D:232:PRO:HD2	2.02	0.41
1:E:238:PHE:O	1:E:242:ARG:HB2	2.21	0.41
1:G:93:VAL:HB	1:G:117:VAL:HG13	2.03	0.41
1:A:131:ALA:C	1:A:133:ALA:H	2.22	0.41
1:B:60:CYS:O	1:B:64:LEU:HG	2.21	0.41
1:E:45:PHE:CZ	6:F:630:HOH:O	2.71	0.41
1:E:33:THR:HG22	1:F:203:ALA:HB1	2.03	0.41
1:E:27:PRO:HB2	1:G:27:PRO:HB2	2.03	0.41
1:G:34:TYR:HD2	1:G:45:PHE:O	2.04	0.41
1:E:281:GLU:OE1	1:E:281:GLU:N	2.48	0.41
1:E:36:ARG:O	1:E:42:PRO:HG3	2.21	0.41
1:E:113:GLN:HB3	1:F:113:GLN:OE1	2.20	0.41
4:E:404:GOL:C1	1:F:48:ARG:HH22	2.34	0.41
1:C:131:ALA:O	1:C:134:GLU:HB2	2.20	0.41
1:C:310:ARG:HA	1:C:310:ARG:NE	2.35	0.41
1:D:96:THR:OG1	1:D:98:ASP:OD2	2.17	0.41
1:E:47:GLY:HA2	1:E:50:GLU:O	2.20	0.41
1:F:213:ARG:HG3	6:F:663:HOH:O	2.21	0.41
1:H:21:THR:OG1	1:H:23:ASP:OD1	2.29	0.41
2:H:401:MES:H82	2:H:401:MES:H31	1.81	0.41
1:A:173:ASN:OD1	1:A:176:ALA:HB3	2.21	0.41
1:B:29:HIS:CD2	1:B:52:PRO:HB2	2.56	0.41
1:D:94:VAL:HA	1:D:118:ARG:O	2.21	0.41
1:E:156:ALA:O	1:E:160:ARG:HD3	2.20	0.41
1:E:214:ASP:CB	1:E:217:LEU:HB3	2.51	0.41
1:F:124:THR:HA	1:F:125:PRO:HD2	1.85	0.41
1:C:257:THR:HG21	1:C:369:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:ARG:HH11	1:D:367:GLN:NE2	2.19	0.41
1:F:179:VAL:HG21	1:F:251:VAL:HG21	2.01	0.41
1:G:36:ARG:CZ	1:G:45:PHE:CD1	3.04	0.41
1:B:95:SER:CB	1:B:141:TRP:HB3	2.50	0.41
1:C:186:LEU:HD11	1:C:291:GLN:HB2	2.02	0.41
1:C:51:ASN:HA	1:C:52:PRO:HD3	1.90	0.41
1:E:121:ASP:O	1:E:127:GLY:HA3	2.20	0.41
1:A:175:PHE:HB3	6:A:513:HOH:O	2.20	0.41
1:B:371:GLU:O	1:B:375:ARG:HG3	2.20	0.41
1:E:107:PHE:HB3	1:E:117:VAL:HG21	2.02	0.41
1:F:226:THR:HG22	6:F:544:HOH:O	2.21	0.41
1:F:4:MSE:HB2	1:F:9:ARG:HG2	2.03	0.41
1:A:35:GLU:O	1:A:39:GLN:NE2	2.37	0.41
1:A:97:ASP:C	1:A:99:VAL:N	2.74	0.41
1:B:43:ARG:HE	1:B:43:ARG:HB3	1.66	0.41
1:D:264:ARG:NH2	1:D:370:ALA:HB1	2.28	0.41
1:F:41:GLU:O	1:F:43:ARG:HG3	2.21	0.41
1:A:379:GLY:CA	6:A:651:HOH:O	2.65	0.41
1:A:50:GLU:HA	6:A:551:HOH:O	2.19	0.41
1:B:16:ARG:NE	1:B:56:GLU:OE1	2.54	0.41
1:D:9:ARG:NH2	6:D:626:HOH:O	2.37	0.41
1:E:144:THR:HA	1:E:145:PRO:C	2.41	0.41
1:F:103:THR:HG22	1:F:107:PHE:CZ	2.55	0.41
1:F:16:ARG:HD3	1:F:17:PRO:CD	2.51	0.41
1:H:215:ALA:O	1:H:218:HIS:HB3	2.21	0.41
1:A:94:VAL:HG22	1:A:118:ARG:HB3	2.02	0.41
1:B:152:VAL:H	1:B:284:GLN:HE21	1.68	0.41
1:D:142:ILE:O	1:D:171:VAL:HA	2.21	0.41
1:D:60:CYS:SG	1:D:244:LEU:HD13	2.61	0.41
1:F:338:THR:C	1:F:340:ARG:H	2.23	0.41
1:F:347:ARG:HB3	1:F:352:ILE:O	2.21	0.41
1:A:347:ARG:HG2	1:A:352:ILE:HD12	2.02	0.41
1:C:92:CYS:HA	1:C:116:ARG:O	2.21	0.41
1:D:336:LEU:HB2	1:D:337:MSE:HE2	2.03	0.41
1:H:318:PHE:CE2	1:H:329:SER:HB3	2.55	0.41
1:B:68:PRO:HG2	1:B:213:ARG:HA	2.02	0.41
1:E:163:HIS:O	6:E:607:HOH:O	2.22	0.41
1:H:100:TYR:HE1	2:H:401:MES:H81	1.85	0.41
3:B:407:GOL:C1	6:B:664:HOH:O	2.68	0.41
1:C:288:VAL:HG13	1:C:292:MSE:CE	2.51	0.41
1:D:284:GLN:O	1:D:288:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:MSE:CB	6:D:656:HOH:O	2.69	0.41
1:F:173:ASN:OD1	1:F:176:ALA:HB3	2.20	0.41
1:G:89:PRO:HD3	6:H:603:HOH:O	2.21	0.41
1:A:330:LEU:HB2	1:A:360:SER:HB3	2.02	0.41
1:C:83:LEU:HA	1:C:83:LEU:HD12	1.87	0.41
1:F:118:ARG:HD2	1:F:134:GLU:OE2	2.21	0.41
1:H:245:HIS:HE1	6:H:532:HOH:O	2.04	0.41
1:H:88:ARG:HB2	1:H:91:GLN:HG3	2.03	0.41
1:A:84:LEU:HD11	1:A:107:PHE:CE1	2.56	0.41
1:B:252:HIS:O	1:B:254:GLN:N	2.52	0.41
1:E:168:ARG:NH1	6:E:527:HOH:O	2.31	0.41
1:A:126:GLU:H	1:A:126:GLU:CD	2.25	0.40
1:C:354:GLU:HG2	1:C:354:GLU:H	1.55	0.40
1:D:116:ARG:HH12	1:D:135:PRO:HD2	1.85	0.40
1:E:16:ARG:HA	1:E:17:PRO:HD3	1.86	0.40
1:F:111:ALA:HA	1:F:115:VAL:O	2.21	0.40
1:D:268:SER:HA	1:D:269:PRO:HD3	1.94	0.40
1:F:98:ASP:HB2	1:F:146:THR:HB	2.02	0.40
1:A:127:GLY:O	6:A:673:HOH:O	2.21	0.40
1:G:147:ASN:ND2	1:G:147:ASN:C	2.74	0.40
1:G:336:LEU:HB3	1:G:337:MSE:SE	2.71	0.40
1:B:343:SER:C	1:B:345:GLU:H	2.24	0.40
1:F:176:ALA:HB2	1:F:292:MSE:HE1	2.02	0.40
1:B:99:VAL:HG13	1:B:103:THR:HB	2.02	0.40
1:B:4:MSE:O	1:B:9:ARG:NE	2.28	0.40
1:C:371:GLU:O	1:C:375:ARG:HD3	2.21	0.40
1:G:175:PHE:HB3	6:G:536:HOH:O	2.21	0.40
1:A:179:VAL:HG13	1:A:251:VAL:HG21	2.02	0.40
1:A:343:SER:HB2	6:A:648:HOH:O	2.21	0.40
1:B:29:HIS:CD2	1:B:52:PRO:HB2	2.56	0.40
1:C:6:PHE:O	1:C:9:ARG:HG2	2.21	0.40
1:C:313:ASP:HA	1:D:37:ARG:CD	2.51	0.40
1:D:95:SER:OG	1:D:96:THR:N	2.54	0.40
1:E:20:GLY:O	1:G:39:GLN:HG2	2.21	0.40
1:A:174:THR:HB	1:A:197:LLP:H2'2	2.03	0.40
1:B:143:GLU:HG3	1:B:172:ASP:HB3	2.03	0.40
1:B:16:ARG:HB3	1:B:16:ARG:HE	1.42	0.40
1:C:232:PRO:HB3	6:C:637:HOH:O	2.21	0.40
1:C:175:PHE:CZ	1:C:298:ILE:HB	2.56	0.40
1:F:164:GLU:HB2	6:F:678:HOH:O	2.21	0.40
1:B:58:GLU:OE1	6:B:588:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:GLN:O	1:E:116:ARG:HB2	2.21	0.40
1:G:281:GLU:CB	6:G:677:HOH:O	2.69	0.40
1:B:340:ARG:O	1:B:342:LEU:N	2.55	0.40
1:B:94:VAL:HG11	1:B:131:ALA:HB1	2.02	0.40
1:C:367:GLN:O	1:C:371:GLU:HG3	2.21	0.40
1:D:134:GLU:HA	1:D:135:PRO:HD3	1.89	0.40
1:E:287:VAL:HG23	6:E:623:HOH:O	2.21	0.40
1:B:89:PRO:HD3	6:B:610:HOH:O	2.21	0.40
2:E:401:MES:O3S	6:E:562:HOH:O	2.21	0.40
1:G:142:ILE:O	1:G:171:VAL:HA	2.21	0.40
1:G:16:ARG:HB3	1:G:16:ARG:HE	1.68	0.40
1:A:354:GLU:HG2	6:A:616:HOH:O	2.19	0.40
1:D:253:ARG:NH2	1:D:256:ALA:HB3	2.35	0.40
1:E:111:ALA:C	1:E:114:GLY:H	2.24	0.40
1:E:34:TYR:CD2	1:E:44:TYR:HB3	2.56	0.40
1:E:365:ASP:OD2	1:H:5:ARG:HB2	2.21	0.40
1:A:175:PHE:C	1:A:175:PHE:CD1	2.95	0.40
1:C:340:ARG:NH2	6:C:502:HOH:O	2.55	0.40
1:H:140:VAL:HB	1:H:169:VAL:HG22	2.02	0.40
1:G:242:ARG:HA	1:G:245:HIS:HD2	1.85	0.40
1:B:132:LEU:CD1	1:B:161:ARG:HB3	2.52	0.40
1:D:6:PHE:O	1:D:10:LEU:HG	2.22	0.40
1:D:175:PHE:HB3	6:D:515:HOH:O	2.21	0.40
1:D:20:GLY:O	6:D:672:HOH:O	2.22	0.40
2:H:401:MES:H32	2:H:401:MES:H82	1.36	0.40
1:E:292:MSE:HG3	1:E:294:ALA:O	2.20	0.40
1:B:255:VAL:O	1:B:259:ARG:HD2	2.21	0.40
1:C:332:GLU:OE2	1:C:338:THR:HG23	2.21	0.40
1:C:36:ARG:HH22	1:D:309:GLU:HG3	1.86	0.40
1:H:147:ASN:HA	1:H:148:PRO:HA	1.85	0.40
1:E:242:ARG:HD3	1:H:242:ARG:HH11	1.86	0.40
1:A:175:PHE:C	1:A:175:PHE:HD1	2.24	0.40
1:A:350:ARG:O	1:A:352:ILE:HG13	2.21	0.40
1:F:96:THR:HB	1:F:98:ASP:HB2	2.03	0.40
1:A:118:ARG:O	1:A:118:ARG:HG3	2.20	0.40
1:C:321:GLY:O	1:C:332:GLU:HB3	2.20	0.40
1:H:110:ALA:HB1	1:H:115:VAL:HB	2.03	0.40
1:H:94:VAL:HG23	1:H:137:LEU:HD13	2.02	0.40
1:D:107:PHE:HB3	1:D:117:VAL:HG21	2.03	0.40
1:D:329:SER:O	1:D:330:LEU:HD23	2.21	0.40
1:H:149:LEU:HB2	6:H:578:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:SER:OG	1:B:99:VAL:HG11	2.21	0.40
1:E:291:GLN:HE21	1:E:292:MSE:HE2	1.86	0.40
1:F:157:GLU:HA	1:F:160:ARG:HH11	1.86	0.40
1:G:32:THR:OG1	1:G:33:THR:HG22	2.22	0.40
1:G:3:GLY:C	1:G:4:MSE:SE	3.09	0.40
1:D:132:LEU:HD22	1:D:162:ALA:HA	2.03	0.40
1:E:152:VAL:HG21	1:E:288:VAL:HG22	2.04	0.40
1:E:249:LEU:HD23	1:E:249:LEU:HA	1.94	0.40
1:G:37:ARG:HD2	1:H:313:ASP:HA	2.03	0.40
1:B:168:ARG:HA	1:B:189:ASP:OD2	2.22	0.40
1:B:276:TYR:HA	1:B:277:PRO:HD3	1.94	0.40
1:B:9:ARG:NH2	1:B:66:ARG:HG2	2.36	0.40
1:C:369:LEU:HD23	1:C:369:LEU:HA	1.94	0.40
1:B:368:ASP:OD1	1:C:3:GLY:N	2.55	0.40
1:D:199:ILE:HG23	1:D:244:LEU:HD21	2.03	0.40
1:D:339:HIS:HB3	1:D:352:ILE:HD13	2.02	0.40
1:F:11:VAL:HA	1:F:245:HIS:ND1	2.37	0.40
1:F:288:VAL:HA	1:F:292:MSE:CE	2.50	0.40
3:G:403:GOL:H31	1:H:102:GLY:HA2	2.03	0.40
1:B:264:ARG:CZ	1:B:370:ALA:HB1	2.52	0.40
1:F:104:ASP:HA	1:F:107:PHE:CD2	2.57	0.40
1:F:337:MSE:HB3	1:F:337:MSE:HE3	1.98	0.40
1:H:110:ALA:O	1:H:115:VAL:HB	2.22	0.40
1:A:340:ARG:HA	1:A:347:ARG:NH1	2.36	0.40
1:D:180:LEU:HA	1:D:293:SER:OG	2.21	0.40
1:E:96:THR:CG2	1:E:143:GLU:H	2.33	0.40
1:F:308:ALA:O	1:F:312:LEU:HG	2.22	0.40
1:G:312:LEU:CD1	1:G:337:MSE:HE1	2.49	0.40
1:H:101:ALA:O	1:H:105:GLY:N	2.54	0.40
1:H:111:ALA:HA	1:H:115:VAL:O	2.22	0.40
1:A:157:GLU:O	1:A:161:ARG:HG2	2.21	0.40
1:C:191:SER:HB3	1:C:193:TYR:CE2	2.56	0.40
2:C:401:MES:H32	6:C:678:HOH:O	2.21	0.40
1:G:262:VAL:HG11	1:G:279:LEU:HD21	2.02	0.40
1:E:112:ARG:NH2	6:E:668:HOH:O	2.53	0.40
1:F:147:ASN:C	6:F:677:HOH:O	2.59	0.40
1:F:319:THR:O	1:F:330:LEU:HA	2.21	0.40
1:H:29:HIS:CD2	1:H:52:PRO:HB2	2.56	0.40
1:A:35:GLU:HB2	1:B:319:THR:HG23	2.03	0.40
1:B:95:SER:HB2	1:B:141:TRP:HB3	2.03	0.40
1:C:92:CYS:HG	1:C:134:GLU:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:TYR:CE1	2:D:401:MES:H81	2.56	0.40
1:G:43:ARG:HD3	1:G:44:TYR:CZ	2.57	0.40
1:H:214:ASP:HB3	1:H:217:LEU:HB3	2.03	0.40
1:D:150:LEU:HD22	1:D:175:PHE:CZ	2.56	0.40
1:F:20:GLY:H	1:H:39:GLN:HA	1.86	0.40
1:F:288:VAL:HG22	1:F:292:MSE:HE3	2.02	0.40
1:F:80:ALA:O	1:F:84:LEU:HB2	2.21	0.40
1:G:160:ARG:HG3	1:G:161:ARG:NE	2.36	0.40
1:H:88:ARG:O	1:H:115:VAL:HG22	2.21	0.40
1:A:16:ARG:HD3	1:A:16:ARG:HA	1.96	0.40
1:B:214:ASP:HB2	6:B:517:HOH:O	2.21	0.40
1:B:282:HIS:CG	1:B:283:PRO:HD2	2.55	0.40
1:C:100:TYR:HA	6:C:655:HOH:O	2.21	0.40
1:C:137:LEU:HD12	1:C:137:LEU:HA	1.95	0.40
1:D:178:PRO:HD3	1:D:193:TYR:CE1	2.56	0.40
1:E:159:SER:HA	1:E:169:VAL:HG21	2.04	0.40
1:E:289:LYS:HE3	1:E:289:LYS:HB3	1.86	0.40
1:F:146:THR:O	1:F:150:LEU:HA	2.22	0.40
1:F:5:ARG:O	1:F:9:ARG:HG3	2.22	0.40
1:A:16:ARG:HA	1:A:17:PRO:HD2	1.67	0.40
1:A:239:LEU:HD22	1:D:242:ARG:CZ	2.51	0.40
1:A:259:ARG:HD3	6:A:572:HOH:O	2.21	0.40
1:B:262:VAL:HG11	1:B:279:LEU:HD21	2.02	0.40
1:B:337:MSE:HA	1:B:340:ARG:HB2	2.03	0.40
1:B:340:ARG:NE	6:B:643:HOH:O	2.51	0.40
1:B:5:ARG:HH12	1:C:371:GLU:CD	2.24	0.40
1:C:16:ARG:NE	6:C:679:HOH:O	2.49	0.40
1:D:146:THR:OG1	1:D:151:THR:N	2.52	0.40
1:D:5:ARG:C	1:D:6:PHE:O	2.59	0.40
1:B:137:LEU:HB3	1:B:165:ARG:HH11	1.87	0.40
1:B:343:SER:C	1:B:347:ARG:HE	2.24	0.40
1:G:333:CYS:O	1:G:337:MSE:HB2	2.22	0.40
1:H:108:ASP:O	1:H:111:ALA:N	2.54	0.40
1:C:251:VAL:HG22	6:C:568:HOH:O	2.21	0.40
1:C:14:GLY:HA2	1:C:59:GLU:OE2	2.22	0.40
1:F:15:ARG:HG3	1:F:26:PRO:CG	2.51	0.40
1:A:240:VAL:O	1:A:244:LEU:HD23	2.21	0.40
1:B:197:LLP:H4'1	2:B:401:MES:H71	2.02	0.40
1:B:88:ARG:O	1:B:91:GLN:HB2	2.21	0.40
1:C:205:VAL:HG23	1:C:236:ASP:OD2	2.22	0.40
1:C:337:MSE:HB3	1:C:337:MSE:HE3	1.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:HIS:HE1	1:F:187:GLY:O	2.04	0.40
1:G:279:LEU:HD23	1:G:279:LEU:HA	1.92	0.40
1:H:19:ALA:O	1:H:21:THR:N	2.54	0.40
1:G:36:ARG:HG2	1:H:320:CYS:O	2.22	0.40
1:A:84:LEU:HG	1:A:141:TRP:HZ3	1.86	0.40
1:A:35:GLU:OE2	1:A:37:ARG:N	2.47	0.40
1:A:100:TYR:CE1	2:A:401:MES:H81	2.56	0.40
1:B:41:GLU:HA	1:B:42:PRO:HD2	1.91	0.40
1:E:285:HIS:O	1:E:288:VAL:HB	2.21	0.40
1:G:116:ARG:NH1	1:G:134:GLU:OE1	2.54	0.40
1:B:118:ARG:NH2	1:B:131:ALA:HA	2.36	0.40
1:C:333:CYS:HA	1:C:334:PRO:HD2	1.93	0.40
1:E:152:VAL:HG21	1:E:288:VAL:HG22	2.03	0.40
1:G:116:ARG:NH1	1:G:134:GLU:HG2	2.37	0.40
1:A:132:LEU:HD12	1:A:137:LEU:CD2	2.52	0.40
1:A:340:ARG:HB3	1:A:341:PRO:HD3	2.02	0.40
1:B:5:ARG:NH1	1:C:371:GLU:OE2	2.54	0.40
1:C:339:HIS:O	1:C:342:LEU:HB2	2.22	0.40
1:D:16:ARG:HA	1:D:17:PRO:HD2	1.72	0.40
1:H:115:VAL:HG12	1:H:117:VAL:HG23	2.03	0.40
1:H:183:PRO:HA	1:H:186:LEU:HD12	2.03	0.40
1:H:41:GLU:O	1:H:43:ARG:N	2.54	0.40
1:H:5:ARG:HB3	1:H:6:PHE:H	1.76	0.40
1:A:178:PRO:HD3	1:A:193:TYR:CE1	2.55	0.40
1:A:36:ARG:HE	1:A:45:PHE:HD1	1.69	0.40
1:A:41:GLU:HA	1:A:42:PRO:HD3	1.91	0.40
1:B:198:SER:OG	6:B:532:HOH:O	2.22	0.40
1:B:365:ASP:CG	1:C:5:ARG:HB2	2.42	0.40
1:B:365:ASP:HB3	1:B:368:ASP:OD2	2.21	0.40
1:D:126:GLU:HG3	1:D:126:GLU:H	1.52	0.40
1:D:347:ARG:HB3	1:D:352:ILE:O	2.21	0.40
1:G:16:ARG:HG2	1:G:16:ARG:H	1.74	0.40
1:C:134:GLU:HG3	1:C:135:PRO:HD2	2.04	0.40
1:C:175:PHE:C	1:C:175:PHE:CD1	2.95	0.40
1:D:17:PRO:HB2	1:D:18:SER:H	1.76	0.40
1:D:32:THR:OG1	1:D:33:THR:HG22	2.21	0.40
1:F:102:GLY:HA2	3:F:402:GOL:H11	2.03	0.40
1:G:213:ARG:NE	3:G:402:GOL:O2	2.47	0.40
1:B:173:ASN:HB3	1:B:193:TYR:CE1	2.56	0.40
1:C:84:LEU:HA	1:C:84:LEU:HD13	1.88	0.40
1:G:290:ALA:O	3:G:404:GOL:H31	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:334:PRO:O	1:G:339:HIS:N	2.46	0.40
1:H:199:ILE:HG23	1:H:244:LEU:HD21	2.02	0.40
1:C:160:ARG:HG2	1:C:161:ARG:CZ	2.52	0.40
1:F:42:PRO:O	1:F:43:ARG:HB2	2.22	0.40
1:H:6:PHE:HE1	1:H:64:LEU:HB3	1.87	0.40
1:B:94:VAL:HG21	1:B:131:ALA:O	2.22	0.40
1:C:92:CYS:HA	1:C:116:ARG:O	2.22	0.40
1:E:365:ASP:O	1:E:368:ASP:HB2	2.22	0.40
1:F:94:VAL:HG22	1:F:118:ARG:HG2	2.03	0.40
1:F:276:TYR:HA	1:F:277:PRO:HD3	1.90	0.40
1:H:185:ALA:HA	3:H:402:GOL:H11	2.03	0.40
1:C:5:ARG:HA	1:C:9:ARG:HH11	1.86	0.40
1:D:97:ASP:N	1:D:119:TYR:HB3	2.36	0.40
1:E:312:LEU:O	1:F:37:ARG:NH2	2.54	0.40
1:F:38:ALA:C	6:F:668:HOH:O	2.46	0.40
1:C:160:ARG:O	1:C:164:GLU:HG3	2.21	0.40
1:C:173:ASN:HB3	1:C:193:TYR:CE1	2.56	0.40
1:C:34:TYR:OH	6:C:585:HOH:O	2.21	0.40
1:C:84:LEU:HD13	1:C:84:LEU:HA	1.83	0.40
1:D:254:GLN:HB3	1:D:297:ALA:HB2	2.03	0.40
1:C:35:GLU:OE1	1:D:319:THR:HG23	2.21	0.40
1:F:264:ARG:HG2	6:F:616:HOH:O	2.22	0.40
1:A:100:TYR:CE2	1:A:102:GLY:HA3	2.57	0.40
1:A:118:ARG:HD3	1:A:118:ARG:HH21	1.77	0.40
1:A:126:GLU:CD	1:A:126:GLU:H	2.25	0.40
1:A:338:THR:HG23	2:A:401:MES:C3	2.52	0.40
1:A:97:ASP:HB2	1:A:98:ASP:OD1	2.22	0.40
1:B:111:ALA:HB3	6:B:608:HOH:O	2.22	0.40
1:C:197:LLP:C4'	2:C:401:MES:H71	2.52	0.40
1:D:146:THR:O	1:D:150:LEU:HA	2.22	0.40
1:A:113:GLN:HE21	1:B:113:GLN:NE2	2.20	0.40
1:A:368:ASP:OD1	1:D:5:ARG:NH1	2.40	0.40
1:E:62:ALA:HB1	1:E:67:ALA:O	2.21	0.40
1:B:112:ARG:HG2	6:B:658:HOH:O	2.20	0.40
1:A:322:VAL:HG11	4:B:409:CL:CL	2.59	0.40
1:C:42:PRO:HB2	1:C:45:PHE:CZ	2.57	0.40
1:D:105:GLY:O	1:D:108:ASP:HB3	2.21	0.40
1:D:9:ARG:HB3	6:D:519:HOH:O	2.22	0.40
1:E:157:GLU:OE1	1:E:160:ARG:NH1	2.41	0.40
1:E:367:GLN:HA	1:E:367:GLN:OE1	2.21	0.40
1:F:320:CYS:HA	1:F:331:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:ARG:O	1:F:9:ARG:HG3	2.22	0.40
1:H:160:ARG:HB3	1:H:161:ARG:NH2	2.36	0.40
1:A:276:TYR:OH	1:A:296:GLY:O	2.23	0.40
1:A:92:CYS:HA	1:A:116:ARG:O	2.22	0.40
1:B:89:PRO:HG3	1:B:113:GLN:O	2.22	0.40
1:C:335:ALA:HB2	1:C:354:GLU:HA	2.03	0.40
1:E:145:PRO:HB2	1:E:175:PHE:CE2	2.57	0.40
1:E:176:ALA:HB1	1:E:180:LEU:HB2	2.03	0.40
1:F:188:ALA:O	1:F:213:ARG:NH1	2.55	0.40
1:F:340:ARG:HA	1:F:347:ARG:NH1	2.36	0.40
1:F:4:MSE:SE	1:F:13:GLY:HA2	2.71	0.40
1:F:9:ARG:HB3	6:F:527:HOH:O	2.21	0.40
1:H:144:THR:HG1	1:H:152:VAL:HG13	1.87	0.40
1:E:21:THR:HG22	1:G:44:TYR:CE2	2.56	0.40
1:F:38:ALA:HB1	1:H:18:SER:O	2.22	0.40
1:B:95:SER:HB2	1:B:141:TRP:HB3	2.04	0.40
1:C:92:CYS:SG	1:C:93:VAL:N	2.94	0.40
1:F:332:GLU:OE2	1:F:334:PRO:HA	2.22	0.40
1:A:139:LEU:HD12	1:A:168:ARG:O	2.21	0.40
1:B:84:LEU:HD11	1:B:107:PHE:CD1	2.57	0.40
1:D:175:PHE:C	1:D:175:PHE:CD1	2.95	0.40
1:F:49:GLY:HA3	1:F:50:GLU:OE2	2.21	0.40
1:G:264:ARG:HD2	1:G:370:ALA:HB1	2.03	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	1-A	373/384 (97%)	347 (93%)	20 (5%)	6 (2%)	<b>11</b> <b>5</b>
1	1-B	375/384 (98%)	350 (93%)	19 (5%)	6 (2%)	<b>11</b> <b>5</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-C	376/384 (98%)	346 (92%)	23 (6%)	7 (2%)	9	4
1	1-D	373/384 (97%)	338 (91%)	23 (6%)	12 (3%)	5	1
1	1-E	373/384 (97%)	347 (93%)	20 (5%)	6 (2%)	11	5
1	1-F	374/384 (97%)	352 (94%)	18 (5%)	4 (1%)	17	11
1	1-G	375/384 (98%)	341 (91%)	27 (7%)	7 (2%)	9	4
1	1-H	375/384 (98%)	341 (91%)	28 (8%)	6 (2%)	11	5
1	2-A	373/384 (97%)	348 (93%)	21 (6%)	4 (1%)	17	11
1	2-B	375/384 (98%)	345 (92%)	24 (6%)	6 (2%)	11	5
1	2-C	376/384 (98%)	348 (93%)	24 (6%)	4 (1%)	17	11
1	2-D	373/384 (97%)	350 (94%)	15 (4%)	8 (2%)	8	3
1	2-E	373/384 (97%)	350 (94%)	17 (5%)	6 (2%)	11	5
1	2-F	374/384 (97%)	345 (92%)	25 (7%)	4 (1%)	17	11
1	2-G	375/384 (98%)	344 (92%)	28 (8%)	3 (1%)	22	17
1	2-H	375/384 (98%)	345 (92%)	24 (6%)	6 (2%)	11	5
1	3-A	373/384 (97%)	341 (91%)	28 (8%)	4 (1%)	17	11
1	3-B	375/384 (98%)	347 (92%)	20 (5%)	8 (2%)	8	3
1	3-C	376/384 (98%)	341 (91%)	30 (8%)	5 (1%)	14	8
1	3-D	373/384 (97%)	342 (92%)	23 (6%)	8 (2%)	8	3
1	3-E	373/384 (97%)	345 (92%)	19 (5%)	9 (2%)	7	2
1	3-F	374/384 (97%)	346 (92%)	17 (4%)	11 (3%)	5	2
1	3-G	375/384 (98%)	339 (90%)	31 (8%)	5 (1%)	14	8
1	3-H	375/384 (98%)	346 (92%)	21 (6%)	8 (2%)	8	3
1	4-A	373/384 (97%)	348 (93%)	21 (6%)	4 (1%)	17	11
1	4-B	375/384 (98%)	350 (93%)	18 (5%)	7 (2%)	9	4
1	4-C	376/384 (98%)	353 (94%)	17 (4%)	6 (2%)	11	5
1	4-D	373/384 (97%)	342 (92%)	25 (7%)	6 (2%)	11	5
1	4-E	373/384 (97%)	347 (93%)	18 (5%)	8 (2%)	8	3
1	4-F	374/384 (97%)	340 (91%)	24 (6%)	10 (3%)	6	2
1	4-G	375/384 (98%)	344 (92%)	24 (6%)	7 (2%)	9	4
1	4-H	375/384 (98%)	348 (93%)	24 (6%)	3 (1%)	22	17
1	5-A	373/384 (97%)	333 (89%)	32 (9%)	8 (2%)	8	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5-B	375/384 (98%)	352 (94%)	19 (5%)	4 (1%)	17	11
1	5-C	376/384 (98%)	347 (92%)	28 (7%)	1 (0%)	44	44
1	5-D	373/384 (97%)	345 (92%)	21 (6%)	7 (2%)	9	4
1	5-E	373/384 (97%)	343 (92%)	17 (5%)	13 (4%)	4	1
1	5-F	374/384 (97%)	349 (93%)	18 (5%)	7 (2%)	9	4
1	5-G	375/384 (98%)	339 (90%)	29 (8%)	7 (2%)	9	4
1	5-H	375/384 (98%)	345 (92%)	25 (7%)	5 (1%)	14	8
1	6-A	373/384 (97%)	342 (92%)	25 (7%)	6 (2%)	11	5
1	6-B	375/384 (98%)	343 (92%)	29 (8%)	3 (1%)	22	17
1	6-C	376/384 (98%)	345 (92%)	28 (7%)	3 (1%)	22	17
1	6-D	373/384 (97%)	340 (91%)	22 (6%)	11 (3%)	5	2
1	6-E	373/384 (97%)	351 (94%)	17 (5%)	5 (1%)	14	8
1	6-F	374/384 (97%)	347 (93%)	24 (6%)	3 (1%)	22	17
1	6-G	375/384 (98%)	351 (94%)	20 (5%)	4 (1%)	17	11
1	6-H	375/384 (98%)	347 (92%)	23 (6%)	5 (1%)	14	8
1	7-A	373/384 (97%)	345 (92%)	22 (6%)	6 (2%)	11	5
1	7-B	375/384 (98%)	349 (93%)	22 (6%)	4 (1%)	17	11
1	7-C	376/384 (98%)	340 (90%)	28 (7%)	8 (2%)	8	3
1	7-D	373/384 (97%)	343 (92%)	24 (6%)	6 (2%)	11	5
1	7-E	373/384 (97%)	344 (92%)	24 (6%)	5 (1%)	14	8
1	7-F	374/384 (97%)	344 (92%)	25 (7%)	5 (1%)	14	8
1	7-G	375/384 (98%)	339 (90%)	30 (8%)	6 (2%)	11	5
1	7-H	375/384 (98%)	349 (93%)	23 (6%)	3 (1%)	22	17
1	8-A	373/384 (97%)	344 (92%)	23 (6%)	6 (2%)	11	5
1	8-B	375/384 (98%)	347 (92%)	23 (6%)	5 (1%)	14	8
1	8-C	376/384 (98%)	347 (92%)	23 (6%)	6 (2%)	11	5
1	8-D	373/384 (97%)	345 (92%)	21 (6%)	7 (2%)	9	4
1	8-E	373/384 (97%)	353 (95%)	15 (4%)	5 (1%)	14	8
1	8-F	374/384 (97%)	341 (91%)	29 (8%)	4 (1%)	17	11
1	8-G	375/384 (98%)	347 (92%)	22 (6%)	6 (2%)	11	5
1	8-H	375/384 (98%)	346 (92%)	25 (7%)	4 (1%)	17	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-A	373/384 (97%)	344 (92%)	18 (5%)	11 (3%)	5	2
1	9-B	375/384 (98%)	345 (92%)	25 (7%)	5 (1%)	14	8
1	9-C	376/384 (98%)	349 (93%)	26 (7%)	1 (0%)	44	44
1	9-D	373/384 (97%)	335 (90%)	32 (9%)	6 (2%)	11	5
1	9-E	373/384 (97%)	342 (92%)	20 (5%)	11 (3%)	5	2
1	9-F	374/384 (97%)	351 (94%)	19 (5%)	4 (1%)	17	11
1	9-G	375/384 (98%)	347 (92%)	24 (6%)	4 (1%)	17	11
1	9-H	375/384 (98%)	350 (93%)	23 (6%)	2 (0%)	32	28
1	10-A	373/384 (97%)	343 (92%)	25 (7%)	5 (1%)	14	8
1	10-B	375/384 (98%)	342 (91%)	27 (7%)	6 (2%)	11	5
1	10-C	376/384 (98%)	340 (90%)	29 (8%)	7 (2%)	9	4
1	10-D	373/384 (97%)	345 (92%)	16 (4%)	12 (3%)	5	1
1	10-E	373/384 (97%)	346 (93%)	20 (5%)	7 (2%)	9	4
1	10-F	374/384 (97%)	347 (93%)	17 (4%)	10 (3%)	6	2
1	10-G	375/384 (98%)	341 (91%)	25 (7%)	9 (2%)	7	2
1	10-H	375/384 (98%)	349 (93%)	23 (6%)	3 (1%)	22	17
All	All	29940/30720 (98%)	27614 (92%)	1841 (6%)	485 (2%)	11	5

All (485) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	17	PRO
1	1-A	40	ASP
1	1-A	122	LEU
1	1-B	15	ARG
1	1-B	17	PRO
1	1-B	39	GLN
1	1-D	19	ALA
1	1-D	39	GLN
1	1-D	40	ASP
1	1-D	122	LEU
1	1-D	339	HIS
1	1-E	40	ASP
1	1-E	337	MSE
1	1-F	36	ARG
1	1-G	337	MSE

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Mol	Chain	Res	Type
1	1-H	6	PHE
1	1-H	40	ASP
1	1-H	347	ARG
1	2-B	16	ARG
1	2-B	97	ASP
1	2-B	341	PRO
1	2-C	342	LEU
1	2-D	40	ASP
1	2-D	347	ARG
1	2-E	341	PRO
1	3-A	40	ASP
1	3-B	16	ARG
1	3-B	17	PRO
1	3-B	132	LEU
1	3-D	19	ALA
1	3-D	39	GLN
1	3-D	323	SER
1	3-D	348	ALA
1	3-E	36	ARG
1	3-E	37	ARG
1	3-E	40	ASP
1	3-E	97	ASP
1	3-E	343	SER
1	3-F	18	SER
1	3-F	40	ASP
1	3-F	42	PRO
1	3-F	342	LEU
1	3-G	19	ALA
1	3-G	344	ALA
1	3-H	16	ARG
1	3-H	19	ALA
1	3-H	42	PRO
1	3-H	343	SER
1	3-H	344	ALA
1	4-A	5	ARG
1	4-A	6	PHE
1	4-A	323	SER
1	4-B	17	PRO
1	4-B	18	SER
1	4-C	16	ARG
1	4-C	323	SER
1	4-C	342	LEU

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Mol	Chain	Res	Type
1	4-D	6	PHE
1	4-D	18	SER
1	4-D	352	ILE
1	4-E	131	ALA
1	4-E	132	LEU
1	4-E	323	SER
1	4-E	346	ALA
1	4-F	36	ARG
1	4-F	338	THR
1	4-F	342	LEU
1	4-G	131	ALA
1	4-G	132	LEU
1	4-G	323	SER
1	4-G	348	ALA
1	4-G	349	ARG
1	4-H	98	ASP
1	5-A	16	ARG
1	5-A	17	PRO
1	5-A	334	PRO
1	5-A	341	PRO
1	5-B	322	VAL
1	5-B	323	SER
1	5-D	17	PRO
1	5-D	18	SER
1	5-D	41	GLU
1	5-D	295	PRO
1	5-D	338	THR
1	5-D	378	ALA
1	5-E	4	MSE
1	5-E	16	ARG
1	5-E	37	ARG
1	5-E	38	ALA
1	5-E	41	GLU
1	5-E	130	ALA
1	5-F	40	ASP
1	5-F	126	GLU
1	5-F	378	ALA
1	5-G	131	ALA
1	5-G	132	LEU
1	5-G	133	ALA
1	5-H	6	PHE
1	5-H	42	PRO

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Mol	Chain	Res	Type
1	6-A	40	ASP
1	6-B	98	ASP
1	6-C	339	HIS
1	6-D	19	ALA
1	6-D	37	ARG
1	6-D	97	ASP
1	6-D	351	GLY
1	6-E	342	LEU
1	6-E	343	SER
1	6-E	346	ALA
1	6-G	323	SER
1	6-H	322	VAL
1	7-B	20	GLY
1	7-C	21	THR
1	7-C	39	GLN
1	7-C	40	ASP
1	7-D	323	SER
1	7-E	295	PRO
1	7-E	377	LEU
1	7-F	21	THR
1	7-G	17	PRO
1	7-G	18	SER
1	7-G	295	PRO
1	8-C	40	ASP
1	8-C	343	SER
1	8-C	346	ALA
1	8-D	18	SER
1	8-D	42	PRO
1	8-D	342	LEU
1	8-D	343	SER
1	8-E	323	SER
1	8-G	20	GLY
1	8-G	338	THR
1	8-G	343	SER
1	8-H	4	MSE
1	8-H	38	ALA
1	8-H	323	SER
1	9-A	98	ASP
1	9-A	131	ALA
1	9-B	37	ARG
1	9-C	119	TYR
1	9-D	17	PRO

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Mol	Chain	Res	Type
1	9-D	43	ARG
1	9-D	98	ASP
1	9-D	343	SER
1	9-D	347	ARG
1	9-E	17	PRO
1	9-E	18	SER
1	9-E	42	PRO
1	9-E	97	ASP
1	9-E	98	ASP
1	9-E	355	SER
1	9-F	344	ALA
1	9-G	337	MSE
1	9-H	40	ASP
1	10-A	17	PRO
1	10-A	281	GLU
1	10-B	18	SER
1	10-C	16	ARG
1	10-C	17	PRO
1	10-C	132	LEU
1	10-D	6	PHE
1	10-D	7	GLY
1	10-D	323	SER
1	10-D	347	ARG
1	10-E	41	GLU
1	10-E	323	SER
1	10-F	4	MSE
1	10-F	42	PRO
1	10-F	344	ALA
1	10-G	131	ALA
1	10-G	132	LEU
1	10-G	295	PRO
1	10-H	97	ASP
1	1-A	5	ARG
1	1-B	41	GLU
1	1-B	346	ALA
1	1-D	37	ARG
1	1-D	338	THR
1	1-E	19	ALA
1	1-E	43	ARG
1	1-E	126	GLU
1	1-F	37	ARG
1	1-G	99	VAL

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Mol	Chain	Res	Type
1	1-G	132	LEU
1	2-D	41	GLU
1	2-D	42	PRO
1	2-D	323	SER
1	2-D	346	ALA
1	2-E	97	ASP
1	2-E	346	ALA
1	2-F	37	ARG
1	2-H	19	ALA
1	2-H	42	PRO
1	2-H	97	ASP
1	2-H	323	SER
1	3-C	44	TYR
1	3-E	346	ALA
1	3-F	343	SER
1	3-F	349	ARG
1	3-G	5	ARG
1	4-B	16	ARG
1	4-C	20	GLY
1	4-C	42	PRO
1	4-D	323	SER
1	4-E	19	ALA
1	4-E	345	GLU
1	4-F	43	ARG
1	4-G	97	ASP
1	4-G	338	THR
1	4-H	323	SER
1	4-H	379	GLY
1	5-A	38	ALA
1	5-A	132	LEU
1	5-B	290	ALA
1	5-C	96	THR
1	5-E	40	ASP
1	5-E	346	ALA
1	5-G	323	SER
1	5-H	323	SER
1	6-B	96	THR
1	6-D	36	ARG
1	6-D	349	ARG
1	6-E	20	GLY
1	6-E	97	ASP
1	6-G	122	LEU

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Mol	Chain	Res	Type
1	6-H	37	ARG
1	7-A	99	VAL
1	7-B	5	ARG
1	7-D	19	ALA
1	7-F	322	VAL
1	7-G	37	ARG
1	7-H	379	GLY
1	8-A	39	GLN
1	8-B	100	TYR
1	8-B	345	GLU
1	8-B	351	GLY
1	8-C	20	GLY
1	8-D	17	PRO
1	8-E	40	ASP
1	8-E	42	PRO
1	8-F	98	ASP
1	8-F	344	ALA
1	8-H	5	ARG
1	9-A	128	ILE
1	9-A	343	SER
1	9-D	352	ILE
1	9-E	19	ALA
1	9-E	323	SER
1	9-G	101	ALA
1	9-H	343	SER
1	10-A	18	SER
1	10-A	20	GLY
1	10-B	137	LEU
1	10-B	343	SER
1	10-C	119	TYR
1	10-D	17	PRO
1	10-F	17	PRO
1	10-F	43	ARG
1	10-F	338	THR
1	10-G	8	THR
1	10-H	40	ASP
1	10-H	98	ASP
1	1-C	17	PRO
1	1-C	19	ALA
1	1-C	339	HIS
1	1-C	342	LEU
1	1-D	343	SER

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Mol	Chain	Res	Type
1	1-G	20	GLY
1	2-A	42	PRO
1	2-A	98	ASP
1	2-A	323	SER
1	2-B	137	LEU
1	2-B	338	THR
1	2-C	40	ASP
1	2-C	119	TYR
1	2-C	349	ARG
1	2-D	97	ASP
1	2-D	337	MSE
1	2-E	340	ARG
1	2-E	351	GLY
1	2-G	43	ARG
1	2-G	323	SER
1	3-A	342	LEU
1	3-B	131	ALA
1	3-B	341	PRO
1	3-C	379	GLY
1	3-F	121	ASP
1	3-F	125	PRO
1	3-F	335	ALA
1	3-H	6	PHE
1	4-B	283	PRO
1	4-C	17	PRO
1	4-E	6	PHE
1	4-F	19	ALA
1	4-F	97	ASP
1	4-F	339	HIS
1	4-F	344	ALA
1	5-A	39	GLN
1	5-B	175	PHE
1	5-E	132	LEU
1	5-E	341	PRO
1	5-F	97	ASP
1	5-G	283	PRO
1	5-G	350	ARG
1	6-A	5	ARG
1	6-D	41	GLU
1	6-D	323	SER
1	6-G	43	ARG
1	7-A	338	THR

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Mol	Chain	Res	Type
1	7-B	137	LEU
1	7-C	98	ASP
1	7-C	343	SER
1	7-C	344	ALA
1	7-D	18	SER
1	7-D	335	ALA
1	7-E	98	ASP
1	7-E	342	LEU
1	7-G	338	THR
1	7-H	37	ARG
1	7-H	42	PRO
1	8-A	132	LEU
1	8-B	323	SER
1	8-D	340	ARG
1	8-F	4	MSE
1	8-F	125	PRO
1	8-G	341	PRO
1	9-A	20	GLY
1	9-A	40	ASP
1	9-A	126	GLU
1	9-A	291	GLN
1	9-B	42	PRO
1	9-E	344	ALA
1	9-F	343	SER
1	9-G	349	ARG
1	10-A	343	SER
1	10-C	5	ARG
1	10-D	18	SER
1	10-E	6	PHE
1	10-E	97	ASP
1	10-F	18	SER
1	10-F	19	ALA
1	1-D	7	GLY
1	1-D	127	GLY
1	1-E	336	LEU
1	1-F	114	GLY
1	1-F	351	GLY
1	2-E	39	GLN
1	2-H	40	ASP
1	3-A	131	ALA
1	3-C	309	GLU
1	3-F	337	MSE

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Mol	Chain	Res	Type
1	3-G	98	ASP
1	4-B	126	GLU
1	5-F	133	ALA
1	5-G	349	ARG
1	6-A	17	PRO
1	6-C	40	ASP
1	6-D	20	GLY
1	6-D	39	GLN
1	6-F	41	GLU
1	6-F	323	SER
1	6-H	5	ARG
1	6-H	42	PRO
1	7-A	6	PHE
1	7-A	42	PRO
1	7-C	37	ARG
1	7-C	42	PRO
1	7-D	334	PRO
1	7-F	323	SER
1	8-A	42	PRO
1	8-A	122	LEU
1	8-G	16	ARG
1	8-G	19	ALA
1	9-B	15	ARG
1	9-B	323	SER
1	9-E	6	PHE
1	9-E	346	ALA
1	10-B	125	PRO
1	10-C	42	PRO
1	10-D	346	ALA
1	10-E	19	ALA
1	10-F	114	GLY
1	10-G	4	MSE
1	10-G	96	THR
1	10-G	133	ALA
1	1-C	338	THR
1	1-D	35	GLU
1	1-D	126	GLU
1	1-G	42	PRO
1	1-G	131	ALA
1	1-H	19	ALA
1	2-B	18	SER
1	2-F	97	ASP

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Mol	Chain	Res	Type
1	2-F	340	ARG
1	3-B	125	PRO
1	3-B	137	LEU
1	3-C	378	ALA
1	3-D	38	ALA
1	3-E	323	SER
1	3-G	335	ALA
1	4-D	42	PRO
1	4-E	100	TYR
1	4-F	18	SER
1	4-F	40	ASP
1	5-A	130	ALA
1	5-E	42	PRO
1	6-A	352	ILE
1	6-D	280	PRO
1	7-B	323	SER
1	7-D	17	PRO
1	8-A	37	ARG
1	8-E	96	THR
1	9-A	42	PRO
1	9-A	127	GLY
1	9-B	36	ARG
1	9-F	97	ASP
1	9-G	340	ARG
1	10-B	97	ASP
1	10-B	338	THR
1	10-D	43	ARG
1	10-D	340	ARG
1	10-E	343	SER
1	1-A	244	LEU
1	1-B	16	ARG
1	1-G	322	VAL
1	2-H	187	GLY
1	3-B	323	SER
1	3-C	17	PRO
1	3-H	306	GLY
1	4-A	37	ARG
1	5-E	115	VAL
1	5-F	38	ALA
1	6-A	97	ASP
1	6-B	16	ARG
1	6-C	18	SER

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Mol	Chain	Res	Type
1	6-F	351	GLY
1	6-G	18	SER
1	6-H	89	PRO
1	7-F	6	PHE
1	7-F	42	PRO
1	7-G	42	PRO
1	8-A	348	ALA
1	8-C	97	ASP
1	8-E	6	PHE
1	9-F	96	THR
1	10-D	41	GLU
1	10-D	281	GLU
1	1-H	305	GLY
1	3-A	305	GLY
1	3-F	17	PRO
1	5-E	322	VAL
1	6-A	166	GLY
1	8-B	20	GLY
1	10-D	16	ARG
1	10-E	322	VAL
1	10-G	283	PRO
1	1-A	41	GLU
1	1-H	17	PRO
1	3-E	17	PRO
1	4-D	99	VAL
1	5-H	114	GLY
1	2-G	115	VAL
1	3-D	283	PRO
1	3-E	42	PRO
1	5-D	280	PRO
1	5-F	127	GLY
1	7-A	322	VAL
1	8-C	327	VAL
1	10-F	128	ILE
1	1-C	295	PRO
1	2-F	322	VAL
1	3-D	17	PRO
1	3-D	334	PRO
1	4-B	125	PRO
1	8-D	199	ILE
1	9-A	334	PRO
1	10-C	322	VAL

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Mol	Chain	Res	Type
1	10-G	128	ILE
1	1-C	322	VAL
1	2-A	99	VAL
1	3-H	20	GLY
1	4-B	42	PRO
1	5-H	340	ARG
1	7-A	16	ARG
1	7-E	334	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	291/293 (99%)	269 (92%)	22 (8%)	15	11
1	1-B	291/293 (99%)	263 (90%)	28 (10%)	10	6
1	1-C	289/293 (99%)	268 (93%)	21 (7%)	16	13
1	1-D	285/293 (97%)	261 (92%)	24 (8%)	13	8
1	1-E	286/293 (98%)	268 (94%)	18 (6%)	21	17
1	1-F	284/293 (97%)	261 (92%)	23 (8%)	14	9
1	1-G	285/293 (97%)	267 (94%)	18 (6%)	21	17
1	1-H	287/293 (98%)	263 (92%)	24 (8%)	13	8
1	2-A	291/293 (99%)	274 (94%)	17 (6%)	23	20
1	2-B	291/293 (99%)	270 (93%)	21 (7%)	17	13
1	2-C	289/293 (99%)	274 (95%)	15 (5%)	27	24
1	2-D	285/293 (97%)	263 (92%)	22 (8%)	15	11
1	2-E	286/293 (98%)	271 (95%)	15 (5%)	27	24
1	2-F	284/293 (97%)	266 (94%)	18 (6%)	21	17
1	2-G	285/293 (97%)	265 (93%)	20 (7%)	18	14
1	2-H	287/293 (98%)	263 (92%)	24 (8%)	13	8
1	3-A	291/293 (99%)	267 (92%)	24 (8%)	13	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3-B	291/293 (99%)	281 (97%)	10 (3%)	42	43
1	3-C	289/293 (99%)	264 (91%)	25 (9%)	12	8
1	3-D	285/293 (97%)	260 (91%)	25 (9%)	12	8
1	3-E	286/293 (98%)	273 (96%)	13 (4%)	32	30
1	3-F	284/293 (97%)	264 (93%)	20 (7%)	18	14
1	3-G	285/293 (97%)	267 (94%)	18 (6%)	21	17
1	3-H	287/293 (98%)	267 (93%)	20 (7%)	18	14
1	4-A	291/293 (99%)	270 (93%)	21 (7%)	17	13
1	4-B	291/293 (99%)	268 (92%)	23 (8%)	14	10
1	4-C	289/293 (99%)	273 (94%)	16 (6%)	25	22
1	4-D	285/293 (97%)	263 (92%)	22 (8%)	15	11
1	4-E	286/293 (98%)	266 (93%)	20 (7%)	18	14
1	4-F	284/293 (97%)	261 (92%)	23 (8%)	14	9
1	4-G	285/293 (97%)	269 (94%)	16 (6%)	25	21
1	4-H	287/293 (98%)	265 (92%)	22 (8%)	15	11
1	5-A	291/293 (99%)	275 (94%)	16 (6%)	25	22
1	5-B	291/293 (99%)	269 (92%)	22 (8%)	15	11
1	5-C	289/293 (99%)	269 (93%)	20 (7%)	18	14
1	5-D	285/293 (97%)	260 (91%)	25 (9%)	12	8
1	5-E	286/293 (98%)	261 (91%)	25 (9%)	12	8
1	5-F	284/293 (97%)	273 (96%)	11 (4%)	37	37
1	5-G	285/293 (97%)	272 (95%)	13 (5%)	31	29
1	5-H	287/293 (98%)	266 (93%)	21 (7%)	16	13
1	6-A	291/293 (99%)	274 (94%)	17 (6%)	23	20
1	6-B	291/293 (99%)	270 (93%)	21 (7%)	17	13
1	6-C	289/293 (99%)	271 (94%)	18 (6%)	21	18
1	6-D	285/293 (97%)	260 (91%)	25 (9%)	12	8
1	6-E	286/293 (98%)	264 (92%)	22 (8%)	15	11
1	6-F	284/293 (97%)	259 (91%)	25 (9%)	12	8
1	6-G	285/293 (97%)	261 (92%)	24 (8%)	13	8
1	6-H	287/293 (98%)	269 (94%)	18 (6%)	21	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7-A	291/293 (99%)	258 (89%)	33 (11%)	7	3
1	7-B	291/293 (99%)	267 (92%)	24 (8%)	13	9
1	7-C	289/293 (99%)	269 (93%)	20 (7%)	18	14
1	7-D	285/293 (97%)	261 (92%)	24 (8%)	13	8
1	7-E	286/293 (98%)	268 (94%)	18 (6%)	21	17
1	7-F	284/293 (97%)	265 (93%)	19 (7%)	19	15
1	7-G	285/293 (97%)	272 (95%)	13 (5%)	31	29
1	7-H	287/293 (98%)	269 (94%)	18 (6%)	21	17
1	8-A	291/293 (99%)	276 (95%)	15 (5%)	27	24
1	8-B	291/293 (99%)	277 (95%)	14 (5%)	30	27
1	8-C	289/293 (99%)	271 (94%)	18 (6%)	21	18
1	8-D	285/293 (97%)	267 (94%)	18 (6%)	21	17
1	8-E	286/293 (98%)	267 (93%)	19 (7%)	19	16
1	8-F	284/293 (97%)	265 (93%)	19 (7%)	19	15
1	8-G	285/293 (97%)	269 (94%)	16 (6%)	25	21
1	8-H	287/293 (98%)	271 (94%)	16 (6%)	25	21
1	9-A	291/293 (99%)	272 (94%)	19 (6%)	20	16
1	9-B	291/293 (99%)	272 (94%)	19 (6%)	20	16
1	9-C	289/293 (99%)	262 (91%)	27 (9%)	10	7
1	9-D	285/293 (97%)	269 (94%)	16 (6%)	25	21
1	9-E	286/293 (98%)	267 (93%)	19 (7%)	19	16
1	9-F	284/293 (97%)	263 (93%)	21 (7%)	16	12
1	9-G	285/293 (97%)	271 (95%)	14 (5%)	29	26
1	9-H	287/293 (98%)	271 (94%)	16 (6%)	25	21
1	10-A	291/293 (99%)	263 (90%)	28 (10%)	10	6
1	10-B	291/293 (99%)	270 (93%)	21 (7%)	17	13
1	10-C	289/293 (99%)	268 (93%)	21 (7%)	16	13
1	10-D	285/293 (97%)	263 (92%)	22 (8%)	15	11
1	10-E	286/293 (98%)	271 (95%)	15 (5%)	27	24
1	10-F	284/293 (97%)	266 (94%)	18 (6%)	21	17
1	10-G	285/293 (97%)	262 (92%)	23 (8%)	14	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	10-H	287/293 (98%)	270 (94%)	17 (6%)	23	19
All	All	22980/23440 (98%)	21389 (93%)	1591 (7%)	18	14

All (1591) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	16	ARG
1	1-A	41	GLU
1	1-A	43	ARG
1	1-A	84	LEU
1	1-A	92	CYS
1	1-A	98	ASP
1	1-A	112	ARG
1	1-A	124	THR
1	1-A	132	LEU
1	1-A	161	ARG
1	1-A	175	PHE
1	1-A	177	SER
1	1-A	206	LEU
1	1-A	214	ASP
1	1-A	226	THR
1	1-A	244	LEU
1	1-A	263	GLU
1	1-A	295	PRO
1	1-A	323	SER
1	1-A	328	HIS
1	1-A	332	GLU
1	1-A	365	ASP
1	1-B	16	ARG
1	1-B	23	ASP
1	1-B	33	THR
1	1-B	36	ARG
1	1-B	40	ASP
1	1-B	41	GLU
1	1-B	43	ARG
1	1-B	66	ARG
1	1-B	84	LEU
1	1-B	92	CYS
1	1-B	96	THR
1	1-B	97	ASP
1	1-B	116	ARG
1	1-B	126	GLU

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Mol	Chain	Res	Type
1	1-B	147	ASN
1	1-B	161	ARG
1	1-B	165	ARG
1	1-B	192	LEU
1	1-B	259	ARG
1	1-B	323	SER
1	1-B	328	HIS
1	1-B	330	LEU
1	1-B	332	GLU
1	1-B	337	MSE
1	1-B	345	GLU
1	1-B	347	ARG
1	1-B	355	SER
1	1-B	367	GLN
1	1-C	16	ARG
1	1-C	23	ASP
1	1-C	35	GLU
1	1-C	36	ARG
1	1-C	39	GLN
1	1-C	104	ASP
1	1-C	108	ASP
1	1-C	112	ARG
1	1-C	116	ARG
1	1-C	149	LEU
1	1-C	161	ARG
1	1-C	231	VAL
1	1-C	289	LYS
1	1-C	292	MSE
1	1-C	327	VAL
1	1-C	332	GLU
1	1-C	337	MSE
1	1-C	342	LEU
1	1-C	343	SER
1	1-C	354	GLU
1	1-C	375	ARG
1	1-D	4	MSE
1	1-D	33	THR
1	1-D	66	ARG
1	1-D	96	THR
1	1-D	98	ASP
1	1-D	116	ARG
1	1-D	119	TYR

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Mol	Chain	Res	Type
1	1-D	126	GLU
1	1-D	160	ARG
1	1-D	161	ARG
1	1-D	165	ARG
1	1-D	192	LEU
1	1-D	213	ARG
1	1-D	252	HIS
1	1-D	253	ARG
1	1-D	264	ARG
1	1-D	292	MSE
1	1-D	300	SER
1	1-D	309	GLU
1	1-D	320	CYS
1	1-D	323	SER
1	1-D	324	LEU
1	1-D	332	GLU
1	1-D	375	ARG
1	1-E	4	MSE
1	1-E	9	ARG
1	1-E	16	ARG
1	1-E	33	THR
1	1-E	39	GLN
1	1-E	43	ARG
1	1-E	96	THR
1	1-E	97	ASP
1	1-E	104	ASP
1	1-E	113	GLN
1	1-E	121	ASP
1	1-E	151	THR
1	1-E	226	THR
1	1-E	259	ARG
1	1-E	281	GLU
1	1-E	309	GLU
1	1-E	336	LEU
1	1-E	337	MSE
1	1-F	23	ASP
1	1-F	37	ARG
1	1-F	66	ARG
1	1-F	74	SER
1	1-F	96	THR
1	1-F	98	ASP
1	1-F	99	VAL

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Mol	Chain	Res	Type
1	1-F	108	ASP
1	1-F	112	ARG
1	1-F	117	VAL
1	1-F	123	THR
1	1-F	124	THR
1	1-F	126	GLU
1	1-F	132	LEU
1	1-F	147	ASN
1	1-F	161	ARG
1	1-F	175	PHE
1	1-F	177	SER
1	1-F	192	LEU
1	1-F	231	VAL
1	1-F	332	GLU
1	1-F	338	THR
1	1-F	352	ILE
1	1-G	16	ARG
1	1-G	33	THR
1	1-G	36	ARG
1	1-G	41	GLU
1	1-G	43	ARG
1	1-G	50	GLU
1	1-G	83	LEU
1	1-G	104	ASP
1	1-G	116	ARG
1	1-G	121	ASP
1	1-G	134	GLU
1	1-G	161	ARG
1	1-G	165	ARG
1	1-G	252	HIS
1	1-G	284	GLN
1	1-G	337	MSE
1	1-G	352	ILE
1	1-G	374	SER
1	1-H	4	MSE
1	1-H	9	ARG
1	1-H	16	ARG
1	1-H	18	SER
1	1-H	23	ASP
1	1-H	33	THR
1	1-H	84	LEU
1	1-H	96	THR

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Mol	Chain	Res	Type
1	1-H	104	ASP
1	1-H	109	LEU
1	1-H	126	GLU
1	1-H	147	ASN
1	1-H	177	SER
1	1-H	213	ARG
1	1-H	214	ASP
1	1-H	231	VAL
1	1-H	236	ASP
1	1-H	244	LEU
1	1-H	323	SER
1	1-H	324	LEU
1	1-H	337	MSE
1	1-H	342	LEU
1	1-H	343	SER
1	1-H	352	ILE
1	2-A	4	MSE
1	2-A	18	SER
1	2-A	33	THR
1	2-A	36	ARG
1	2-A	84	LEU
1	2-A	97	ASP
1	2-A	160	ARG
1	2-A	175	PHE
1	2-A	179	VAL
1	2-A	206	LEU
1	2-A	213	ARG
1	2-A	231	VAL
1	2-A	244	LEU
1	2-A	248	SER
1	2-A	328	HIS
1	2-A	338	THR
1	2-A	350	ARG
1	2-B	4	MSE
1	2-B	15	ARG
1	2-B	36	ARG
1	2-B	59	GLU
1	2-B	84	LEU
1	2-B	96	THR
1	2-B	97	ASP
1	2-B	104	ASP
1	2-B	124	THR

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Mol	Chain	Res	Type
1	2-B	126	GLU
1	2-B	147	ASN
1	2-B	161	ARG
1	2-B	194	SER
1	2-B	213	ARG
1	2-B	242	ARG
1	2-B	300	SER
1	2-B	332	GLU
1	2-B	337	MSE
1	2-B	338	THR
1	2-B	340	ARG
1	2-B	367	GLN
1	2-C	4	MSE
1	2-C	23	ASP
1	2-C	96	THR
1	2-C	99	VAL
1	2-C	109	LEU
1	2-C	112	ARG
1	2-C	117	VAL
1	2-C	231	VAL
1	2-C	244	LEU
1	2-C	327	VAL
1	2-C	332	GLU
1	2-C	333	CYS
1	2-C	337	MSE
1	2-C	342	LEU
1	2-C	381	THR
1	2-D	6	PHE
1	2-D	39	GLN
1	2-D	43	ARG
1	2-D	84	LEU
1	2-D	95	SER
1	2-D	98	ASP
1	2-D	107	PHE
1	2-D	116	ARG
1	2-D	124	THR
1	2-D	132	LEU
1	2-D	147	ASN
1	2-D	152	VAL
1	2-D	160	ARG
1	2-D	191	SER
1	2-D	252	HIS

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Mol	Chain	Res	Type
1	2-D	281	GLU
1	2-D	310	ARG
1	2-D	330	LEU
1	2-D	337	MSE
1	2-D	340	ARG
1	2-D	350	ARG
1	2-D	365	ASP
1	2-E	16	ARG
1	2-E	18	SER
1	2-E	23	ASP
1	2-E	33	THR
1	2-E	84	LEU
1	2-E	97	ASP
1	2-E	98	ASP
1	2-E	126	GLU
1	2-E	132	LEU
1	2-E	146	THR
1	2-E	309	GLU
1	2-E	310	ARG
1	2-E	328	HIS
1	2-E	332	GLU
1	2-E	367	GLN
1	2-F	4	MSE
1	2-F	9	ARG
1	2-F	23	ASP
1	2-F	33	THR
1	2-F	37	ARG
1	2-F	66	ARG
1	2-F	96	THR
1	2-F	98	ASP
1	2-F	109	LEU
1	2-F	123	THR
1	2-F	124	THR
1	2-F	147	ASN
1	2-F	160	ARG
1	2-F	161	ARG
1	2-F	231	VAL
1	2-F	309	GLU
1	2-F	328	HIS
1	2-F	350	ARG
1	2-G	4	MSE
1	2-G	9	ARG

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Mol	Chain	Res	Type
1	2-G	16	ARG
1	2-G	23	ASP
1	2-G	40	ASP
1	2-G	74	SER
1	2-G	88	ARG
1	2-G	97	ASP
1	2-G	117	VAL
1	2-G	124	THR
1	2-G	161	ARG
1	2-G	175	PHE
1	2-G	206	LEU
1	2-G	231	VAL
1	2-G	284	GLN
1	2-G	328	HIS
1	2-G	332	GLU
1	2-G	354	GLU
1	2-G	355	SER
1	2-G	367	GLN
1	2-H	16	ARG
1	2-H	17	PRO
1	2-H	36	ARG
1	2-H	43	ARG
1	2-H	91	GLN
1	2-H	96	THR
1	2-H	97	ASP
1	2-H	98	ASP
1	2-H	104	ASP
1	2-H	108	ASP
1	2-H	124	THR
1	2-H	147	ASN
1	2-H	161	ARG
1	2-H	165	ARG
1	2-H	175	PHE
1	2-H	226	THR
1	2-H	248	SER
1	2-H	263	GLU
1	2-H	266	ARG
1	2-H	285	HIS
1	2-H	288	VAL
1	2-H	292	MSE
1	2-H	323	SER
1	2-H	332	GLU

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Mol	Chain	Res	Type
1	3-A	4	MSE
1	3-A	21	THR
1	3-A	23	ASP
1	3-A	36	ARG
1	3-A	37	ARG
1	3-A	43	ARG
1	3-A	97	ASP
1	3-A	99	VAL
1	3-A	112	ARG
1	3-A	118	ARG
1	3-A	126	GLU
1	3-A	132	LEU
1	3-A	136	ASP
1	3-A	148	PRO
1	3-A	177	SER
1	3-A	205	VAL
1	3-A	236	ASP
1	3-A	264	ARG
1	3-A	281	GLU
1	3-A	300	SER
1	3-A	309	GLU
1	3-A	328	HIS
1	3-A	338	THR
1	3-A	367	GLN
1	3-B	23	ASP
1	3-B	36	ARG
1	3-B	97	ASP
1	3-B	161	ARG
1	3-B	177	SER
1	3-B	214	ASP
1	3-B	328	HIS
1	3-B	332	GLU
1	3-B	337	MSE
1	3-B	338	THR
1	3-C	5	ARG
1	3-C	8	THR
1	3-C	16	ARG
1	3-C	23	ASP
1	3-C	36	ARG
1	3-C	84	LEU
1	3-C	96	THR
1	3-C	99	VAL

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Mol	Chain	Res	Type
1	3-C	104	ASP
1	3-C	112	ARG
1	3-C	124	THR
1	3-C	134	GLU
1	3-C	136	ASP
1	3-C	161	ARG
1	3-C	175	PHE
1	3-C	281	GLU
1	3-C	313	ASP
1	3-C	327	VAL
1	3-C	328	HIS
1	3-C	332	GLU
1	3-C	337	MSE
1	3-C	338	THR
1	3-C	340	ARG
1	3-C	367	GLN
1	3-C	381	THR
1	3-D	4	MSE
1	3-D	23	ASP
1	3-D	33	THR
1	3-D	36	ARG
1	3-D	39	GLN
1	3-D	66	ARG
1	3-D	84	LEU
1	3-D	97	ASP
1	3-D	99	VAL
1	3-D	104	ASP
1	3-D	123	THR
1	3-D	151	THR
1	3-D	175	PHE
1	3-D	214	ASP
1	3-D	244	LEU
1	3-D	264	ARG
1	3-D	300	SER
1	3-D	310	ARG
1	3-D	336	LEU
1	3-D	337	MSE
1	3-D	339	HIS
1	3-D	349	ARG
1	3-D	350	ARG
1	3-D	358	ARG
1	3-D	371	GLU

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Mol	Chain	Res	Type
1	3-E	17	PRO
1	3-E	23	ASP
1	3-E	35	GLU
1	3-E	43	ARG
1	3-E	50	GLU
1	3-E	132	LEU
1	3-E	160	ARG
1	3-E	175	PHE
1	3-E	177	SER
1	3-E	191	SER
1	3-E	206	LEU
1	3-E	328	HIS
1	3-E	345	GLU
1	3-F	4	MSE
1	3-F	23	ASP
1	3-F	37	ARG
1	3-F	66	ARG
1	3-F	84	LEU
1	3-F	96	THR
1	3-F	97	ASP
1	3-F	98	ASP
1	3-F	112	ARG
1	3-F	132	LEU
1	3-F	161	ARG
1	3-F	177	SER
1	3-F	213	ARG
1	3-F	248	SER
1	3-F	309	GLU
1	3-F	328	HIS
1	3-F	332	GLU
1	3-F	337	MSE
1	3-F	340	ARG
1	3-F	350	ARG
1	3-G	33	THR
1	3-G	36	ARG
1	3-G	41	GLU
1	3-G	43	ARG
1	3-G	83	LEU
1	3-G	112	ARG
1	3-G	134	GLU
1	3-G	147	ASN
1	3-G	161	ARG

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Mol	Chain	Res	Type
1	3-G	175	PHE
1	3-G	213	ARG
1	3-G	231	VAL
1	3-G	248	SER
1	3-G	284	GLN
1	3-G	332	GLU
1	3-G	354	GLU
1	3-G	371	GLU
1	3-G	375	ARG
1	3-H	4	MSE
1	3-H	9	ARG
1	3-H	16	ARG
1	3-H	18	SER
1	3-H	23	ASP
1	3-H	39	GLN
1	3-H	93	VAL
1	3-H	97	ASP
1	3-H	99	VAL
1	3-H	118	ARG
1	3-H	124	THR
1	3-H	175	PHE
1	3-H	213	ARG
1	3-H	231	VAL
1	3-H	253	ARG
1	3-H	300	SER
1	3-H	320	CYS
1	3-H	332	GLU
1	3-H	339	HIS
1	3-H	375	ARG
1	4-A	9	ARG
1	4-A	23	ASP
1	4-A	33	THR
1	4-A	37	ARG
1	4-A	41	GLU
1	4-A	50	GLU
1	4-A	88	ARG
1	4-A	97	ASP
1	4-A	99	VAL
1	4-A	104	ASP
1	4-A	112	ARG
1	4-A	113	GLN
1	4-A	118	ARG

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Mol	Chain	Res	Type
1	4-A	132	LEU
1	4-A	161	ARG
1	4-A	192	LEU
1	4-A	244	LEU
1	4-A	328	HIS
1	4-A	332	GLU
1	4-A	340	ARG
1	4-A	349	ARG
1	4-B	16	ARG
1	4-B	33	THR
1	4-B	36	ARG
1	4-B	41	GLU
1	4-B	96	THR
1	4-B	97	ASP
1	4-B	99	VAL
1	4-B	109	LEU
1	4-B	128	ILE
1	4-B	147	ASN
1	4-B	161	ARG
1	4-B	206	LEU
1	4-B	231	VAL
1	4-B	253	ARG
1	4-B	292	MSE
1	4-B	293	SER
1	4-B	328	HIS
1	4-B	330	LEU
1	4-B	332	GLU
1	4-B	347	ARG
1	4-B	349	ARG
1	4-B	365	ASP
1	4-B	367	GLN
1	4-C	4	MSE
1	4-C	8	THR
1	4-C	23	ASP
1	4-C	33	THR
1	4-C	40	ASP
1	4-C	43	ARG
1	4-C	96	THR
1	4-C	160	ARG
1	4-C	285	HIS
1	4-C	292	MSE
1	4-C	327	VAL

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Mol	Chain	Res	Type
1	4-C	332	GLU
1	4-C	338	THR
1	4-C	342	LEU
1	4-C	350	ARG
1	4-C	381	THR
1	4-D	6	PHE
1	4-D	36	ARG
1	4-D	95	SER
1	4-D	97	ASP
1	4-D	98	ASP
1	4-D	99	VAL
1	4-D	108	ASP
1	4-D	112	ARG
1	4-D	121	ASP
1	4-D	136	ASP
1	4-D	151	THR
1	4-D	161	ARG
1	4-D	177	SER
1	4-D	244	LEU
1	4-D	264	ARG
1	4-D	281	GLU
1	4-D	292	MSE
1	4-D	310	ARG
1	4-D	328	HIS
1	4-D	332	GLU
1	4-D	338	THR
1	4-D	354	GLU
1	4-E	4	MSE
1	4-E	6	PHE
1	4-E	96	THR
1	4-E	97	ASP
1	4-E	98	ASP
1	4-E	116	ARG
1	4-E	123	THR
1	4-E	124	THR
1	4-E	160	ARG
1	4-E	161	ARG
1	4-E	175	PHE
1	4-E	177	SER
1	4-E	289	LYS
1	4-E	292	MSE
1	4-E	309	GLU

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Mol	Chain	Res	Type
1	4-E	313	ASP
1	4-E	332	GLU
1	4-E	336	LEU
1	4-E	343	SER
1	4-E	350	ARG
1	4-F	4	MSE
1	4-F	18	SER
1	4-F	37	ARG
1	4-F	39	GLN
1	4-F	96	THR
1	4-F	104	ASP
1	4-F	112	ARG
1	4-F	119	TYR
1	4-F	123	THR
1	4-F	132	LEU
1	4-F	136	ASP
1	4-F	147	ASN
1	4-F	161	ARG
1	4-F	165	ARG
1	4-F	177	SER
1	4-F	292	MSE
1	4-F	328	HIS
1	4-F	332	GLU
1	4-F	337	MSE
1	4-F	338	THR
1	4-F	350	ARG
1	4-F	367	GLN
1	4-F	375	ARG
1	4-G	8	THR
1	4-G	40	ASP
1	4-G	41	GLU
1	4-G	84	LEU
1	4-G	98	ASP
1	4-G	99	VAL
1	4-G	161	ARG
1	4-G	244	LEU
1	4-G	284	GLN
1	4-G	289	LYS
1	4-G	309	GLU
1	4-G	330	LEU
1	4-G	333	CYS
1	4-G	342	LEU

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Mol	Chain	Res	Type
1	4-G	343	SER
1	4-G	347	ARG
1	4-H	4	MSE
1	4-H	5	ARG
1	4-H	9	ARG
1	4-H	16	ARG
1	4-H	39	GLN
1	4-H	45	PHE
1	4-H	66	ARG
1	4-H	74	SER
1	4-H	84	LEU
1	4-H	98	ASP
1	4-H	104	ASP
1	4-H	118	ARG
1	4-H	124	THR
1	4-H	192	LEU
1	4-H	253	ARG
1	4-H	281	GLU
1	4-H	300	SER
1	4-H	309	GLU
1	4-H	328	HIS
1	4-H	332	GLU
1	4-H	339	HIS
1	4-H	355	SER
1	5-A	21	THR
1	5-A	39	GLN
1	5-A	99	VAL
1	5-A	132	LEU
1	5-A	136	ASP
1	5-A	147	ASN
1	5-A	151	THR
1	5-A	165	ARG
1	5-A	179	VAL
1	5-A	231	VAL
1	5-A	281	GLU
1	5-A	328	HIS
1	5-A	332	GLU
1	5-A	337	MSE
1	5-A	347	ARG
1	5-A	371	GLU
1	5-B	4	MSE
1	5-B	16	ARG

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Mol	Chain	Res	Type
1	5-B	23	ASP
1	5-B	36	ARG
1	5-B	40	ASP
1	5-B	41	GLU
1	5-B	43	ARG
1	5-B	66	ARG
1	5-B	97	ASP
1	5-B	99	VAL
1	5-B	108	ASP
1	5-B	109	LEU
1	5-B	118	ARG
1	5-B	126	GLU
1	5-B	161	ARG
1	5-B	177	SER
1	5-B	198	SER
1	5-B	244	LEU
1	5-B	323	SER
1	5-B	328	HIS
1	5-B	332	GLU
1	5-B	340	ARG
1	5-C	4	MSE
1	5-C	8	THR
1	5-C	23	ASP
1	5-C	98	ASP
1	5-C	99	VAL
1	5-C	124	THR
1	5-C	181	GLN
1	5-C	244	LEU
1	5-C	292	MSE
1	5-C	300	SER
1	5-C	313	ASP
1	5-C	324	LEU
1	5-C	332	GLU
1	5-C	333	CYS
1	5-C	334	PRO
1	5-C	338	THR
1	5-C	340	ARG
1	5-C	342	LEU
1	5-C	355	SER
1	5-C	375	ARG
1	5-D	33	THR
1	5-D	36	ARG

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Mol	Chain	Res	Type
1	5-D	43	ARG
1	5-D	66	ARG
1	5-D	96	THR
1	5-D	98	ASP
1	5-D	104	ASP
1	5-D	113	GLN
1	5-D	119	TYR
1	5-D	175	PHE
1	5-D	206	LEU
1	5-D	231	VAL
1	5-D	253	ARG
1	5-D	264	ARG
1	5-D	281	GLU
1	5-D	292	MSE
1	5-D	330	LEU
1	5-D	332	GLU
1	5-D	336	LEU
1	5-D	337	MSE
1	5-D	340	ARG
1	5-D	350	ARG
1	5-D	360	SER
1	5-D	367	GLN
1	5-D	375	ARG
1	5-E	4	MSE
1	5-E	8	THR
1	5-E	9	ARG
1	5-E	16	ARG
1	5-E	18	SER
1	5-E	23	ASP
1	5-E	33	THR
1	5-E	35	GLU
1	5-E	39	GLN
1	5-E	43	ARG
1	5-E	96	THR
1	5-E	98	ASP
1	5-E	109	LEU
1	5-E	113	GLN
1	5-E	123	THR
1	5-E	124	THR
1	5-E	126	GLU
1	5-E	134	GLU
1	5-E	160	ARG

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Mol	Chain	Res	Type
1	5-E	213	ARG
1	5-E	292	MSE
1	5-E	309	GLU
1	5-E	336	LEU
1	5-E	337	MSE
1	5-E	342	LEU
1	5-F	4	MSE
1	5-F	18	SER
1	5-F	39	GLN
1	5-F	84	LEU
1	5-F	99	VAL
1	5-F	113	GLN
1	5-F	124	THR
1	5-F	192	LEU
1	5-F	313	ASP
1	5-F	332	GLU
1	5-F	340	ARG
1	5-G	4	MSE
1	5-G	23	ASP
1	5-G	36	ARG
1	5-G	83	LEU
1	5-G	84	LEU
1	5-G	89	PRO
1	5-G	112	ARG
1	5-G	161	ARG
1	5-G	216	ASP
1	5-G	284	GLN
1	5-G	309	GLU
1	5-G	328	HIS
1	5-G	332	GLU
1	5-H	4	MSE
1	5-H	16	ARG
1	5-H	18	SER
1	5-H	23	ASP
1	5-H	35	GLU
1	5-H	50	GLU
1	5-H	74	SER
1	5-H	104	ASP
1	5-H	109	LEU
1	5-H	126	GLU
1	5-H	152	VAL
1	5-H	177	SER

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Mol	Chain	Res	Type
1	5-H	213	ARG
1	5-H	231	VAL
1	5-H	236	ASP
1	5-H	259	ARG
1	5-H	322	VAL
1	5-H	330	LEU
1	5-H	332	GLU
1	5-H	333	CYS
1	5-H	337	MSE
1	6-A	4	MSE
1	6-A	23	ASP
1	6-A	32	THR
1	6-A	40	ASP
1	6-A	108	ASP
1	6-A	132	LEU
1	6-A	179	VAL
1	6-A	213	ARG
1	6-A	242	ARG
1	6-A	244	LEU
1	6-A	263	GLU
1	6-A	264	ARG
1	6-A	328	HIS
1	6-A	332	GLU
1	6-A	338	THR
1	6-A	340	ARG
1	6-A	342	LEU
1	6-B	4	MSE
1	6-B	18	SER
1	6-B	36	ARG
1	6-B	40	ASP
1	6-B	84	LEU
1	6-B	96	THR
1	6-B	98	ASP
1	6-B	99	VAL
1	6-B	104	ASP
1	6-B	126	GLU
1	6-B	161	ARG
1	6-B	177	SER
1	6-B	242	ARG
1	6-B	244	LEU
1	6-B	259	ARG
1	6-B	266	ARG

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Mol	Chain	Res	Type
1	6-B	284	GLN
1	6-B	292	MSE
1	6-B	324	LEU
1	6-B	339	HIS
1	6-B	365	ASP
1	6-C	9	ARG
1	6-C	23	ASP
1	6-C	36	ARG
1	6-C	84	LEU
1	6-C	96	THR
1	6-C	98	ASP
1	6-C	116	ARG
1	6-C	121	ASP
1	6-C	152	VAL
1	6-C	175	PHE
1	6-C	231	VAL
1	6-C	264	ARG
1	6-C	281	GLU
1	6-C	300	SER
1	6-C	342	LEU
1	6-C	354	GLU
1	6-C	355	SER
1	6-C	381	THR
1	6-D	33	THR
1	6-D	36	ARG
1	6-D	43	ARG
1	6-D	74	SER
1	6-D	98	ASP
1	6-D	104	ASP
1	6-D	112	ARG
1	6-D	113	GLN
1	6-D	124	THR
1	6-D	136	ASP
1	6-D	151	THR
1	6-D	160	ARG
1	6-D	165	ARG
1	6-D	226	THR
1	6-D	227	THR
1	6-D	231	VAL
1	6-D	264	ARG
1	6-D	281	GLU
1	6-D	284	GLN

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Mol	Chain	Res	Type
1	6-D	292	MSE
1	6-D	319	THR
1	6-D	323	SER
1	6-D	340	ARG
1	6-D	350	ARG
1	6-D	375	ARG
1	6-E	16	ARG
1	6-E	23	ASP
1	6-E	35	GLU
1	6-E	84	LEU
1	6-E	88	ARG
1	6-E	96	THR
1	6-E	98	ASP
1	6-E	99	VAL
1	6-E	116	ARG
1	6-E	124	THR
1	6-E	126	GLU
1	6-E	150	LEU
1	6-E	151	THR
1	6-E	161	ARG
1	6-E	177	SER
1	6-E	179	VAL
1	6-E	231	VAL
1	6-E	310	ARG
1	6-E	313	ASP
1	6-E	332	GLU
1	6-E	337	MSE
1	6-E	342	LEU
1	6-F	37	ARG
1	6-F	92	CYS
1	6-F	96	THR
1	6-F	97	ASP
1	6-F	99	VAL
1	6-F	104	ASP
1	6-F	118	ARG
1	6-F	124	THR
1	6-F	132	LEU
1	6-F	136	ASP
1	6-F	147	ASN
1	6-F	161	ARG
1	6-F	165	ARG
1	6-F	177	SER

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Mol	Chain	Res	Type
1	6-F	216	ASP
1	6-F	244	LEU
1	6-F	309	GLU
1	6-F	310	ARG
1	6-F	319	THR
1	6-F	324	LEU
1	6-F	337	MSE
1	6-F	343	SER
1	6-F	367	GLN
1	6-F	371	GLU
1	6-F	375	ARG
1	6-G	4	MSE
1	6-G	23	ASP
1	6-G	36	ARG
1	6-G	43	ARG
1	6-G	66	ARG
1	6-G	83	LEU
1	6-G	97	ASP
1	6-G	109	LEU
1	6-G	123	THR
1	6-G	124	THR
1	6-G	136	ASP
1	6-G	161	ARG
1	6-G	175	PHE
1	6-G	231	VAL
1	6-G	288	VAL
1	6-G	292	MSE
1	6-G	302	ASP
1	6-G	309	GLU
1	6-G	322	VAL
1	6-G	323	SER
1	6-G	328	HIS
1	6-G	337	MSE
1	6-G	343	SER
1	6-G	371	GLU
1	6-H	4	MSE
1	6-H	9	ARG
1	6-H	23	ASP
1	6-H	43	ARG
1	6-H	66	ARG
1	6-H	97	ASP
1	6-H	99	VAL

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Mol	Chain	Res	Type
1	6-H	109	LEU
1	6-H	116	ARG
1	6-H	118	ARG
1	6-H	148	PRO
1	6-H	175	PHE
1	6-H	177	SER
1	6-H	231	VAL
1	6-H	328	HIS
1	6-H	332	GLU
1	6-H	354	GLU
1	6-H	367	GLN
1	7-A	4	MSE
1	7-A	6	PHE
1	7-A	16	ARG
1	7-A	23	ASP
1	7-A	33	THR
1	7-A	36	ARG
1	7-A	40	ASP
1	7-A	41	GLU
1	7-A	43	ARG
1	7-A	66	ARG
1	7-A	83	LEU
1	7-A	84	LEU
1	7-A	98	ASP
1	7-A	104	ASP
1	7-A	112	ARG
1	7-A	124	THR
1	7-A	126	GLU
1	7-A	132	LEU
1	7-A	136	ASP
1	7-A	147	ASN
1	7-A	161	ARG
1	7-A	175	PHE
1	7-A	231	VAL
1	7-A	244	LEU
1	7-A	253	ARG
1	7-A	264	ARG
1	7-A	266	ARG
1	7-A	291	GLN
1	7-A	292	MSE
1	7-A	328	HIS
1	7-A	332	GLU

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Mol	Chain	Res	Type
1	7-A	342	LEU
1	7-A	367	GLN
1	7-B	4	MSE
1	7-B	5	ARG
1	7-B	6	PHE
1	7-B	16	ARG
1	7-B	33	THR
1	7-B	36	ARG
1	7-B	40	ASP
1	7-B	98	ASP
1	7-B	99	VAL
1	7-B	109	LEU
1	7-B	126	GLU
1	7-B	128	ILE
1	7-B	161	ARG
1	7-B	263	GLU
1	7-B	264	ARG
1	7-B	266	ARG
1	7-B	284	GLN
1	7-B	292	MSE
1	7-B	332	GLU
1	7-B	337	MSE
1	7-B	338	THR
1	7-B	340	ARG
1	7-B	343	SER
1	7-B	345	GLU
1	7-C	4	MSE
1	7-C	23	ASP
1	7-C	35	GLU
1	7-C	39	GLN
1	7-C	40	ASP
1	7-C	42	PRO
1	7-C	43	ARG
1	7-C	96	THR
1	7-C	97	ASP
1	7-C	117	VAL
1	7-C	231	VAL
1	7-C	263	GLU
1	7-C	281	GLU
1	7-C	300	SER
1	7-C	313	ASP
1	7-C	324	LEU

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Mol	Chain	Res	Type
1	7-C	337	MSE
1	7-C	342	LEU
1	7-C	350	ARG
1	7-C	381	THR
1	7-D	4	MSE
1	7-D	23	ASP
1	7-D	84	LEU
1	7-D	93	VAL
1	7-D	95	SER
1	7-D	96	THR
1	7-D	98	ASP
1	7-D	99	VAL
1	7-D	112	ARG
1	7-D	123	THR
1	7-D	124	THR
1	7-D	126	GLU
1	7-D	227	THR
1	7-D	231	VAL
1	7-D	244	LEU
1	7-D	252	HIS
1	7-D	281	GLU
1	7-D	324	LEU
1	7-D	333	CYS
1	7-D	338	THR
1	7-D	340	ARG
1	7-D	343	SER
1	7-D	350	ARG
1	7-D	375	ARG
1	7-E	4	MSE
1	7-E	16	ARG
1	7-E	23	ASP
1	7-E	33	THR
1	7-E	54	ARG
1	7-E	84	LEU
1	7-E	98	ASP
1	7-E	104	ASP
1	7-E	108	ASP
1	7-E	132	LEU
1	7-E	161	ARG
1	7-E	177	SER
1	7-E	191	SER
1	7-E	242	ARG

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Mol	Chain	Res	Type
1	7-E	292	MSE
1	7-E	309	GLU
1	7-E	328	HIS
1	7-E	354	GLU
1	7-F	23	ASP
1	7-F	37	ARG
1	7-F	43	ARG
1	7-F	97	ASP
1	7-F	118	ARG
1	7-F	161	ARG
1	7-F	175	PHE
1	7-F	177	SER
1	7-F	213	ARG
1	7-F	242	ARG
1	7-F	244	LEU
1	7-F	248	SER
1	7-F	323	SER
1	7-F	328	HIS
1	7-F	330	LEU
1	7-F	332	GLU
1	7-F	354	GLU
1	7-F	367	GLN
1	7-F	375	ARG
1	7-G	4	MSE
1	7-G	16	ARG
1	7-G	18	SER
1	7-G	104	ASP
1	7-G	112	ARG
1	7-G	117	VAL
1	7-G	136	ASP
1	7-G	147	ASN
1	7-G	161	ARG
1	7-G	213	ARG
1	7-G	292	MSE
1	7-G	309	GLU
1	7-G	371	GLU
1	7-H	16	ARG
1	7-H	18	SER
1	7-H	23	ASP
1	7-H	36	ARG
1	7-H	43	ARG
1	7-H	116	ARG

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Mol	Chain	Res	Type
1	7-H	118	ARG
1	7-H	124	THR
1	7-H	147	ASN
1	7-H	175	PHE
1	7-H	244	LEU
1	7-H	253	ARG
1	7-H	259	ARG
1	7-H	266	ARG
1	7-H	309	GLU
1	7-H	324	LEU
1	7-H	367	GLN
1	7-H	375	ARG
1	8-A	33	THR
1	8-A	37	ARG
1	8-A	40	ASP
1	8-A	43	ARG
1	8-A	98	ASP
1	8-A	116	ARG
1	8-A	118	ARG
1	8-A	124	THR
1	8-A	161	ARG
1	8-A	179	VAL
1	8-A	244	LEU
1	8-A	248	SER
1	8-A	338	THR
1	8-A	340	ARG
1	8-A	349	ARG
1	8-B	4	MSE
1	8-B	74	SER
1	8-B	84	LEU
1	8-B	95	SER
1	8-B	98	ASP
1	8-B	128	ILE
1	8-B	161	ARG
1	8-B	231	VAL
1	8-B	248	SER
1	8-B	302	ASP
1	8-B	328	HIS
1	8-B	332	GLU
1	8-B	337	MSE
1	8-B	350	ARG
1	8-C	36	ARG

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Mol	Chain	Res	Type
1	8-C	112	ARG
1	8-C	161	ARG
1	8-C	175	PHE
1	8-C	177	SER
1	8-C	236	ASP
1	8-C	244	LEU
1	8-C	248	SER
1	8-C	253	ARG
1	8-C	264	ARG
1	8-C	281	GLU
1	8-C	313	ASP
1	8-C	337	MSE
1	8-C	338	THR
1	8-C	340	ARG
1	8-C	342	LEU
1	8-C	343	SER
1	8-C	367	GLN
1	8-D	23	ASP
1	8-D	33	THR
1	8-D	36	ARG
1	8-D	104	ASP
1	8-D	112	ARG
1	8-D	144	THR
1	8-D	157	GLU
1	8-D	165	ARG
1	8-D	242	ARG
1	8-D	253	ARG
1	8-D	279	LEU
1	8-D	281	GLU
1	8-D	324	LEU
1	8-D	330	LEU
1	8-D	332	GLU
1	8-D	337	MSE
1	8-D	339	HIS
1	8-D	356	LEU
1	8-E	16	ARG
1	8-E	18	SER
1	8-E	124	THR
1	8-E	147	ASN
1	8-E	151	THR
1	8-E	161	ARG
1	8-E	264	ARG

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Mol	Chain	Res	Type
1	8-E	289	LYS
1	8-E	292	MSE
1	8-E	313	ASP
1	8-E	324	LEU
1	8-E	328	HIS
1	8-E	332	GLU
1	8-E	336	LEU
1	8-E	341	PRO
1	8-E	347	ARG
1	8-E	349	ARG
1	8-E	355	SER
1	8-E	371	GLU
1	8-F	4	MSE
1	8-F	23	ASP
1	8-F	35	GLU
1	8-F	37	ARG
1	8-F	43	ARG
1	8-F	84	LEU
1	8-F	99	VAL
1	8-F	126	GLU
1	8-F	147	ASN
1	8-F	149	LEU
1	8-F	177	SER
1	8-F	213	ARG
1	8-F	292	MSE
1	8-F	309	GLU
1	8-F	330	LEU
1	8-F	338	THR
1	8-F	339	HIS
1	8-F	355	SER
1	8-F	375	ARG
1	8-G	16	ARG
1	8-G	33	THR
1	8-G	99	VAL
1	8-G	112	ARG
1	8-G	152	VAL
1	8-G	161	ARG
1	8-G	248	SER
1	8-G	289	LYS
1	8-G	302	ASP
1	8-G	309	GLU
1	8-G	328	HIS

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Mol	Chain	Res	Type
1	8-G	332	GLU
1	8-G	337	MSE
1	8-G	342	LEU
1	8-G	355	SER
1	8-G	374	SER
1	8-H	4	MSE
1	8-H	16	ARG
1	8-H	23	ASP
1	8-H	36	ARG
1	8-H	84	LEU
1	8-H	93	VAL
1	8-H	96	THR
1	8-H	99	VAL
1	8-H	118	ARG
1	8-H	147	ASN
1	8-H	161	ARG
1	8-H	177	SER
1	8-H	263	GLU
1	8-H	317	LEU
1	8-H	328	HIS
1	8-H	337	MSE
1	9-A	4	MSE
1	9-A	18	SER
1	9-A	23	ASP
1	9-A	84	LEU
1	9-A	97	ASP
1	9-A	99	VAL
1	9-A	116	ARG
1	9-A	132	LEU
1	9-A	147	ASN
1	9-A	161	ARG
1	9-A	179	VAL
1	9-A	226	THR
1	9-A	264	ARG
1	9-A	322	VAL
1	9-A	328	HIS
1	9-A	332	GLU
1	9-A	337	MSE
1	9-A	340	ARG
1	9-A	343	SER
1	9-B	33	THR
1	9-B	39	GLN

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Mol	Chain	Res	Type
1	9-B	43	ARG
1	9-B	66	ARG
1	9-B	98	ASP
1	9-B	104	ASP
1	9-B	116	ARG
1	9-B	126	GLU
1	9-B	147	ASN
1	9-B	161	ARG
1	9-B	206	LEU
1	9-B	213	ARG
1	9-B	231	VAL
1	9-B	284	GLN
1	9-B	289	LYS
1	9-B	319	THR
1	9-B	328	HIS
1	9-B	332	GLU
1	9-B	354	GLU
1	9-C	23	ASP
1	9-C	33	THR
1	9-C	36	ARG
1	9-C	39	GLN
1	9-C	43	ARG
1	9-C	84	LEU
1	9-C	88	ARG
1	9-C	96	THR
1	9-C	98	ASP
1	9-C	104	ASP
1	9-C	124	THR
1	9-C	143	GLU
1	9-C	161	ARG
1	9-C	175	PHE
1	9-C	177	SER
1	9-C	226	THR
1	9-C	231	VAL
1	9-C	248	SER
1	9-C	252	HIS
1	9-C	253	ARG
1	9-C	300	SER
1	9-C	322	VAL
1	9-C	327	VAL
1	9-C	339	HIS
1	9-C	340	ARG

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Mol	Chain	Res	Type
1	9-C	343	SER
1	9-C	375	ARG
1	9-D	17	PRO
1	9-D	23	ASP
1	9-D	66	ARG
1	9-D	95	SER
1	9-D	98	ASP
1	9-D	99	VAL
1	9-D	109	LEU
1	9-D	112	ARG
1	9-D	124	THR
1	9-D	216	ASP
1	9-D	253	ARG
1	9-D	313	ASP
1	9-D	328	HIS
1	9-D	332	GLU
1	9-D	337	MSE
1	9-D	347	ARG
1	9-E	23	ASP
1	9-E	84	LEU
1	9-E	98	ASP
1	9-E	104	ASP
1	9-E	112	ARG
1	9-E	132	LEU
1	9-E	161	ARG
1	9-E	214	ASP
1	9-E	231	VAL
1	9-E	244	LEU
1	9-E	289	LYS
1	9-E	291	GLN
1	9-E	292	MSE
1	9-E	309	GLU
1	9-E	324	LEU
1	9-E	332	GLU
1	9-E	342	LEU
1	9-E	343	SER
1	9-E	350	ARG
1	9-F	23	ASP
1	9-F	33	THR
1	9-F	84	LEU
1	9-F	96	THR
1	9-F	97	ASP

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Mol	Chain	Res	Type
1	9-F	98	ASP
1	9-F	108	ASP
1	9-F	126	GLU
1	9-F	128	ILE
1	9-F	147	ASN
1	9-F	149	LEU
1	9-F	160	ARG
1	9-F	161	ARG
1	9-F	231	VAL
1	9-F	242	ARG
1	9-F	244	LEU
1	9-F	253	ARG
1	9-F	292	MSE
1	9-F	324	LEU
1	9-F	332	GLU
1	9-F	343	SER
1	9-G	4	MSE
1	9-G	83	LEU
1	9-G	97	ASP
1	9-G	99	VAL
1	9-G	123	THR
1	9-G	134	GLU
1	9-G	147	ASN
1	9-G	161	ARG
1	9-G	213	ARG
1	9-G	231	VAL
1	9-G	309	GLU
1	9-G	332	GLU
1	9-G	337	MSE
1	9-G	367	GLN
1	9-H	9	ARG
1	9-H	50	GLU
1	9-H	84	LEU
1	9-H	93	VAL
1	9-H	95	SER
1	9-H	109	LEU
1	9-H	118	ARG
1	9-H	124	THR
1	9-H	126	GLU
1	9-H	165	ARG
1	9-H	231	VAL
1	9-H	266	ARG

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Mol	Chain	Res	Type
1	9-H	302	ASP
1	9-H	337	MSE
1	9-H	367	GLN
1	9-H	375	ARG
1	10-A	4	MSE
1	10-A	16	ARG
1	10-A	17	PRO
1	10-A	18	SER
1	10-A	23	ASP
1	10-A	33	THR
1	10-A	35	GLU
1	10-A	36	ARG
1	10-A	39	GLN
1	10-A	40	ASP
1	10-A	66	ARG
1	10-A	108	ASP
1	10-A	118	ARG
1	10-A	121	ASP
1	10-A	124	THR
1	10-A	132	LEU
1	10-A	161	ARG
1	10-A	198	SER
1	10-A	226	THR
1	10-A	236	ASP
1	10-A	322	VAL
1	10-A	328	HIS
1	10-A	332	GLU
1	10-A	337	MSE
1	10-A	340	ARG
1	10-A	342	LEU
1	10-A	343	SER
1	10-A	374	SER
1	10-B	23	ASP
1	10-B	41	GLU
1	10-B	84	LEU
1	10-B	98	ASP
1	10-B	109	LEU
1	10-B	118	ARG
1	10-B	124	THR
1	10-B	147	ASN
1	10-B	161	ARG
1	10-B	177	SER

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Mol	Chain	Res	Type
1	10-B	192	LEU
1	10-B	206	LEU
1	10-B	213	ARG
1	10-B	214	ASP
1	10-B	242	ARG
1	10-B	259	ARG
1	10-B	284	GLN
1	10-B	289	LYS
1	10-B	302	ASP
1	10-B	323	SER
1	10-B	328	HIS
1	10-C	5	ARG
1	10-C	16	ARG
1	10-C	23	ASP
1	10-C	43	ARG
1	10-C	96	THR
1	10-C	99	VAL
1	10-C	103	THR
1	10-C	116	ARG
1	10-C	161	ARG
1	10-C	175	PHE
1	10-C	198	SER
1	10-C	231	VAL
1	10-C	253	ARG
1	10-C	283	PRO
1	10-C	285	HIS
1	10-C	313	ASP
1	10-C	323	SER
1	10-C	327	VAL
1	10-C	332	GLU
1	10-C	342	LEU
1	10-C	347	ARG
1	10-D	6	PHE
1	10-D	33	THR
1	10-D	36	ARG
1	10-D	39	GLN
1	10-D	43	ARG
1	10-D	116	ARG
1	10-D	126	GLU
1	10-D	213	ARG
1	10-D	236	ASP
1	10-D	244	LEU

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Mol	Chain	Res	Type
1	10-D	248	SER
1	10-D	270	VAL
1	10-D	292	MSE
1	10-D	300	SER
1	10-D	328	HIS
1	10-D	332	GLU
1	10-D	333	CYS
1	10-D	347	ARG
1	10-D	350	ARG
1	10-D	354	GLU
1	10-D	367	GLN
1	10-D	375	ARG
1	10-E	16	ARG
1	10-E	18	SER
1	10-E	23	ASP
1	10-E	33	THR
1	10-E	98	ASP
1	10-E	126	GLU
1	10-E	160	ARG
1	10-E	161	ARG
1	10-E	175	PHE
1	10-E	281	GLU
1	10-E	292	MSE
1	10-E	324	LEU
1	10-E	332	GLU
1	10-E	345	GLU
1	10-E	355	SER
1	10-F	4	MSE
1	10-F	33	THR
1	10-F	39	GLN
1	10-F	83	LEU
1	10-F	123	THR
1	10-F	124	THR
1	10-F	136	ASP
1	10-F	147	ASN
1	10-F	151	THR
1	10-F	160	ARG
1	10-F	161	ARG
1	10-F	175	PHE
1	10-F	213	ARG
1	10-F	253	ARG
1	10-F	259	ARG

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Mol	Chain	Res	Type
1	10-F	292	MSE
1	10-F	338	THR
1	10-F	352	ILE
1	10-G	4	MSE
1	10-G	16	ARG
1	10-G	18	SER
1	10-G	23	ASP
1	10-G	33	THR
1	10-G	40	ASP
1	10-G	66	ARG
1	10-G	74	SER
1	10-G	83	LEU
1	10-G	96	THR
1	10-G	104	ASP
1	10-G	112	ARG
1	10-G	121	ASP
1	10-G	132	LEU
1	10-G	151	THR
1	10-G	161	ARG
1	10-G	165	ARG
1	10-G	198	SER
1	10-G	214	ASP
1	10-G	231	VAL
1	10-G	244	LEU
1	10-G	292	MSE
1	10-G	293	SER
1	10-H	6	PHE
1	10-H	16	ARG
1	10-H	23	ASP
1	10-H	36	ARG
1	10-H	43	ARG
1	10-H	66	ARG
1	10-H	124	THR
1	10-H	192	LEU
1	10-H	213	ARG
1	10-H	226	THR
1	10-H	253	ARG
1	10-H	300	SER
1	10-H	309	GLU
1	10-H	324	LEU
1	10-H	328	HIS
1	10-H	342	LEU

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Mol	Chain	Res	Type
1	10-H	347	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (186) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	252	HIS
1	1-A	367	GLN
1	1-B	285	HIS
1	1-C	147	ASN
1	1-D	254	GLN
1	1-E	113	GLN
1	1-E	252	HIS
1	1-E	275	HIS
1	1-F	181	GLN
1	1-F	252	HIS
1	1-G	284	GLN
1	1-G	367	GLN
1	1-H	147	ASN
1	1-H	245	HIS
1	1-H	254	GLN
1	2-A	163	HIS
1	2-B	163	HIS
1	2-B	252	HIS
1	2-B	284	GLN
1	2-C	147	ASN
1	2-C	339	HIS
1	2-C	367	GLN
1	2-D	39	GLN
1	2-D	254	GLN
1	2-E	285	HIS
1	2-F	367	GLN
1	2-G	113	GLN
1	2-G	284	GLN
1	2-H	113	GLN
1	2-H	147	ASN
1	2-H	245	HIS
1	2-H	254	GLN
1	3-A	252	HIS
1	3-A	367	GLN
1	3-B	252	HIS
1	3-C	147	ASN
1	3-D	91	GLN

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Mol	Chain	Res	Type
1	3-D	254	GLN
1	3-D	339	HIS
1	3-E	113	GLN
1	3-E	163	HIS
1	3-E	285	HIS
1	3-F	181	GLN
1	3-F	285	HIS
1	3-G	284	GLN
1	3-H	245	HIS
1	3-H	252	HIS
1	3-H	254	GLN
1	4-A	275	HIS
1	4-A	339	HIS
1	4-A	367	GLN
1	4-B	113	GLN
1	4-B	181	GLN
1	4-B	284	GLN
1	4-B	285	HIS
1	4-B	339	HIS
1	4-C	39	GLN
1	4-C	147	ASN
1	4-D	91	GLN
1	4-D	113	GLN
1	4-D	252	HIS
1	4-D	254	GLN
1	4-D	285	HIS
1	4-D	367	GLN
1	4-E	113	GLN
1	4-E	147	ASN
1	4-F	181	GLN
1	4-F	285	HIS
1	4-F	367	GLN
1	4-G	252	HIS
1	4-G	284	GLN
1	4-G	367	GLN
1	4-H	245	HIS
1	4-H	284	GLN
1	5-B	113	GLN
1	5-B	284	GLN
1	5-B	339	HIS
1	5-C	39	GLN
1	5-C	113	GLN

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Mol	Chain	Res	Type
1	5-C	181	GLN
1	5-C	254	GLN
1	5-D	39	GLN
1	5-D	91	GLN
1	5-D	113	GLN
1	5-D	147	ASN
1	5-E	39	GLN
1	5-E	113	GLN
1	5-E	339	HIS
1	5-F	39	GLN
1	5-F	181	GLN
1	5-F	252	HIS
1	5-F	285	HIS
1	5-G	113	GLN
1	5-G	147	ASN
1	5-G	367	GLN
1	5-H	245	HIS
1	5-H	284	GLN
1	6-B	113	GLN
1	6-B	284	GLN
1	6-C	29	HIS
1	6-C	39	GLN
1	6-C	113	GLN
1	6-C	147	ASN
1	6-D	91	GLN
1	6-D	113	GLN
1	6-D	147	ASN
1	6-D	285	HIS
1	6-D	339	HIS
1	6-E	113	GLN
1	6-F	181	GLN
1	6-H	147	ASN
1	6-H	245	HIS
1	6-H	285	HIS
1	6-H	367	GLN
1	7-A	163	HIS
1	7-B	113	GLN
1	7-B	252	HIS
1	7-B	284	GLN
1	7-B	339	HIS
1	7-C	39	GLN
1	7-C	113	GLN

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Mol	Chain	Res	Type
1	7-C	147	ASN
1	7-C	252	HIS
1	7-D	91	GLN
1	7-D	147	ASN
1	7-D	285	HIS
1	7-E	39	GLN
1	7-F	181	GLN
1	7-F	367	GLN
1	7-H	147	ASN
1	7-H	339	HIS
1	8-A	39	GLN
1	8-B	113	GLN
1	8-B	367	GLN
1	8-C	39	GLN
1	8-C	113	GLN
1	8-C	339	HIS
1	8-D	91	GLN
1	8-D	181	GLN
1	8-E	147	ASN
1	8-E	252	HIS
1	8-E	285	HIS
1	8-F	181	GLN
1	8-G	147	ASN
1	8-H	147	ASN
1	8-H	245	HIS
1	8-H	254	GLN
1	8-H	339	HIS
1	9-A	39	GLN
1	9-A	163	HIS
1	9-A	252	HIS
1	9-B	284	GLN
1	9-C	39	GLN
1	9-C	275	HIS
1	9-C	367	GLN
1	9-D	91	GLN
1	9-D	252	HIS
1	9-E	39	GLN
1	9-E	367	GLN
1	9-F	39	GLN
1	9-F	147	ASN
1	9-F	181	GLN
1	9-F	252	HIS

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Mol	Chain	Res	Type
1	9-G	147	ASN
1	9-G	163	HIS
1	9-H	245	HIS
1	9-H	367	GLN
1	10-A	181	GLN
1	10-A	252	HIS
1	10-B	163	HIS
1	10-B	252	HIS
1	10-B	284	GLN
1	10-C	285	HIS
1	10-C	367	GLN
1	10-D	91	GLN
1	10-D	367	GLN
1	10-E	39	GLN
1	10-E	147	ASN
1	10-E	252	HIS
1	10-F	147	ASN
1	10-F	181	GLN
1	10-F	252	HIS
1	10-F	339	HIS
1	10-G	328	HIS
1	10-H	245	HIS
1	10-H	254	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	1-A	197	1	24,24,25	2.57	7 (29%)	28,32,34	1.34	4 (14%)
1	LLP	1-B	197	1	24,24,25	2.71	7 (29%)	28,32,34	1.19	2 (7%)
1	LLP	1-C	197	1	24,24,25	2.63	7 (29%)	28,32,34	1.37	5 (17%)
1	LLP	1-D	197	1	24,24,25	2.63	6 (25%)	28,32,34	1.16	4 (14%)
1	LLP	1-E	197	1	24,24,25	2.64	7 (29%)	28,32,34	1.15	4 (14%)
1	LLP	1-F	197	1	24,24,25	2.65	7 (29%)	28,32,34	1.29	6 (21%)
1	LLP	1-G	197	1	24,24,25	2.73	7 (29%)	28,32,34	1.14	2 (7%)
1	LLP	1-H	197	1	24,24,25	2.60	5 (20%)	28,32,34	1.19	3 (10%)
1	LLP	10-A	197	1	24,24,25	2.74	7 (29%)	28,32,34	1.29	4 (14%)
1	LLP	10-B	197	1	24,24,25	2.67	6 (25%)	28,32,34	1.52	7 (25%)
1	LLP	10-C	197	1	24,24,25	2.72	7 (29%)	28,32,34	1.29	4 (14%)
1	LLP	10-D	197	1	24,24,25	2.62	5 (20%)	28,32,34	1.10	3 (10%)
1	LLP	10-E	197	1	24,24,25	2.67	6 (25%)	28,32,34	1.07	3 (10%)
1	LLP	10-F	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.24	5 (17%)
1	LLP	10-G	197	1	24,24,25	2.70	7 (29%)	28,32,34	1.43	5 (17%)
1	LLP	10-H	197	1	24,24,25	2.69	7 (29%)	28,32,34	1.25	3 (10%)
1	LLP	2-A	197	1	24,24,25	2.77	7 (29%)	28,32,34	1.32	3 (10%)
1	LLP	2-B	197	1	24,24,25	2.72	6 (25%)	28,32,34	1.13	4 (14%)
1	LLP	2-C	197	1	24,24,25	2.70	7 (29%)	28,32,34	1.30	3 (10%)
1	LLP	2-D	197	1	24,24,25	2.60	6 (25%)	28,32,34	1.13	3 (10%)
1	LLP	2-E	197	1	24,24,25	2.79	7 (29%)	28,32,34	1.26	3 (10%)
1	LLP	2-F	197	1	24,24,25	2.67	7 (29%)	28,32,34	1.40	6 (21%)
1	LLP	2-G	197	1	24,24,25	2.78	7 (29%)	28,32,34	1.19	2 (7%)
1	LLP	2-H	197	1	24,24,25	2.60	7 (29%)	28,32,34	1.67	6 (21%)
1	LLP	3-A	197	1	24,24,25	2.71	7 (29%)	28,32,34	1.31	5 (17%)
1	LLP	3-B	197	1	24,24,25	2.75	6 (25%)	28,32,34	1.34	6 (21%)
1	LLP	3-C	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.38	5 (17%)
1	LLP	3-D	197	1	24,24,25	2.60	5 (20%)	28,32,34	1.16	4 (14%)
1	LLP	3-E	197	1	24,24,25	2.79	7 (29%)	28,32,34	1.14	2 (7%)
1	LLP	3-F	197	1	24,24,25	2.64	6 (25%)	28,32,34	1.28	3 (10%)
1	LLP	3-G	197	1	24,24,25	2.69	7 (29%)	28,32,34	1.25	3 (10%)
1	LLP	3-H	197	1	24,24,25	2.80	7 (29%)	28,32,34	1.37	5 (17%)
1	LLP	4-A	197	1	24,24,25	2.67	7 (29%)	28,32,34	1.32	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	4-B	197	1	24,24,25	2.69	7 (29%)	28,32,34	1.28	3 (10%)
1	LLP	4-C	197	1	24,24,25	2.83	7 (29%)	28,32,34	1.38	6 (21%)
1	LLP	4-D	197	1	24,24,25	2.56	6 (25%)	28,32,34	1.25	3 (10%)
1	LLP	4-E	197	1	24,24,25	2.70	7 (29%)	28,32,34	1.30	4 (14%)
1	LLP	4-F	197	1	24,24,25	2.65	7 (29%)	28,32,34	1.29	6 (21%)
1	LLP	4-G	197	1	24,24,25	2.67	7 (29%)	28,32,34	1.33	4 (14%)
1	LLP	4-H	197	1	24,24,25	2.80	7 (29%)	28,32,34	1.26	3 (10%)
1	LLP	5-A	197	1	24,24,25	2.78	7 (29%)	28,32,34	1.34	5 (17%)
1	LLP	5-B	197	1	24,24,25	2.71	7 (29%)	28,32,34	1.11	3 (10%)
1	LLP	5-C	197	1	24,24,25	2.69	7 (29%)	28,32,34	1.46	6 (21%)
1	LLP	5-D	197	1	24,24,25	2.57	5 (20%)	28,32,34	1.33	4 (14%)
1	LLP	5-E	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.18	3 (10%)
1	LLP	5-F	197	1	24,24,25	2.49	6 (25%)	28,32,34	1.32	4 (14%)
1	LLP	5-G	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.36	4 (14%)
1	LLP	5-H	197	1	24,24,25	2.63	7 (29%)	28,32,34	1.45	5 (17%)
1	LLP	6-A	197	1	24,24,25	2.71	7 (29%)	28,32,34	1.32	4 (14%)
1	LLP	6-B	197	1	24,24,25	2.62	6 (25%)	28,32,34	1.26	4 (14%)
1	LLP	6-C	197	1	24,24,25	2.84	7 (29%)	28,32,34	1.47	6 (21%)
1	LLP	6-D	197	1	24,24,25	2.60	6 (25%)	28,32,34	1.23	4 (14%)
1	LLP	6-E	197	1	24,24,25	2.63	7 (29%)	28,32,34	1.19	2 (7%)
1	LLP	6-F	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.23	4 (14%)
1	LLP	6-G	197	1	24,24,25	2.73	7 (29%)	28,32,34	1.26	4 (14%)
1	LLP	6-H	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.23	3 (10%)
1	LLP	7-A	197	1	24,24,25	2.76	7 (29%)	28,32,34	1.28	5 (17%)
1	LLP	7-B	197	1	24,24,25	2.64	6 (25%)	28,32,34	1.34	5 (17%)
1	LLP	7-C	197	1	24,24,25	2.65	6 (25%)	28,32,34	1.36	4 (14%)
1	LLP	7-D	197	1	24,24,25	2.65	6 (25%)	28,32,34	1.60	5 (17%)
1	LLP	7-E	197	1	24,24,25	2.73	7 (29%)	28,32,34	1.12	3 (10%)
1	LLP	7-F	197	1	24,24,25	2.70	7 (29%)	28,32,34	1.34	6 (21%)
1	LLP	7-G	197	1	24,24,25	2.75	7 (29%)	28,32,34	1.33	5 (17%)
1	LLP	7-H	197	1	24,24,25	2.65	7 (29%)	28,32,34	1.64	5 (17%)
1	LLP	8-A	197	1	24,24,25	2.73	7 (29%)	28,32,34	1.27	4 (14%)
1	LLP	8-B	197	1	24,24,25	2.65	6 (25%)	28,32,34	1.19	3 (10%)
1	LLP	8-C	197	1	24,24,25	2.72	7 (29%)	28,32,34	1.40	5 (17%)
1	LLP	8-D	197	1	24,24,25	2.60	6 (25%)	28,32,34	1.52	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	8-E	197	1	24,24,25	2.71	7 (29%)	28,32,34	1.18	4 (14%)
1	LLP	8-F	197	1	24,24,25	2.62	7 (29%)	28,32,34	1.37	6 (21%)
1	LLP	8-G	197	1	24,24,25	2.62	7 (29%)	28,32,34	1.34	2 (7%)
1	LLP	8-H	197	1	24,24,25	2.69	7 (29%)	28,32,34	1.29	4 (14%)
1	LLP	9-A	197	1	24,24,25	2.64	7 (29%)	28,32,34	1.22	4 (14%)
1	LLP	9-B	197	1	24,24,25	2.40	5 (20%)	28,32,34	1.60	8 (28%)
1	LLP	9-C	197	1	24,24,25	2.74	7 (29%)	28,32,34	1.26	4 (14%)
1	LLP	9-D	197	1	24,24,25	2.55	5 (20%)	28,32,34	1.20	3 (10%)
1	LLP	9-E	197	1	24,24,25	2.66	7 (29%)	28,32,34	1.25	4 (14%)
1	LLP	9-F	197	1	24,24,25	2.65	7 (29%)	28,32,34	1.36	5 (17%)
1	LLP	9-G	197	1	24,24,25	2.71	7 (29%)	28,32,34	1.14	2 (7%)
1	LLP	9-H	197	1	24,24,25	2.65	7 (29%)	28,32,34	1.20	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	1-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	1-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	10-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-E	197	1	-	0/15/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	2-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	2-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	3-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	4-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	5-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	6-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	7-G	197	1	-	0/15/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	7-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	8-H	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-A	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-B	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-C	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-D	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-E	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-F	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-G	197	1	-	0/15/17/19	0/1/1/1
1	LLP	9-H	197	1	-	0/15/17/19	0/1/1/1

All (532) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-C	197	LLP	C4-C5	-4.12	1.36	1.42
1	4-C	197	LLP	C4-C5	-4.04	1.36	1.42
1	4-A	197	LLP	C4-C5	-4.03	1.36	1.42
1	5-A	197	LLP	C4-C5	-3.97	1.36	1.42
1	9-A	197	LLP	C4-C5	-3.86	1.37	1.42
1	5-D	197	LLP	C4-C5	-3.86	1.37	1.42
1	7-C	197	LLP	C4-C5	-3.85	1.37	1.42
1	7-A	197	LLP	C4-C5	-3.72	1.37	1.42
1	1-D	197	LLP	C4-C5	-3.71	1.37	1.42
1	3-A	197	LLP	C4-C5	-3.70	1.37	1.42
1	2-A	197	LLP	C4-C5	-3.70	1.37	1.42
1	3-B	197	LLP	C4-C5	-3.68	1.37	1.42
1	10-E	197	LLP	C4-C5	-3.67	1.37	1.42
1	7-D	197	LLP	C4-C5	-3.67	1.37	1.42
1	10-A	197	LLP	C4-C5	-3.67	1.37	1.42
1	2-C	197	LLP	C4-C5	-3.66	1.37	1.42
1	6-D	197	LLP	C4-C5	-3.66	1.37	1.42
1	10-C	197	LLP	C4-C5	-3.64	1.37	1.42
1	7-B	197	LLP	C4-C5	-3.62	1.37	1.42
1	8-D	197	LLP	C4-C5	-3.60	1.37	1.42
1	8-A	197	LLP	C4-C5	-3.57	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	9-D	197	LLP	C4-C5	-3.53	1.37	1.42
1	6-B	197	LLP	C4-C5	-3.53	1.37	1.42
1	5-F	197	LLP	C4-C5	-3.49	1.37	1.42
1	2-F	197	LLP	C4-C5	-3.48	1.37	1.42
1	2-D	197	LLP	C4-C5	-3.47	1.37	1.42
1	1-A	197	LLP	C4-C5	-3.45	1.37	1.42
1	6-A	197	LLP	C4-C5	-3.45	1.37	1.42
1	8-E	197	LLP	C4-C5	-3.42	1.37	1.42
1	1-C	197	LLP	C4-C5	-3.42	1.37	1.42
1	7-F	197	LLP	C4-C5	-3.40	1.37	1.42
1	6-E	197	LLP	C4-C5	-3.39	1.37	1.42
1	9-F	197	LLP	C4-C5	-3.36	1.37	1.42
1	10-D	197	LLP	C4-C5	-3.35	1.37	1.42
1	8-B	197	LLP	C4-C5	-3.31	1.37	1.42
1	4-F	197	LLP	C4-C5	-3.30	1.37	1.42
1	3-D	197	LLP	C4-C5	-3.29	1.37	1.42
1	6-F	197	LLP	C4-C5	-3.27	1.37	1.42
1	8-C	197	LLP	C4-C5	-3.26	1.37	1.42
1	8-F	197	LLP	C4-C5	-3.25	1.37	1.42
1	9-B	197	LLP	C4-C5	-3.24	1.37	1.42
1	9-E	197	LLP	C4-C5	-3.23	1.37	1.42
1	3-F	197	LLP	C4-C5	-3.22	1.37	1.42
1	10-B	197	LLP	C4-C5	-3.22	1.37	1.42
1	9-G	197	LLP	C4-C5	-3.19	1.37	1.42
1	4-D	197	LLP	C4-C5	-3.19	1.37	1.42
1	6-G	197	LLP	C4-C5	-3.18	1.37	1.42
1	3-G	197	LLP	C4-C5	-3.16	1.37	1.42
1	5-C	197	LLP	C4-C5	-3.15	1.37	1.42
1	2-E	197	LLP	C4-C5	-3.14	1.37	1.42
1	1-F	197	LLP	C4-C5	-3.14	1.37	1.42
1	3-E	197	LLP	C4-C5	-3.12	1.38	1.42
1	2-B	197	LLP	C4-C5	-3.11	1.38	1.42
1	3-H	197	LLP	C4-C5	-3.10	1.38	1.42
1	5-E	197	LLP	C4-C5	-3.10	1.38	1.42
1	7-H	197	LLP	C4-C5	-3.10	1.38	1.42
1	7-E	197	LLP	C4-C5	-3.07	1.38	1.42
1	10-F	197	LLP	C4-C5	-3.07	1.38	1.42
1	1-E	197	LLP	C4-C5	-3.07	1.38	1.42
1	8-G	197	LLP	C4-C5	-3.06	1.38	1.42
1	1-B	197	LLP	C4-C5	-3.05	1.38	1.42
1	6-C	197	LLP	C4-C5	-2.97	1.38	1.42
1	2-G	197	LLP	C4-C5	-2.94	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-G	197	LLP	C4-C5	-2.92	1.38	1.42
1	4-G	197	LLP	C4-C5	-2.92	1.38	1.42
1	5-B	197	LLP	C4-C5	-2.91	1.38	1.42
1	1-G	197	LLP	C4-C5	-2.91	1.38	1.42
1	2-H	197	LLP	C4-C5	-2.89	1.38	1.42
1	5-H	197	LLP	C4-C5	-2.84	1.38	1.42
1	1-H	197	LLP	C4-C5	-2.80	1.38	1.42
1	9-H	197	LLP	C4-C5	-2.80	1.38	1.42
1	7-G	197	LLP	C4-C5	-2.73	1.38	1.42
1	3-C	197	LLP	C4-C5	-2.72	1.38	1.42
1	4-H	197	LLP	C4-C5	-2.68	1.38	1.42
1	8-H	197	LLP	C4-C5	-2.66	1.38	1.42
1	4-B	197	LLP	C4-C5	-2.66	1.38	1.42
1	10-H	197	LLP	C4-C5	-2.65	1.38	1.42
1	10-G	197	LLP	C4-C5	-2.64	1.38	1.42
1	4-E	197	LLP	C4-C5	-2.61	1.38	1.42
1	6-H	197	LLP	C4-C5	-2.45	1.38	1.42
1	7-H	197	LLP	CB-CA	-2.13	1.50	1.53
1	6-E	197	LLP	C5'-C5	2.00	1.56	1.50
1	5-A	197	LLP	C5'-C5	2.00	1.56	1.50
1	5-B	197	LLP	C5'-C5	2.02	1.56	1.50
1	9-C	197	LLP	C5'-C5	2.02	1.56	1.50
1	10-G	197	LLP	C5'-C5	2.02	1.56	1.50
1	8-E	197	LLP	C5'-C5	2.03	1.56	1.50
1	7-A	197	LLP	C5'-C5	2.04	1.56	1.50
1	1-D	197	LLP	C3-C2	2.04	1.42	1.40
1	5-H	197	LLP	C5'-C5	2.05	1.56	1.50
1	4-A	197	LLP	C5'-C5	2.06	1.56	1.50
1	6-D	197	LLP	C5'-C5	2.06	1.56	1.50
1	9-G	197	LLP	C5'-C5	2.06	1.56	1.50
1	9-F	197	LLP	C5'-C5	2.07	1.56	1.50
1	9-E	197	LLP	C5'-C5	2.07	1.56	1.50
1	4-C	197	LLP	C5'-C5	2.08	1.56	1.50
1	5-E	197	LLP	C5'-C5	2.09	1.56	1.50
1	7-C	197	LLP	C5'-C5	2.09	1.56	1.50
1	5-G	197	LLP	C6-N1	2.09	1.38	1.34
1	10-C	197	LLP	C5'-C5	2.11	1.56	1.50
1	10-A	197	LLP	C5'-C5	2.12	1.56	1.50
1	5-G	197	LLP	C5'-C5	2.12	1.56	1.50
1	8-D	197	LLP	C5'-C5	2.13	1.56	1.50
1	1-A	197	LLP	C3-C2	2.14	1.42	1.40
1	1-E	197	LLP	C5'-C5	2.14	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-H	197	LLP	C5'-C5	2.15	1.56	1.50
1	3-G	197	LLP	C5'-C5	2.15	1.56	1.50
1	3-F	197	LLP	C5'-C5	2.16	1.56	1.50
1	3-A	197	LLP	C5'-C5	2.16	1.56	1.50
1	4-D	197	LLP	C5'-C5	2.16	1.56	1.50
1	7-H	197	LLP	C5'-C5	2.17	1.57	1.50
1	6-G	197	LLP	C5'-C5	2.17	1.57	1.50
1	5-H	197	LLP	C3-C2	2.17	1.42	1.40
1	4-E	197	LLP	C5'-C5	2.18	1.57	1.50
1	2-A	197	LLP	C5'-C5	2.18	1.57	1.50
1	1-B	197	LLP	C5'-C5	2.18	1.57	1.50
1	1-G	197	LLP	C5'-C5	2.18	1.57	1.50
1	10-F	197	LLP	C5'-C5	2.18	1.57	1.50
1	8-F	197	LLP	C3-C2	2.19	1.42	1.40
1	4-G	197	LLP	C5'-C5	2.19	1.57	1.50
1	9-A	197	LLP	C5'-C5	2.19	1.57	1.50
1	7-G	197	LLP	C5'-C5	2.20	1.57	1.50
1	7-F	197	LLP	C5'-C5	2.20	1.57	1.50
1	7-G	197	LLP	C6-N1	2.21	1.39	1.34
1	3-E	197	LLP	C5'-C5	2.21	1.57	1.50
1	10-H	197	LLP	C3-C2	2.22	1.42	1.40
1	8-A	197	LLP	C5'-C5	2.22	1.57	1.50
1	2-H	197	LLP	C5'-C5	2.22	1.57	1.50
1	2-G	197	LLP	C5'-C5	2.23	1.57	1.50
1	6-F	197	LLP	C5'-C5	2.23	1.57	1.50
1	2-C	197	LLP	C5'-C5	2.23	1.57	1.50
1	8-C	197	LLP	C5'-C5	2.23	1.57	1.50
1	7-E	197	LLP	C5'-C5	2.24	1.57	1.50
1	8-F	197	LLP	C5'-C5	2.26	1.57	1.50
1	7-B	197	LLP	C3-C2	2.26	1.42	1.40
1	6-H	197	LLP	C5'-C5	2.27	1.57	1.50
1	2-E	197	LLP	C5'-C5	2.27	1.57	1.50
1	6-A	197	LLP	C5'-C5	2.28	1.57	1.50
1	2-F	197	LLP	C5'-C5	2.28	1.57	1.50
1	5-F	197	LLP	C5'-C5	2.29	1.57	1.50
1	6-B	197	LLP	C6-N1	2.29	1.39	1.34
1	4-F	197	LLP	C5'-C5	2.30	1.57	1.50
1	1-G	197	LLP	C6-N1	2.30	1.39	1.34
1	4-B	197	LLP	C5'-C5	2.30	1.57	1.50
1	3-B	197	LLP	C3-C2	2.31	1.42	1.40
1	1-A	197	LLP	C5'-C5	2.33	1.57	1.50
1	6-C	197	LLP	C5'-C5	2.33	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-C	197	LLP	C5'-C5	2.34	1.57	1.50
1	10-B	197	LLP	C3-C2	2.34	1.42	1.40
1	1-F	197	LLP	C5'-C5	2.35	1.57	1.50
1	7-D	197	LLP	C3-C2	2.35	1.42	1.40
1	3-D	197	LLP	C6-N1	2.36	1.39	1.34
1	10-G	197	LLP	C6-N1	2.36	1.39	1.34
1	1-C	197	LLP	C5'-C5	2.37	1.57	1.50
1	2-G	197	LLP	C6-N1	2.37	1.39	1.34
1	10-H	197	LLP	C5'-C5	2.38	1.57	1.50
1	3-H	197	LLP	C5'-C5	2.38	1.57	1.50
1	9-G	197	LLP	C6-N1	2.39	1.39	1.34
1	7-D	197	LLP	C6-N1	2.39	1.39	1.34
1	6-G	197	LLP	C6-N1	2.40	1.39	1.34
1	2-H	197	LLP	C3-C2	2.40	1.42	1.40
1	9-H	197	LLP	C5'-C5	2.40	1.57	1.50
1	10-E	197	LLP	C6-N1	2.41	1.39	1.34
1	5-D	197	LLP	C6-N1	2.42	1.39	1.34
1	10-D	197	LLP	C6-N1	2.42	1.39	1.34
1	5-C	197	LLP	C6-N1	2.43	1.39	1.34
1	4-G	197	LLP	C6-N1	2.43	1.39	1.34
1	1-F	197	LLP	C3-C2	2.43	1.42	1.40
1	4-H	197	LLP	C5'-C5	2.44	1.57	1.50
1	7-H	197	LLP	C6-N1	2.44	1.39	1.34
1	8-G	197	LLP	C3-C2	2.45	1.42	1.40
1	5-E	197	LLP	C6-N1	2.45	1.39	1.34
1	3-G	197	LLP	C6-N1	2.47	1.39	1.34
1	2-D	197	LLP	C6-N1	2.47	1.39	1.34
1	1-H	197	LLP	C6-N1	2.48	1.39	1.34
1	2-H	197	LLP	C6-N1	2.48	1.39	1.34
1	9-F	197	LLP	C3-C2	2.48	1.42	1.40
1	9-E	197	LLP	C6-N1	2.48	1.39	1.34
1	1-C	197	LLP	C6-N1	2.49	1.39	1.34
1	9-B	197	LLP	C6-N1	2.49	1.39	1.34
1	3-C	197	LLP	C5'-C5	2.49	1.57	1.50
1	2-D	197	LLP	C3-C2	2.49	1.42	1.40
1	1-D	197	LLP	C6-N1	2.49	1.39	1.34
1	9-D	197	LLP	C6-N1	2.50	1.39	1.34
1	8-G	197	LLP	C5'-C5	2.50	1.57	1.50
1	6-D	197	LLP	C6-N1	2.51	1.39	1.34
1	8-G	197	LLP	C6-N1	2.51	1.39	1.34
1	4-D	197	LLP	C6-N1	2.52	1.39	1.34
1	1-B	197	LLP	C6-N1	2.52	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3-H	197	LLP	C6-N1	2.53	1.39	1.34
1	2-B	197	LLP	C6-N1	2.54	1.39	1.34
1	8-H	197	LLP	C6-N1	2.54	1.39	1.34
1	10-H	197	LLP	C6-N1	2.54	1.39	1.34
1	8-C	197	LLP	C6-N1	2.54	1.39	1.34
1	2-F	197	LLP	C3-C2	2.54	1.42	1.40
1	8-E	197	LLP	C6-N1	2.55	1.39	1.34
1	8-B	197	LLP	C6-N1	2.55	1.39	1.34
1	6-E	197	LLP	C3-C2	2.55	1.42	1.40
1	2-C	197	LLP	C6-N1	2.56	1.39	1.34
1	5-B	197	LLP	C2'-C2	2.57	1.55	1.50
1	6-C	197	LLP	C6-N1	2.57	1.39	1.34
1	7-E	197	LLP	C6-N1	2.57	1.39	1.34
1	9-H	197	LLP	C6-N1	2.58	1.40	1.34
1	4-E	197	LLP	C6-N1	2.58	1.40	1.34
1	7-B	197	LLP	C6-N1	2.58	1.40	1.34
1	5-C	197	LLP	C3-C2	2.58	1.42	1.40
1	10-C	197	LLP	C6-N1	2.59	1.40	1.34
1	1-A	197	LLP	C6-N1	2.59	1.40	1.34
1	6-F	197	LLP	C3-C2	2.60	1.42	1.40
1	4-H	197	LLP	C6-N1	2.60	1.40	1.34
1	4-C	197	LLP	C6-N1	2.60	1.40	1.34
1	5-B	197	LLP	C6-N1	2.61	1.40	1.34
1	6-H	197	LLP	C6-N1	2.61	1.40	1.34
1	5-A	197	LLP	C6-N1	2.62	1.40	1.34
1	9-C	197	LLP	C6-N1	2.63	1.40	1.34
1	2-A	197	LLP	C6-N1	2.64	1.40	1.34
1	4-B	197	LLP	C6-N1	2.64	1.40	1.34
1	6-B	197	LLP	C2'-C2	2.65	1.55	1.50
1	7-A	197	LLP	C6-N1	2.66	1.40	1.34
1	4-A	197	LLP	C3-C2	2.67	1.42	1.40
1	6-E	197	LLP	C6-N1	2.67	1.40	1.34
1	10-A	197	LLP	C6-N1	2.67	1.40	1.34
1	10-B	197	LLP	C6-N1	2.68	1.40	1.34
1	3-C	197	LLP	C3-C2	2.68	1.42	1.40
1	8-E	197	LLP	C3-C2	2.69	1.42	1.40
1	8-A	197	LLP	C6-N1	2.69	1.40	1.34
1	5-H	197	LLP	C6-N1	2.70	1.40	1.34
1	8-B	197	LLP	C2'-C2	2.72	1.55	1.50
1	3-C	197	LLP	C6-N1	2.72	1.40	1.34
1	10-A	197	LLP	C3-C2	2.72	1.42	1.40
1	7-C	197	LLP	C6-N1	2.73	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4-H	197	LLP	C3-C2	2.73	1.42	1.40
1	8-F	197	LLP	C2'-C2	2.74	1.55	1.50
1	9-A	197	LLP	C6-N1	2.74	1.40	1.34
1	6-A	197	LLP	C6-N1	2.74	1.40	1.34
1	6-H	197	LLP	C3-C2	2.75	1.42	1.40
1	10-F	197	LLP	C3-C2	2.76	1.42	1.40
1	2-C	197	LLP	C3-C2	2.76	1.42	1.40
1	8-D	197	LLP	C6-N1	2.76	1.40	1.34
1	2-E	197	LLP	C6-N1	2.76	1.40	1.34
1	4-A	197	LLP	C6-N1	2.78	1.40	1.34
1	3-E	197	LLP	C6-N1	2.78	1.40	1.34
1	10-F	197	LLP	C6-N1	2.78	1.40	1.34
1	1-E	197	LLP	C6-N1	2.79	1.40	1.34
1	8-H	197	LLP	C3-C2	2.80	1.42	1.40
1	3-F	197	LLP	C2'-C2	2.81	1.55	1.50
1	5-F	197	LLP	C6-N1	2.82	1.40	1.34
1	9-B	197	LLP	C2'-C2	2.83	1.55	1.50
1	1-B	197	LLP	C2'-C2	2.85	1.55	1.50
1	4-B	197	LLP	C3-C2	2.85	1.42	1.40
1	6-F	197	LLP	C2'-C2	2.85	1.55	1.50
1	3-A	197	LLP	C6-N1	2.86	1.40	1.34
1	4-B	197	LLP	C2'-C2	2.86	1.55	1.50
1	2-F	197	LLP	C2'-C2	2.87	1.55	1.50
1	5-E	197	LLP	C3-C2	2.87	1.42	1.40
1	4-F	197	LLP	C2'-C2	2.88	1.55	1.50
1	1-E	197	LLP	C3-C2	2.88	1.42	1.40
1	3-B	197	LLP	C6-N1	2.88	1.40	1.34
1	6-F	197	LLP	C6-N1	2.89	1.40	1.34
1	2-B	197	LLP	C2'-C2	2.89	1.55	1.50
1	9-F	197	LLP	C2'-C2	2.89	1.55	1.50
1	4-F	197	LLP	C3-C2	2.90	1.42	1.40
1	1-C	197	LLP	C3-C2	2.90	1.42	1.40
1	5-B	197	LLP	C3-C2	2.91	1.42	1.40
1	6-B	197	LLP	C3-C2	2.92	1.42	1.40
1	3-F	197	LLP	C6-N1	2.93	1.40	1.34
1	5-G	197	LLP	C3-C2	2.93	1.42	1.40
1	7-B	197	LLP	C2'-C2	2.94	1.55	1.50
1	3-A	197	LLP	C3-C2	2.95	1.42	1.40
1	8-A	197	LLP	C3-C2	2.96	1.42	1.40
1	7-F	197	LLP	C2'-C2	2.96	1.55	1.50
1	10-B	197	LLP	C2'-C2	2.96	1.55	1.50
1	7-F	197	LLP	C3-C2	2.97	1.42	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-F	197	LLP	C6-N1	2.97	1.40	1.34
1	3-H	197	LLP	C3-C2	2.98	1.42	1.40
1	3-B	197	LLP	C2'-C2	2.99	1.55	1.50
1	5-F	197	LLP	C2'-C2	2.99	1.55	1.50
1	2-F	197	LLP	C6-N1	3.01	1.40	1.34
1	8-B	197	LLP	C3-C2	3.03	1.42	1.40
1	2-E	197	LLP	C3-C2	3.04	1.42	1.40
1	10-F	197	LLP	C2'-C2	3.05	1.56	1.50
1	9-H	197	LLP	C3-C2	3.05	1.42	1.40
1	3-G	197	LLP	C2'-C2	3.05	1.56	1.50
1	5-D	197	LLP	C2'-C2	3.06	1.56	1.50
1	5-A	197	LLP	C3-C2	3.06	1.42	1.40
1	1-F	197	LLP	C2'-C2	3.07	1.56	1.50
1	9-A	197	LLP	C3-C2	3.08	1.42	1.40
1	9-F	197	LLP	C6-N1	3.11	1.41	1.34
1	4-D	197	LLP	C2'-C2	3.12	1.56	1.50
1	3-A	197	LLP	C2'-C2	3.12	1.56	1.50
1	4-F	197	LLP	C6-N1	3.12	1.41	1.34
1	4-G	197	LLP	C2'-C2	3.14	1.56	1.50
1	10-G	197	LLP	C2'-C2	3.14	1.56	1.50
1	3-D	197	LLP	C2'-C2	3.17	1.56	1.50
1	6-D	197	LLP	C2'-C2	3.17	1.56	1.50
1	7-D	197	LLP	C2'-C2	3.17	1.56	1.50
1	2-G	197	LLP	C2'-C2	3.19	1.56	1.50
1	1-F	197	LLP	C6-N1	3.20	1.41	1.34
1	10-D	197	LLP	C2'-C2	3.22	1.56	1.50
1	9-G	197	LLP	C3-C2	3.23	1.43	1.40
1	4-A	197	LLP	C2'-C2	3.23	1.56	1.50
1	7-A	197	LLP	C3-C2	3.25	1.43	1.40
1	9-G	197	LLP	C2'-C2	3.25	1.56	1.50
1	9-C	197	LLP	C3-C2	3.26	1.43	1.40
1	8-C	197	LLP	C3-C2	3.26	1.43	1.40
1	7-F	197	LLP	C6-N1	3.26	1.41	1.34
1	9-D	197	LLP	C2'-C2	3.26	1.56	1.50
1	2-D	197	LLP	C2'-C2	3.27	1.56	1.50
1	6-H	197	LLP	C2'-C2	3.28	1.56	1.50
1	7-G	197	LLP	C2'-C2	3.29	1.56	1.50
1	8-D	197	LLP	C2'-C2	3.30	1.56	1.50
1	4-G	197	LLP	C3-C2	3.31	1.43	1.40
1	2-A	197	LLP	C2'-C2	3.31	1.56	1.50
1	9-E	197	LLP	C3-C2	3.31	1.43	1.40
1	10-C	197	LLP	C3-C2	3.33	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	197	LLP	C2'-C2	3.33	1.56	1.50
1	7-A	197	LLP	C2'-C2	3.34	1.56	1.50
1	7-C	197	LLP	C2'-C2	3.34	1.56	1.50
1	3-H	197	LLP	C2'-C2	3.35	1.56	1.50
1	8-A	197	LLP	C2'-C2	3.35	1.56	1.50
1	5-G	197	LLP	C2'-C2	3.35	1.56	1.50
1	10-E	197	LLP	C3-C2	3.35	1.43	1.40
1	4-E	197	LLP	C3-C2	3.36	1.43	1.40
1	10-C	197	LLP	C2'-C2	3.38	1.56	1.50
1	9-A	197	LLP	C2'-C2	3.38	1.56	1.50
1	6-E	197	LLP	C2'-C2	3.38	1.56	1.50
1	4-C	197	LLP	C2'-C2	3.38	1.56	1.50
1	7-E	197	LLP	C3-C2	3.39	1.43	1.40
1	9-C	197	LLP	C2'-C2	3.40	1.56	1.50
1	6-C	197	LLP	C2'-C2	3.40	1.56	1.50
1	3-G	197	LLP	C3-C2	3.40	1.43	1.40
1	1-D	197	LLP	C2'-C2	3.40	1.56	1.50
1	3-C	197	LLP	C2'-C2	3.40	1.56	1.50
1	4-H	197	LLP	C2'-C2	3.41	1.56	1.50
1	1-G	197	LLP	C2'-C2	3.41	1.56	1.50
1	5-H	197	LLP	C2'-C2	3.43	1.56	1.50
1	7-H	197	LLP	C2'-C2	3.43	1.56	1.50
1	6-A	197	LLP	C2'-C2	3.43	1.56	1.50
1	10-A	197	LLP	C2'-C2	3.43	1.56	1.50
1	6-G	197	LLP	C2'-C2	3.44	1.56	1.50
1	1-H	197	LLP	C2'-C2	3.45	1.56	1.50
1	9-H	197	LLP	C2'-C2	3.45	1.56	1.50
1	8-H	197	LLP	C2'-C2	3.46	1.56	1.50
1	10-G	197	LLP	C3-C2	3.46	1.43	1.40
1	6-A	197	LLP	C3-C2	3.47	1.43	1.40
1	8-C	197	LLP	C2'-C2	3.50	1.56	1.50
1	2-C	197	LLP	C2'-C2	3.50	1.56	1.50
1	1-C	197	LLP	C2'-C2	3.51	1.56	1.50
1	3-E	197	LLP	C2'-C2	3.51	1.56	1.50
1	1-A	197	LLP	C2'-C2	3.51	1.56	1.50
1	1-E	197	LLP	C2'-C2	3.53	1.56	1.50
1	2-A	197	LLP	C3-C2	3.54	1.43	1.40
1	10-H	197	LLP	C2'-C2	3.54	1.56	1.50
1	4-E	197	LLP	C2'-C2	3.56	1.56	1.50
1	10-E	197	LLP	C2'-C2	3.56	1.56	1.50
1	8-G	197	LLP	C2'-C2	3.56	1.56	1.50
1	2-H	197	LLP	C2'-C2	3.58	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	7-G	197	LLP	C3-C2	3.59	1.43	1.40
1	8-E	197	LLP	C2'-C2	3.60	1.57	1.50
1	5-E	197	LLP	C2'-C2	3.60	1.57	1.50
1	9-E	197	LLP	C2'-C2	3.61	1.57	1.50
1	2-E	197	LLP	C2'-C2	3.61	1.57	1.50
1	5-C	197	LLP	C2'-C2	3.64	1.57	1.50
1	7-E	197	LLP	C2'-C2	3.67	1.57	1.50
1	2-B	197	LLP	C3-C2	3.78	1.43	1.40
1	6-G	197	LLP	C3-C2	3.81	1.43	1.40
1	1-B	197	LLP	C3-C2	3.93	1.43	1.40
1	1-G	197	LLP	C3-C2	3.98	1.43	1.40
1	2-G	197	LLP	C3-C2	4.00	1.43	1.40
1	6-C	197	LLP	C3-C2	4.19	1.43	1.40
1	3-E	197	LLP	C3-C2	4.40	1.43	1.40
1	4-C	197	LLP	C3-C2	4.48	1.43	1.40
1	9-B	197	LLP	C4'-NZ	4.80	1.41	1.27
1	5-F	197	LLP	C4'-NZ	5.24	1.42	1.27
1	4-D	197	LLP	C4'-NZ	5.30	1.42	1.27
1	9-D	197	LLP	C4'-NZ	5.38	1.43	1.27
1	8-G	197	LLP	C4'-NZ	5.43	1.43	1.27
1	1-D	197	LLP	C4'-NZ	5.49	1.43	1.27
1	6-D	197	LLP	C4'-NZ	5.50	1.43	1.27
1	7-D	197	LLP	C4'-NZ	5.51	1.43	1.27
1	10-E	197	LLP	C4'-NZ	5.51	1.43	1.27
1	6-E	197	LLP	C4'-NZ	5.52	1.43	1.27
1	2-D	197	LLP	C4'-NZ	5.54	1.43	1.27
1	1-C	197	LLP	C4'-NZ	5.54	1.43	1.27
1	3-E	197	LLP	C4'-NZ	5.56	1.43	1.27
1	2-A	197	LLP	C4'-NZ	5.57	1.43	1.27
1	5-D	197	LLP	C4'-NZ	5.59	1.43	1.27
1	4-A	197	LLP	C4'-NZ	5.59	1.43	1.27
1	9-E	197	LLP	C4'-NZ	5.59	1.43	1.27
1	3-D	197	LLP	C4'-NZ	5.59	1.43	1.27
1	1-A	197	LLP	C4'-NZ	5.59	1.43	1.27
1	10-C	197	LLP	C4'-NZ	5.60	1.43	1.27
1	2-H	197	LLP	C4'-NZ	5.60	1.43	1.27
1	9-A	197	LLP	C4'-NZ	5.60	1.43	1.27
1	9-F	197	LLP	C4'-NZ	5.65	1.43	1.27
1	4-G	197	LLP	C4'-NZ	5.65	1.43	1.27
1	5-E	197	LLP	C4'-NZ	5.67	1.43	1.27
1	1-E	197	LLP	C4'-NZ	5.68	1.43	1.27
1	1-F	197	LLP	C4'-NZ	5.68	1.43	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	197	LLP	C4'-NZ	5.68	1.43	1.27
1	10-D	197	LLP	C4'-NZ	5.69	1.43	1.27
1	7-A	197	LLP	C4'-NZ	5.69	1.43	1.27
1	9-C	197	LLP	C4'-NZ	5.70	1.43	1.27
1	4-F	197	LLP	C4'-NZ	5.70	1.43	1.27
1	8-E	197	LLP	C4'-NZ	5.70	1.43	1.27
1	10-F	197	LLP	C4'-NZ	5.71	1.43	1.27
1	5-G	197	LLP	C4'-NZ	5.71	1.43	1.27
1	6-B	197	LLP	C4'-NZ	5.72	1.43	1.27
1	5-C	197	LLP	C4'-NZ	5.73	1.44	1.27
1	7-E	197	LLP	C4'-NZ	5.73	1.44	1.27
1	7-F	197	LLP	C4'-NZ	5.75	1.44	1.27
1	6-G	197	LLP	C4'-NZ	5.75	1.44	1.27
1	3-A	197	LLP	C4'-NZ	5.76	1.44	1.27
1	1-G	197	LLP	C4'-NZ	5.76	1.44	1.27
1	7-G	197	LLP	C4'-NZ	5.76	1.44	1.27
1	4-E	197	LLP	C4'-NZ	5.77	1.44	1.27
1	9-G	197	LLP	C4'-NZ	5.77	1.44	1.27
1	7-B	197	LLP	C4'-NZ	5.78	1.44	1.27
1	3-G	197	LLP	C4'-NZ	5.79	1.44	1.27
1	3-C	197	LLP	C4'-NZ	5.81	1.44	1.27
1	2-C	197	LLP	C4'-NZ	5.82	1.44	1.27
1	9-H	197	LLP	C4'-NZ	5.82	1.44	1.27
1	7-C	197	LLP	C4'-NZ	5.83	1.44	1.27
1	2-B	197	LLP	C4'-NZ	5.84	1.44	1.27
1	2-F	197	LLP	C4'-NZ	5.84	1.44	1.27
1	6-F	197	LLP	C4'-NZ	5.84	1.44	1.27
1	7-H	197	LLP	C4'-NZ	5.85	1.44	1.27
1	4-C	197	LLP	C4'-NZ	5.85	1.44	1.27
1	8-A	197	LLP	C4'-NZ	5.85	1.44	1.27
1	8-D	197	LLP	C4'-NZ	5.85	1.44	1.27
1	3-F	197	LLP	C4'-NZ	5.86	1.44	1.27
1	1-B	197	LLP	C4'-NZ	5.87	1.44	1.27
1	5-H	197	LLP	C4'-NZ	5.87	1.44	1.27
1	8-F	197	LLP	C4'-NZ	5.89	1.44	1.27
1	6-A	197	LLP	C4'-NZ	5.89	1.44	1.27
1	8-H	197	LLP	C4'-NZ	5.89	1.44	1.27
1	2-E	197	LLP	C4'-NZ	5.90	1.44	1.27
1	10-G	197	LLP	C4'-NZ	5.91	1.44	1.27
1	1-H	197	LLP	C4'-NZ	5.91	1.44	1.27
1	2-G	197	LLP	C4'-NZ	5.92	1.44	1.27
1	10-A	197	LLP	C4'-NZ	5.93	1.44	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-B	197	LLP	C4'-NZ	5.94	1.44	1.27
1	4-B	197	LLP	C4'-NZ	5.95	1.44	1.27
1	6-H	197	LLP	C4'-NZ	5.99	1.44	1.27
1	10-B	197	LLP	C4'-NZ	6.00	1.44	1.27
1	8-C	197	LLP	C4'-NZ	6.02	1.44	1.27
1	6-C	197	LLP	C4'-NZ	6.04	1.44	1.27
1	3-B	197	LLP	C4'-NZ	6.06	1.44	1.27
1	10-H	197	LLP	C4'-NZ	6.06	1.44	1.27
1	5-B	197	LLP	C4'-NZ	6.09	1.45	1.27
1	3-H	197	LLP	C4'-NZ	6.28	1.45	1.27
1	4-H	197	LLP	C4'-NZ	6.34	1.45	1.27
1	5-F	197	LLP	C4-C4'	8.23	1.61	1.46
1	9-B	197	LLP	C4-C4'	8.27	1.61	1.46
1	2-H	197	LLP	C4-C4'	8.38	1.61	1.46
1	1-A	197	LLP	C4-C4'	8.45	1.61	1.46
1	9-A	197	LLP	C4-C4'	8.49	1.62	1.46
1	8-D	197	LLP	C4-C4'	8.50	1.62	1.46
1	9-H	197	LLP	C4-C4'	8.62	1.62	1.46
1	9-E	197	LLP	C4-C4'	8.65	1.62	1.46
1	4-F	197	LLP	C4-C4'	8.66	1.62	1.46
1	6-A	197	LLP	C4-C4'	8.66	1.62	1.46
1	8-F	197	LLP	C4-C4'	8.67	1.62	1.46
1	6-H	197	LLP	C4-C4'	8.69	1.62	1.46
1	1-H	197	LLP	C4-C4'	8.69	1.62	1.46
1	1-E	197	LLP	C4-C4'	8.72	1.62	1.46
1	2-F	197	LLP	C4-C4'	8.73	1.62	1.46
1	5-H	197	LLP	C4-C4'	8.74	1.62	1.46
1	1-C	197	LLP	C4-C4'	8.74	1.62	1.46
1	4-A	197	LLP	C4-C4'	8.75	1.62	1.46
1	9-F	197	LLP	C4-C4'	8.76	1.62	1.46
1	9-D	197	LLP	C4-C4'	8.77	1.62	1.46
1	8-B	197	LLP	C4-C4'	8.78	1.62	1.46
1	7-C	197	LLP	C4-C4'	8.79	1.62	1.46
1	8-G	197	LLP	C4-C4'	8.80	1.62	1.46
1	3-F	197	LLP	C4-C4'	8.82	1.62	1.46
1	6-E	197	LLP	C4-C4'	8.82	1.62	1.46
1	5-D	197	LLP	C4-C4'	8.82	1.62	1.46
1	10-E	197	LLP	C4-C4'	8.83	1.62	1.46
1	6-F	197	LLP	C4-C4'	8.83	1.62	1.46
1	7-H	197	LLP	C4-C4'	8.83	1.62	1.46
1	1-F	197	LLP	C4-C4'	8.83	1.62	1.46
1	7-F	197	LLP	C4-C4'	8.85	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2-D	197	LLP	C4-C4'	8.87	1.62	1.46
1	6-B	197	LLP	C4-C4'	8.89	1.62	1.46
1	4-D	197	LLP	C4-C4'	8.90	1.62	1.46
1	8-H	197	LLP	C4-C4'	8.91	1.62	1.46
1	7-B	197	LLP	C4-C4'	8.91	1.62	1.46
1	5-E	197	LLP	C4-C4'	8.91	1.62	1.46
1	10-H	197	LLP	C4-C4'	8.93	1.62	1.46
1	10-F	197	LLP	C4-C4'	8.94	1.62	1.46
1	10-B	197	LLP	C4-C4'	8.95	1.62	1.46
1	3-G	197	LLP	C4-C4'	8.95	1.62	1.46
1	2-C	197	LLP	C4-C4'	8.98	1.62	1.46
1	8-C	197	LLP	C4-C4'	8.98	1.62	1.46
1	3-C	197	LLP	C4-C4'	8.99	1.62	1.46
1	3-A	197	LLP	C4-C4'	9.00	1.62	1.46
1	1-B	197	LLP	C4-C4'	9.00	1.62	1.46
1	4-G	197	LLP	C4-C4'	9.00	1.62	1.46
1	10-G	197	LLP	C4-C4'	9.01	1.62	1.46
1	6-G	197	LLP	C4-C4'	9.02	1.62	1.46
1	4-E	197	LLP	C4-C4'	9.02	1.62	1.46
1	10-A	197	LLP	C4-C4'	9.02	1.62	1.46
1	6-D	197	LLP	C4-C4'	9.02	1.62	1.46
1	1-D	197	LLP	C4-C4'	9.04	1.63	1.46
1	10-C	197	LLP	C4-C4'	9.05	1.63	1.46
1	5-G	197	LLP	C4-C4'	9.05	1.63	1.46
1	7-E	197	LLP	C4-C4'	9.05	1.63	1.46
1	10-D	197	LLP	C4-C4'	9.06	1.63	1.46
1	9-C	197	LLP	C4-C4'	9.06	1.63	1.46
1	8-A	197	LLP	C4-C4'	9.07	1.63	1.46
1	5-C	197	LLP	C4-C4'	9.07	1.63	1.46
1	3-D	197	LLP	C4-C4'	9.09	1.63	1.46
1	8-E	197	LLP	C4-C4'	9.09	1.63	1.46
1	1-G	197	LLP	C4-C4'	9.11	1.63	1.46
1	4-C	197	LLP	C4-C4'	9.16	1.63	1.46
1	4-B	197	LLP	C4-C4'	9.20	1.63	1.46
1	9-G	197	LLP	C4-C4'	9.21	1.63	1.46
1	2-B	197	LLP	C4-C4'	9.22	1.63	1.46
1	3-E	197	LLP	C4-C4'	9.23	1.63	1.46
1	3-H	197	LLP	C4-C4'	9.23	1.63	1.46
1	7-D	197	LLP	C4-C4'	9.24	1.63	1.46
1	3-B	197	LLP	C4-C4'	9.25	1.63	1.46
1	7-A	197	LLP	C4-C4'	9.30	1.63	1.46
1	2-E	197	LLP	C4-C4'	9.30	1.63	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	197	LLP	C4-C4'	9.31	1.63	1.46
1	5-B	197	LLP	C4-C4'	9.31	1.63	1.46
1	4-H	197	LLP	C4-C4'	9.36	1.63	1.46
1	2-G	197	LLP	C4-C4'	9.39	1.63	1.46
1	2-A	197	LLP	C4-C4'	9.44	1.63	1.46
1	6-C	197	LLP	C4-C4'	9.51	1.63	1.46
1	7-G	197	LLP	C4-C4'	9.54	1.63	1.46

All (331) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	197	LLP	CE-NZ-C4'	-4.05	107.28	119.03
1	8-D	197	LLP	CB-CA-C	-3.94	105.16	111.65
1	4-G	197	LLP	CE-NZ-C4'	-3.83	107.91	119.03
1	8-G	197	LLP	C4-C4'-NZ	-3.82	106.08	124.66
1	9-B	197	LLP	CE-NZ-C4'	-3.78	108.05	119.03
1	10-G	197	LLP	CE-NZ-C4'	-3.77	108.09	119.03
1	3-F	197	LLP	C4-C4'-NZ	-3.64	106.98	124.66
1	6-B	197	LLP	CE-NZ-C4'	-3.62	108.52	119.03
1	8-B	197	LLP	CE-NZ-C4'	-3.55	108.73	119.03
1	2-C	197	LLP	CE-NZ-C4'	-3.53	108.79	119.03
1	4-E	197	LLP	C4-C4'-NZ	-3.52	107.57	124.66
1	2-H	197	LLP	CE-NZ-C4'	-3.49	108.89	119.03
1	5-C	197	LLP	C4-C4'-NZ	-3.48	107.78	124.66
1	6-C	197	LLP	CE-NZ-C4'	-3.46	108.99	119.03
1	5-G	197	LLP	CE-NZ-C4'	-3.44	109.04	119.03
1	3-G	197	LLP	C4-C4'-NZ	-3.44	107.96	124.66
1	5-D	197	LLP	C4-C4'-NZ	-3.42	108.07	124.66
1	4-D	197	LLP	C4-C4'-NZ	-3.39	108.21	124.66
1	7-C	197	LLP	C4-C4'-NZ	-3.38	108.23	124.66
1	1-C	197	LLP	C4-C4'-NZ	-3.29	108.70	124.66
1	4-A	197	LLP	CE-NZ-C4'	-3.25	109.61	119.03
1	10-H	197	LLP	CE-NZ-C4'	-3.24	109.63	119.03
1	7-D	197	LLP	O-C-CA	-3.23	116.09	125.02
1	6-E	197	LLP	C4-C4'-NZ	-3.20	109.09	124.66
1	6-G	197	LLP	CE-NZ-C4'	-3.16	109.85	119.03
1	5-F	197	LLP	C4-C4'-NZ	-3.15	109.38	124.66
1	10-C	197	LLP	C4-C4'-NZ	-3.10	109.58	124.66
1	1-A	197	LLP	CE-NZ-C4'	-3.10	110.04	119.03
1	2-G	197	LLP	CE-NZ-C4'	-3.09	110.06	119.03
1	9-H	197	LLP	CE-NZ-C4'	-3.09	110.06	119.03
1	9-D	197	LLP	CE-NZ-C4'	-3.08	110.09	119.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-H	197	LLP	CE-NZ-C4'	-3.07	110.11	119.03
1	1-B	197	LLP	CE-NZ-C4'	-3.07	110.12	119.03
1	7-B	197	LLP	CE-NZ-C4'	-3.07	110.13	119.03
1	1-D	197	LLP	C4-C4'-NZ	-3.02	110.02	124.66
1	9-A	197	LLP	C4-C4'-NZ	-3.02	110.02	124.66
1	6-F	197	LLP	CE-NZ-C4'	-3.01	110.28	119.03
1	7-H	197	LLP	CE-NZ-C4'	-3.01	110.30	119.03
1	9-E	197	LLP	C4-C4'-NZ	-2.93	110.44	124.66
1	6-D	197	LLP	CE-NZ-C4'	-2.92	110.54	119.03
1	5-E	197	LLP	CE-NZ-C4'	-2.91	110.58	119.03
1	8-C	197	LLP	CE-NZ-C4'	-2.91	110.59	119.03
1	9-G	197	LLP	CE-NZ-C4'	-2.90	110.62	119.03
1	5-H	197	LLP	CE-NZ-C4'	-2.90	110.62	119.03
1	2-F	197	LLP	C4-C4'-NZ	-2.89	110.62	124.66
1	8-H	197	LLP	CE-NZ-C4'	-2.89	110.64	119.03
1	9-C	197	LLP	CE-NZ-C4'	-2.89	110.65	119.03
1	1-E	197	LLP	C4-C4'-NZ	-2.88	110.69	124.66
1	1-A	197	LLP	C4-C4'-NZ	-2.87	110.72	124.66
1	2-D	197	LLP	C4-C4'-NZ	-2.85	110.84	124.66
1	8-D	197	LLP	CE-NZ-C4'	-2.83	110.80	119.03
1	10-D	197	LLP	C4-C4'-NZ	-2.83	110.94	124.66
1	3-C	197	LLP	C4-C4'-NZ	-2.82	110.96	124.66
1	9-C	197	LLP	C4-C4'-NZ	-2.81	111.00	124.66
1	6-D	197	LLP	C4-C4'-NZ	-2.81	111.03	124.66
1	9-B	197	LLP	C4-C4'-NZ	-2.80	111.04	124.66
1	8-F	197	LLP	C4-C4'-NZ	-2.80	111.04	124.66
1	8-F	197	LLP	CE-NZ-C4'	-2.79	110.92	119.03
1	10-B	197	LLP	CE-NZ-C4'	-2.79	110.92	119.03
1	5-A	197	LLP	C4-C4'-NZ	-2.79	111.10	124.66
1	6-A	197	LLP	C4-C4'-NZ	-2.79	111.13	124.66
1	5-H	197	LLP	C4-C4'-NZ	-2.78	111.16	124.66
1	7-D	197	LLP	CE-NZ-C4'	-2.77	110.99	119.03
1	8-A	197	LLP	CE-NZ-C4'	-2.76	111.01	119.03
1	5-D	197	LLP	CE-NZ-C4'	-2.76	111.01	119.03
1	3-D	197	LLP	C4-C4'-NZ	-2.76	111.26	124.66
1	7-E	197	LLP	CE-NZ-C4'	-2.73	111.09	119.03
1	4-A	197	LLP	C4-C4'-NZ	-2.73	111.42	124.66
1	1-H	197	LLP	CE-NZ-C4'	-2.72	111.13	119.03
1	3-A	197	LLP	CE-NZ-C4'	-2.72	111.13	119.03
1	3-E	197	LLP	CE-NZ-C4'	-2.72	111.13	119.03
1	4-H	197	LLP	C4-C4'-NZ	-2.72	111.46	124.66
1	7-H	197	LLP	O-C-CA	-2.71	117.53	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3-A	197	LLP	C4-C4'-NZ	-2.71	111.50	124.66
1	2-B	197	LLP	CE-NZ-C4'	-2.70	111.20	119.03
1	9-B	197	LLP	C5-C6-N1	-2.70	119.31	123.87
1	9-F	197	LLP	C5-C6-N1	-2.70	119.31	123.87
1	10-D	197	LLP	CE-NZ-C4'	-2.69	111.23	119.03
1	10-A	197	LLP	CE-NZ-C4'	-2.68	111.24	119.03
1	5-A	197	LLP	O-C-CA	-2.68	117.62	125.02
1	4-C	197	LLP	CE-NZ-C4'	-2.68	111.25	119.03
1	1-G	197	LLP	C4-C4'-NZ	-2.68	111.67	124.66
1	1-G	197	LLP	CE-NZ-C4'	-2.67	111.29	119.03
1	4-F	197	LLP	CE-NZ-C4'	-2.66	111.29	119.03
1	5-C	197	LLP	C5'-C5-C6	-2.66	114.75	119.33
1	10-B	197	LLP	O-C-CA	-2.66	117.66	125.02
1	7-F	197	LLP	C4-C4'-NZ	-2.66	111.74	124.66
1	1-F	197	LLP	C4-C4'-NZ	-2.65	111.78	124.66
1	7-H	197	LLP	C4-C4'-NZ	-2.64	111.82	124.66
1	4-B	197	LLP	CE-NZ-C4'	-2.64	111.36	119.03
1	8-A	197	LLP	C4-C4'-NZ	-2.63	111.87	124.66
1	8-C	197	LLP	C4-C4'-NZ	-2.63	111.88	124.66
1	4-F	197	LLP	C4-C4'-NZ	-2.63	111.89	124.66
1	10-E	197	LLP	CE-NZ-C4'	-2.62	111.41	119.03
1	9-E	197	LLP	CE-NZ-C4'	-2.62	111.42	119.03
1	7-H	197	LLP	C5-C6-N1	-2.62	119.43	123.87
1	3-C	197	LLP	CE-NZ-C4'	-2.61	111.46	119.03
1	8-E	197	LLP	CE-NZ-C4'	-2.60	111.49	119.03
1	1-D	197	LLP	CE-NZ-C4'	-2.59	111.51	119.03
1	7-A	197	LLP	O-C-CA	-2.58	117.89	125.02
1	2-H	197	LLP	O-C-CA	-2.58	117.89	125.02
1	10-E	197	LLP	C4-C4'-NZ	-2.58	112.13	124.66
1	6-C	197	LLP	C5'-C5-C6	-2.58	114.89	119.33
1	9-F	197	LLP	C4-C4'-NZ	-2.58	112.14	124.66
1	5-H	197	LLP	O-C-CA	-2.58	117.90	125.02
1	7-D	197	LLP	C4-C4'-NZ	-2.58	112.15	124.66
1	2-H	197	LLP	C4-C4'-NZ	-2.57	112.19	124.66
1	1-H	197	LLP	C5-C6-N1	-2.56	119.53	123.87
1	2-D	197	LLP	CE-NZ-C4'	-2.56	111.60	119.03
1	6-G	197	LLP	O-C-CA	-2.56	117.95	125.02
1	1-F	197	LLP	CE-NZ-C4'	-2.55	111.61	119.03
1	9-D	197	LLP	C5-C6-N1	-2.55	119.55	123.87
1	9-F	197	LLP	O-C-CA	-2.55	117.98	125.02
1	10-F	197	LLP	C4-C4'-NZ	-2.54	112.31	124.66
1	3-H	197	LLP	C4-C4'-NZ	-2.53	112.37	124.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-E	197	LLP	CE-NZ-C4'	-2.53	111.69	119.03
1	7-F	197	LLP	O-C-CA	-2.53	118.04	125.02
1	5-A	197	LLP	CE-NZ-C4'	-2.52	111.70	119.03
1	10-A	197	LLP	O-C-CA	-2.52	118.06	125.02
1	10-C	197	LLP	CE-NZ-C4'	-2.52	111.72	119.03
1	7-A	197	LLP	C4-C4'-NZ	-2.52	112.42	124.66
1	5-D	197	LLP	C5-C6-N1	-2.52	119.61	123.87
1	3-H	197	LLP	O-C-CA	-2.51	118.08	125.02
1	9-A	197	LLP	CE-NZ-C4'	-2.51	111.75	119.03
1	3-B	197	LLP	CE-NZ-C4'	-2.50	111.78	119.03
1	5-F	197	LLP	C5-C6-N1	-2.50	119.64	123.87
1	2-H	197	LLP	C5-C6-N1	-2.50	119.64	123.87
1	4-C	197	LLP	O-C-CA	-2.49	118.15	125.02
1	10-B	197	LLP	C2'-C2-C3	-2.49	118.00	120.96
1	9-D	197	LLP	C4-C4'-NZ	-2.48	112.61	124.66
1	6-A	197	LLP	O-C-CA	-2.48	118.17	125.02
1	9-B	197	LLP	C2'-C2-C3	-2.48	118.01	120.96
1	8-A	197	LLP	O-C-CA	-2.47	118.19	125.02
1	7-C	197	LLP	CE-NZ-C4'	-2.47	111.86	119.03
1	7-A	197	LLP	CE-NZ-C4'	-2.47	111.87	119.03
1	10-A	197	LLP	C4-C4'-NZ	-2.46	112.71	124.66
1	2-B	197	LLP	C4-C4'-NZ	-2.46	112.72	124.66
1	6-F	197	LLP	C5-C6-N1	-2.45	119.72	123.87
1	5-E	197	LLP	C4-C4'-NZ	-2.44	112.81	124.66
1	5-B	197	LLP	CE-NZ-C4'	-2.44	111.95	119.03
1	7-D	197	LLP	C5-C6-N1	-2.44	119.74	123.87
1	4-D	197	LLP	O-C-CA	-2.44	118.29	125.02
1	9-H	197	LLP	C5-C6-N1	-2.43	119.77	123.87
1	10-H	197	LLP	C5-C6-N1	-2.42	119.77	123.87
1	9-F	197	LLP	CE-NZ-C4'	-2.42	112.00	119.03
1	6-A	197	LLP	CE-NZ-C4'	-2.42	112.00	119.03
1	5-F	197	LLP	CE-NZ-C4'	-2.42	112.01	119.03
1	6-B	197	LLP	C5-C6-N1	-2.41	119.79	123.87
1	8-H	197	LLP	C5-C6-N1	-2.41	119.79	123.87
1	7-G	197	LLP	CE-NZ-C4'	-2.41	112.03	119.03
1	7-B	197	LLP	C5-C6-N1	-2.41	119.79	123.87
1	4-C	197	LLP	C4-C4'-NZ	-2.41	112.96	124.66
1	2-C	197	LLP	C4-C4'-NZ	-2.41	112.97	124.66
1	3-F	197	LLP	C5-C6-N1	-2.40	119.81	123.87
1	2-F	197	LLP	O-C-CA	-2.39	118.41	125.02
1	2-E	197	LLP	CE-NZ-C4'	-2.39	112.09	119.03
1	2-D	197	LLP	C5-C6-N1	-2.39	119.83	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	7-F	197	LLP	CE-NZ-C4'	-2.39	112.10	119.03
1	7-B	197	LLP	O-C-CA	-2.39	118.43	125.02
1	6-F	197	LLP	C4-C4'-NZ	-2.38	113.08	124.66
1	3-D	197	LLP	CE-NZ-C4'	-2.38	112.12	119.03
1	8-H	197	LLP	C4-C4'-NZ	-2.38	113.11	124.66
1	2-F	197	LLP	C5-C6-N1	-2.38	119.85	123.87
1	9-C	197	LLP	O-C-CA	-2.36	118.50	125.02
1	10-B	197	LLP	C4-C4'-NZ	-2.36	113.20	124.66
1	8-D	197	LLP	C4-C4'-NZ	-2.36	113.22	124.66
1	6-H	197	LLP	C4-C4'-NZ	-2.34	113.28	124.66
1	5-H	197	LLP	C5-C6-N1	-2.34	119.91	123.87
1	10-F	197	LLP	CE-NZ-C4'	-2.33	112.26	119.03
1	1-D	197	LLP	C5-C6-N1	-2.33	119.92	123.87
1	8-E	197	LLP	O-C-CA	-2.32	118.61	125.02
1	1-C	197	LLP	CE-NZ-C4'	-2.31	112.32	119.03
1	3-A	197	LLP	O-C-CA	-2.31	118.63	125.02
1	4-A	197	LLP	O-C-CA	-2.31	118.64	125.02
1	1-H	197	LLP	C4-C4'-NZ	-2.29	113.52	124.66
1	3-B	197	LLP	O-C-CA	-2.29	118.70	125.02
1	6-G	197	LLP	C4-C4'-NZ	-2.28	113.56	124.66
1	8-D	197	LLP	CG-CD-CE	-2.28	104.82	113.59
1	6-D	197	LLP	C5-C6-N1	-2.28	120.01	123.87
1	8-C	197	LLP	O-C-CA	-2.27	118.74	125.02
1	6-D	197	LLP	O-C-CA	-2.27	118.74	125.02
1	4-F	197	LLP	O-C-CA	-2.27	118.76	125.02
1	6-H	197	LLP	C5-C6-N1	-2.26	120.04	123.87
1	10-D	197	LLP	C5-C6-N1	-2.26	120.04	123.87
1	2-C	197	LLP	C5-C6-N1	-2.26	120.04	123.87
1	3-D	197	LLP	C5-C6-N1	-2.26	120.04	123.87
1	8-E	197	LLP	C4-C4'-NZ	-2.26	113.68	124.66
1	10-E	197	LLP	C5-C6-N1	-2.26	120.05	123.87
1	2-F	197	LLP	CE-NZ-C4'	-2.24	112.52	119.03
1	10-F	197	LLP	O-C-CA	-2.24	118.82	125.02
1	1-E	197	LLP	C5-C6-N1	-2.24	120.07	123.87
1	4-E	197	LLP	O-C-CA	-2.22	118.88	125.02
1	8-E	197	LLP	C5-C6-N1	-2.22	120.11	123.87
1	8-F	197	LLP	C5-C6-N1	-2.22	120.11	123.87
1	8-B	197	LLP	C5-C6-N1	-2.22	120.11	123.87
1	4-B	197	LLP	O-C-CA	-2.22	118.89	125.02
1	8-D	197	LLP	C5-C6-N1	-2.21	120.13	123.87
1	1-A	197	LLP	O-C-CA	-2.21	118.92	125.02
1	10-F	197	LLP	C5-C6-N1	-2.20	120.14	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-F	197	LLP	C5-C6-N1	-2.20	120.14	123.87
1	1-F	197	LLP	C5-C6-N1	-2.20	120.15	123.87
1	6-B	197	LLP	C4-C4'-NZ	-2.20	113.99	124.66
1	5-B	197	LLP	O-C-CA	-2.19	118.96	125.02
1	4-E	197	LLP	C5-C6-N1	-2.19	120.16	123.87
1	5-B	197	LLP	C4-C4'-NZ	-2.19	114.03	124.66
1	3-G	197	LLP	O-C-CA	-2.19	118.98	125.02
1	9-G	197	LLP	C5-C6-N1	-2.19	120.17	123.87
1	2-B	197	LLP	C5-C6-N1	-2.18	120.17	123.87
1	3-E	197	LLP	O-C-CA	-2.18	118.99	125.02
1	3-B	197	LLP	C5-C6-N1	-2.18	120.18	123.87
1	2-G	197	LLP	C4-C4'-NZ	-2.18	114.09	124.66
1	9-H	197	LLP	C4-C4'-NZ	-2.17	114.10	124.66
1	10-G	197	LLP	C4-C4'-NZ	-2.17	114.11	124.66
1	1-F	197	LLP	O-C-CA	-2.17	119.02	125.02
1	9-E	197	LLP	C5-C6-N1	-2.17	120.20	123.87
1	7-C	197	LLP	C5-C6-N1	-2.17	120.20	123.87
1	7-E	197	LLP	C4-C4'-NZ	-2.17	114.14	124.66
1	6-E	197	LLP	O-C-CA	-2.16	119.05	125.02
1	7-G	197	LLP	O-C-CA	-2.15	119.08	125.02
1	1-B	197	LLP	C4-C4'-NZ	-2.15	114.22	124.66
1	1-C	197	LLP	O-C-CA	-2.14	119.10	125.02
1	5-C	197	LLP	O-C-CA	-2.14	119.10	125.02
1	3-A	197	LLP	C5-C6-N1	-2.14	120.25	123.87
1	5-E	197	LLP	C5-C6-N1	-2.14	120.25	123.87
1	5-G	197	LLP	C5-C6-N1	-2.14	120.25	123.87
1	10-B	197	LLP	C5-C6-N1	-2.13	120.26	123.87
1	7-B	197	LLP	C4-C4'-NZ	-2.13	114.31	124.66
1	3-F	197	LLP	O-C-CA	-2.13	119.14	125.02
1	9-A	197	LLP	C5-C6-N1	-2.13	120.27	123.87
1	8-F	197	LLP	O-C-CA	-2.12	119.15	125.02
1	9-B	197	LLP	O-C-CA	-2.12	119.16	125.02
1	2-B	197	LLP	O-C-CA	-2.12	119.17	125.02
1	7-F	197	LLP	C5-C6-N1	-2.11	120.29	123.87
1	5-G	197	LLP	O-C-CA	-2.11	119.19	125.02
1	3-G	197	LLP	CE-NZ-C4'	-2.11	112.92	119.03
1	8-H	197	LLP	O-C-CA	-2.10	119.22	125.02
1	1-C	197	LLP	C5'-C5-C6	-2.10	115.72	119.33
1	4-G	197	LLP	C5-C6-N1	-2.10	120.32	123.87
1	7-C	197	LLP	O-C-CA	-2.09	119.23	125.02
1	4-G	197	LLP	O-C-CA	-2.08	119.26	125.02
1	7-A	197	LLP	C5-C6-N1	-2.08	120.35	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	197	LLP	C4-C4'-NZ	-2.08	114.58	124.66
1	6-C	197	LLP	O-C-CA	-2.08	119.28	125.02
1	4-C	197	LLP	C5-C6-N1	-2.07	120.36	123.87
1	6-F	197	LLP	O-C-CA	-2.07	119.31	125.02
1	1-A	197	LLP	C5-C6-N1	-2.07	120.37	123.87
1	3-B	197	LLP	C4-C4'-NZ	-2.06	114.67	124.66
1	4-A	197	LLP	C5-C6-N1	-2.05	120.39	123.87
1	8-C	197	LLP	C5'-C5-C6	-2.05	115.81	119.33
1	3-H	197	LLP	C5-C6-N1	-2.05	120.40	123.87
1	5-A	197	LLP	C5-C6-N1	-2.04	120.42	123.87
1	7-E	197	LLP	O-C-CA	-2.04	119.39	125.02
1	3-D	197	LLP	O-C-CA	-2.03	119.41	125.02
1	10-H	197	LLP	O-C-CA	-2.03	119.41	125.02
1	1-D	197	LLP	O-C-CA	-2.03	119.41	125.02
1	4-D	197	LLP	C5-C6-N1	-2.03	120.44	123.87
1	4-H	197	LLP	C5-C6-N1	-2.03	120.44	123.87
1	7-G	197	LLP	C4-C4'-NZ	-2.02	114.83	124.66
1	7-G	197	LLP	C5-C6-N1	-2.02	120.45	123.87
1	5-D	197	LLP	O-C-CA	-2.02	119.44	125.02
1	3-C	197	LLP	C5'-C5-C6	-2.02	115.86	119.33
1	5-C	197	LLP	C5-C6-N1	-2.02	120.45	123.87
1	10-G	197	LLP	O-C-CA	-2.01	119.45	125.02
1	6-B	197	LLP	O-C-CA	-2.01	119.46	125.02
1	8-B	197	LLP	C4-C4'-NZ	-2.01	114.90	124.66
1	3-C	197	LLP	C4-C3-C2	2.01	121.39	120.15
1	10-B	197	LLP	OP4-C5'-C5	2.02	113.37	109.32
1	5-C	197	LLP	OP4-C5'-C5	2.02	113.39	109.32
1	1-E	197	LLP	C3-C4-C5	2.03	119.79	118.24
1	4-C	197	LLP	CB-CA-C	2.03	115.00	111.65
1	10-C	197	LLP	CB-CA-C	2.03	115.00	111.65
1	2-H	197	LLP	C3-C4-C5	2.04	119.80	118.24
1	6-A	197	LLP	CB-CA-C	2.04	115.02	111.65
1	1-C	197	LLP	OP4-C5'-C5	2.05	113.43	109.32
1	2-E	197	LLP	OP3-P-OP4	2.05	112.19	106.73
1	3-C	197	LLP	OP4-C5'-C5	2.11	113.56	109.32
1	6-G	197	LLP	CD-CE-NZ	2.14	115.61	110.88
1	6-C	197	LLP	C5'-C5-C4	2.16	125.44	121.66
1	1-F	197	LLP	CB-CA-C	2.17	115.23	111.65
1	8-A	197	LLP	OP4-C5'-C5	2.19	113.72	109.32
1	9-B	197	LLP	C2'-C2-N1	2.19	122.27	117.89
1	4-F	197	LLP	OP4-C5'-C5	2.20	113.74	109.32
1	10-A	197	LLP	CB-CA-C	2.20	115.27	111.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	9-A	197	LLP	C3-C4-C5	2.21	119.93	118.24
1	10-G	197	LLP	CD-CE-NZ	2.22	115.78	110.88
1	8-D	197	LLP	CD-CE-NZ	2.23	115.81	110.88
1	9-E	197	LLP	C3-C4-C5	2.25	119.96	118.24
1	5-C	197	LLP	C5'-C5-C4	2.26	125.61	121.66
1	8-F	197	LLP	OP4-C5'-C5	2.28	113.89	109.32
1	3-H	197	LLP	OP4-C5'-C5	2.28	113.89	109.32
1	10-F	197	LLP	OP4-C5'-C5	2.29	113.93	109.32
1	2-F	197	LLP	OP4-C5'-C5	2.32	113.98	109.32
1	1-F	197	LLP	OP4-C5'-C5	2.36	114.06	109.32
1	10-C	197	LLP	OP4-C5'-C5	2.40	114.15	109.32
1	3-B	197	LLP	OP4-C5'-C5	2.45	114.24	109.32
1	9-B	197	LLP	CB-CA-C	2.51	115.79	111.65
1	4-E	197	LLP	CB-CA-C	2.51	115.80	111.65
1	4-G	197	LLP	CB-CA-C	2.52	115.80	111.65
1	4-F	197	LLP	CB-CA-C	2.53	115.82	111.65
1	7-F	197	LLP	OP4-C5'-C5	2.53	114.41	109.32
1	7-B	197	LLP	CB-CA-C	2.58	115.90	111.65
1	4-H	197	LLP	OP4-C5'-C5	2.59	114.53	109.32
1	8-G	197	LLP	C3-C4-C5	2.60	120.22	118.24
1	4-A	197	LLP	OP4-C5'-C5	2.65	114.65	109.32
1	6-C	197	LLP	OP4-C5'-C5	2.66	114.66	109.32
1	5-G	197	LLP	CB-CA-C	2.72	116.13	111.65
1	2-E	197	LLP	CD-CE-NZ	2.73	116.91	110.88
1	3-B	197	LLP	CD-CE-NZ	2.76	116.99	110.88
1	6-C	197	LLP	CB-CA-C	2.78	116.23	111.65
1	8-F	197	LLP	CB-CA-C	2.79	116.26	111.65
1	9-B	197	LLP	C3-C4-C5	2.80	120.37	118.24
1	7-F	197	LLP	CB-CA-C	2.82	116.30	111.65
1	7-A	197	LLP	OP4-C5'-C5	2.82	114.99	109.32
1	5-A	197	LLP	CB-CA-C	2.86	116.37	111.65
1	2-A	197	LLP	OP4-C5'-C5	2.91	115.16	109.32
1	9-F	197	LLP	CB-CA-C	2.94	116.50	111.65
1	9-C	197	LLP	CB-CA-C	2.95	116.51	111.65
1	5-F	197	LLP	C3-C4-C5	2.97	120.50	118.24
1	4-B	197	LLP	CB-CA-C	3.03	116.64	111.65
1	3-A	197	LLP	OP4-C5'-C5	3.10	115.54	109.32
1	4-C	197	LLP	OP4-C5'-C5	3.11	115.57	109.32
1	10-G	197	LLP	CB-CA-C	3.17	116.87	111.65
1	2-F	197	LLP	CB-CA-C	3.23	116.98	111.65
1	8-C	197	LLP	CB-CA-C	3.25	117.01	111.65
1	7-G	197	LLP	CB-CA-C	3.62	117.62	111.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-H	197	LLP	CB-CA-C	3.63	117.64	111.65
1	3-H	197	LLP	CB-CA-C	3.97	118.19	111.65
1	10-B	197	LLP	CB-CA-C	3.99	118.22	111.65
1	7-D	197	LLP	CB-CA-C	4.85	119.64	111.65
1	2-H	197	LLP	CB-CA-C	4.91	119.74	111.65
1	7-H	197	LLP	CB-CA-C	5.25	120.30	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

48 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1-A	197	LLP	1	0
1	1-D	197	LLP	3	0
1	1-G	197	LLP	2	0
1	1-H	197	LLP	1	0
1	10-B	197	LLP	1	0
1	10-C	197	LLP	2	0
1	10-E	197	LLP	2	0
1	10-F	197	LLP	1	0
1	10-G	197	LLP	1	0
1	2-B	197	LLP	1	0
1	2-C	197	LLP	1	0
1	2-F	197	LLP	1	0
1	2-H	197	LLP	1	0
1	3-A	197	LLP	1	0
1	3-B	197	LLP	3	0
1	3-C	197	LLP	2	0
1	3-D	197	LLP	2	0
1	3-E	197	LLP	1	0
1	3-G	197	LLP	1	0
1	3-H	197	LLP	1	0
1	4-C	197	LLP	1	0
1	4-D	197	LLP	1	0
1	4-F	197	LLP	2	0
1	4-H	197	LLP	3	0
1	5-B	197	LLP	1	0
1	5-D	197	LLP	1	0
1	5-F	197	LLP	1	0
1	5-H	197	LLP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	6-A	197	LLP	2	0
1	6-C	197	LLP	1	0
1	6-F	197	LLP	1	0
1	6-H	197	LLP	2	0
1	7-A	197	LLP	1	0
1	7-B	197	LLP	2	0
1	7-F	197	LLP	2	0
1	7-G	197	LLP	2	0
1	7-H	197	LLP	2	0
1	8-A	197	LLP	2	0
1	8-B	197	LLP	2	0
1	8-D	197	LLP	2	0
1	8-E	197	LLP	1	0
1	8-F	197	LLP	1	0
1	8-H	197	LLP	1	0
1	9-A	197	LLP	3	0
1	9-B	197	LLP	1	0
1	9-C	197	LLP	2	0
1	9-E	197	LLP	1	0
1	9-F	197	LLP	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 494 ligands modelled in this entry, 107 are monoatomic - leaving 387 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	$\# Z  > 2$
2	MES	1-A	401	-	12,12,12	2.15	1 (8%)	14,16,16	2.44	6 (42%)
3	GOL	1-A	402	-	5,5,5	0.33	0	5,5,5	0.23	0
3	GOL	1-A	403	-	5,5,5	0.36	0	5,5,5	0.40	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	1-A	404	-	5,5,5	0.40	0	5,5,5	0.39	0
2	MES	1-B	401	-	12,12,12	1.84	1 (8%)	14,16,16	2.53	6 (42%)
3	GOL	1-B	402	-	5,5,5	0.37	0	5,5,5	0.41	0
3	GOL	1-B	403	-	5,5,5	0.37	0	5,5,5	0.26	0
3	GOL	1-B	404	-	5,5,5	0.31	0	5,5,5	0.69	0
3	GOL	1-B	405	-	5,5,5	0.37	0	5,5,5	0.50	0
3	GOL	1-B	406	-	5,5,5	0.36	0	5,5,5	0.32	0
3	GOL	1-B	407	-	5,5,5	0.38	0	5,5,5	0.37	0
4	GOL	1-B	408	-	5,5,5	0.35	0	5,5,5	0.28	0
2	MES	1-C	401	-	12,12,12	2.19	1 (8%)	14,16,16	2.80	7 (50%)
3	GOL	1-C	402	-	5,5,5	0.31	0	5,5,5	0.33	0
3	FMT	1-C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	1-D	401	-	12,12,12	2.12	1 (8%)	14,16,16	3.00	8 (57%)
3	GOL	1-D	402	-	5,5,5	0.40	0	5,5,5	0.37	0
3	GOL	1-D	403	-	5,5,5	1.04	0	5,5,5	1.24	1 (20%)
3	GOL	1-D	404	-	5,5,5	0.42	0	5,5,5	0.13	0
2	MES	1-E	401	-	12,12,12	1.99	1 (8%)	14,16,16	2.51	4 (28%)
3	GOL	1-E	402	-	5,5,5	0.26	0	5,5,5	0.68	0
3	GOL	1-E	403	-	5,5,5	0.39	0	5,5,5	0.21	0
2	MES	1-F	401	-	12,12,12	1.73	1 (8%)	14,16,16	3.17	8 (57%)
3	GOL	1-F	402	-	5,5,5	0.40	0	5,5,5	0.22	0
3	GOL	1-F	403	-	5,5,5	0.34	0	5,5,5	0.45	0
3	GOL	1-F	404	-	5,5,5	0.37	0	5,5,5	0.55	0
3	GOL	1-F	405	-	5,5,5	0.36	0	5,5,5	0.29	0
3	GOL	1-F	406	-	5,5,5	1.40	1 (20%)	5,5,5	1.38	1 (20%)
5	GOL	1-F	407	-	5,5,5	0.38	0	5,5,5	0.25	0
4	FMT	1-F	408	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	1-G	401	-	12,12,12	2.00	1 (8%)	14,16,16	2.56	7 (50%)
3	GOL	1-G	402	-	5,5,5	0.45	0	5,5,5	0.59	0
3	GOL	1-G	403	-	5,5,5	0.41	0	5,5,5	0.50	0
3	GOL	1-G	404	-	5,5,5	0.41	0	5,5,5	0.32	0
5	GOL	1-G	405	-	5,5,5	0.32	0	5,5,5	0.55	0
4	FMT	1-G	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	1-H	401	-	12,12,12	1.75	1 (8%)	14,16,16	2.75	8 (57%)
3	GOL	1-H	402	-	5,5,5	0.40	0	5,5,5	0.42	0
3	GOL	1-H	403	-	5,5,5	0.36	0	5,5,5	0.26	0
2	MES	10-A	401	-	12,12,12	2.12	1 (8%)	14,16,16	2.15	4 (28%)
3	GOL	10-A	402	-	5,5,5	0.33	0	5,5,5	0.17	0
3	GOL	10-A	403	-	5,5,5	0.39	0	5,5,5	0.33	0
3	GOL	10-A	404	-	5,5,5	0.34	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MES	10-B	401	-	12,12,12	1.89	1 (8%)	14,16,16	2.48	7 (50%)
3	GOL	10-B	402	-	5,5,5	0.33	0	5,5,5	0.27	0
3	GOL	10-B	403	-	5,5,5	0.28	0	5,5,5	0.54	0
3	GOL	10-B	404	-	5,5,5	0.29	0	5,5,5	0.54	0
3	GOL	10-B	405	-	5,5,5	0.38	0	5,5,5	0.35	0
3	GOL	10-B	406	-	5,5,5	0.32	0	5,5,5	0.45	0
3	GOL	10-B	407	-	5,5,5	0.39	0	5,5,5	0.41	0
2	MES	10-C	401	-	12,12,12	1.59	1 (8%)	14,16,16	4.37	7 (50%)
3	GOL	10-C	402	-	5,5,5	0.28	0	5,5,5	0.34	0
3	GOL	10-C	403	-	5,5,5	0.34	0	5,5,5	0.17	0
5	FMT	10-C	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	10-D	401	-	12,12,12	1.92	1 (8%)	14,16,16	2.09	5 (35%)
3	GOL	10-D	402	-	5,5,5	0.43	0	5,5,5	0.51	0
3	GOL	10-D	403	-	5,5,5	0.28	0	5,5,5	0.46	0
3	GOL	10-D	404	-	5,5,5	0.27	0	5,5,5	0.22	0
2	MES	10-E	401	-	12,12,12	1.87	1 (8%)	14,16,16	2.84	7 (50%)
3	GOL	10-E	402	-	5,5,5	0.24	0	5,5,5	0.85	0
3	GOL	10-E	403	-	5,5,5	0.34	0	5,5,5	0.50	0
2	MES	10-F	401	-	12,12,12	2.37	1 (8%)	14,16,16	2.91	8 (57%)
3	GOL	10-F	402	-	5,5,5	0.36	0	5,5,5	0.30	0
3	GOL	10-F	403	-	5,5,5	0.38	0	5,5,5	0.43	0
3	GOL	10-F	404	-	5,5,5	0.38	0	5,5,5	0.20	0
3	GOL	10-F	405	-	5,5,5	0.39	0	5,5,5	0.43	0
3	GOL	10-F	406	-	5,5,5	0.30	0	5,5,5	0.23	0
5	FMT	10-F	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	10-G	401	-	12,12,12	1.83	1 (8%)	14,16,16	3.12	8 (57%)
3	GOL	10-G	402	-	5,5,5	0.34	0	5,5,5	0.82	0
3	GOL	10-G	403	-	5,5,5	0.37	0	5,5,5	0.40	0
3	GOL	10-G	404	-	5,5,5	0.36	0	5,5,5	0.31	0
5	FMT	10-G	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	10-H	401	-	12,12,12	2.11	1 (8%)	14,16,16	2.72	5 (35%)
3	GOL	10-H	402	-	5,5,5	0.38	0	5,5,5	0.32	0
3	GOL	10-H	403	-	5,5,5	0.39	0	5,5,5	0.66	0
3	GOL	10-H	404	-	5,5,5	0.21	0	5,5,5	0.36	0
3	GOL	10-H	405	-	5,5,5	0.33	0	5,5,5	0.39	0
2	MES	2-A	401	-	12,12,12	1.96	1 (8%)	14,16,16	2.07	3 (21%)
3	GOL	2-A	402	-	5,5,5	0.39	0	5,5,5	0.30	0
3	GOL	2-A	403	-	5,5,5	0.32	0	5,5,5	0.48	0
3	GOL	2-A	404	-	5,5,5	0.35	0	5,5,5	0.32	0
2	MES	2-B	401	-	12,12,12	2.00	1 (8%)	14,16,16	2.36	5 (35%)
3	GOL	2-B	402	-	5,5,5	0.31	0	5,5,5	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	2-B	403	-	5,5,5	1.06	0	5,5,5	2.52	2 (40%)
3	GOL	2-B	404	-	5,5,5	0.41	0	5,5,5	0.40	0
3	GOL	2-B	405	-	5,5,5	0.34	0	5,5,5	0.28	0
3	GOL	2-B	406	-	5,5,5	0.43	0	5,5,5	0.29	0
3	GOL	2-B	407	-	5,5,5	0.39	0	5,5,5	0.38	0
2	MES	2-C	401	-	12,12,12	1.72	1 (8%)	14,16,16	2.66	7 (50%)
3	GOL	2-C	402	-	5,5,5	0.35	0	5,5,5	0.46	0
3	GOL	2-C	403	-	5,5,5	0.44	0	5,5,5	0.18	0
5	GOL	2-C	404	-	5,5,5	0.36	0	5,5,5	0.27	0
4	FMT	2-C	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	2-D	401	-	12,12,12	1.91	1 (8%)	14,16,16	3.11	8 (57%)
3	GOL	2-D	402	-	5,5,5	0.39	0	5,5,5	0.45	0
3	GOL	2-D	403	-	5,5,5	0.33	0	5,5,5	0.32	0
2	MES	2-E	401	-	12,12,12	1.74	1 (8%)	14,16,16	3.11	5 (35%)
3	GOL	2-E	402	-	5,5,5	0.26	0	5,5,5	0.32	0
3	GOL	2-E	403	-	5,5,5	0.36	0	5,5,5	0.44	0
4	GOL	2-E	404	-	5,5,5	0.32	0	5,5,5	0.32	0
2	MES	2-F	401	-	12,12,12	1.82	1 (8%)	14,16,16	3.20	7 (50%)
3	GOL	2-F	402	-	5,5,5	0.36	0	5,5,5	0.64	0
3	GOL	2-F	403	-	5,5,5	0.44	0	5,5,5	0.32	0
3	GOL	2-F	404	-	5,5,5	0.44	0	5,5,5	0.15	0
3	GOL	2-F	405	-	5,5,5	0.35	0	5,5,5	0.23	0
3	FMT	2-F	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	2-G	401	-	12,12,12	2.14	1 (8%)	14,16,16	2.56	3 (21%)
3	GOL	2-G	402	-	5,5,5	0.34	0	5,5,5	0.38	0
3	GOL	2-G	403	-	5,5,5	0.33	0	5,5,5	0.52	0
3	GOL	2-G	404	-	5,5,5	1.25	0	5,5,5	0.85	0
5	FMT	2-G	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	2-H	401	-	12,12,12	2.55	1 (8%)	14,16,16	2.11	5 (35%)
3	GOL	2-H	402	-	5,5,5	0.36	0	5,5,5	0.21	0
3	GOL	2-H	403	-	5,5,5	1.17	1 (20%)	5,5,5	1.04	0
3	GOL	2-H	404	-	5,5,5	0.24	0	5,5,5	0.53	0
2	MES	3-A	401	-	12,12,12	1.53	1 (8%)	14,16,16	2.61	6 (42%)
3	GOL	3-A	402	-	5,5,5	0.23	0	5,5,5	0.23	0
3	GOL	3-A	403	-	5,5,5	0.33	0	5,5,5	0.33	0
3	GOL	3-A	404	-	5,5,5	0.32	0	5,5,5	0.37	0
4	GOL	3-A	405	-	5,5,5	0.36	0	5,5,5	0.25	0
2	MES	3-B	401	-	12,12,12	2.11	1 (8%)	14,16,16	5.08	7 (50%)
3	GOL	3-B	402	-	5,5,5	0.39	0	5,5,5	0.36	0
3	GOL	3-B	403	-	5,5,5	0.35	0	5,5,5	0.51	0
3	GOL	3-B	404	-	5,5,5	0.31	0	5,5,5	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	3-B	405	-	5,5,5	0.39	0	5,5,5	0.40	0
3	GOL	3-B	406	-	5,5,5	0.39	0	5,5,5	0.32	0
3	GOL	3-B	407	-	5,5,5	0.27	0	5,5,5	0.42	0
2	MES	3-C	401	-	12,12,12	1.95	1 (8%)	14,16,16	4.74	7 (50%)
3	GOL	3-C	402	-	5,5,5	0.40	0	5,5,5	0.30	0
3	GOL	3-C	403	-	5,5,5	0.27	0	5,5,5	0.62	0
5	FMT	3-C	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	3-D	401	-	12,12,12	1.68	1 (8%)	14,16,16	3.26	8 (57%)
3	GOL	3-D	402	-	5,5,5	0.40	0	5,5,5	0.61	0
3	GOL	3-D	403	-	5,5,5	0.35	0	5,5,5	0.19	0
2	MES	3-E	401	-	12,12,12	1.86	1 (8%)	14,16,16	4.68	12 (85%)
3	GOL	3-E	402	-	5,5,5	0.40	0	5,5,5	0.38	0
3	GOL	3-E	403	-	5,5,5	0.32	0	5,5,5	0.76	0
4	GOL	3-E	404	-	5,5,5	0.43	0	5,5,5	0.23	0
2	MES	3-F	401	-	12,12,12	1.86	1 (8%)	14,16,16	3.49	5 (35%)
3	GOL	3-F	402	-	5,5,5	0.32	0	5,5,5	0.20	0
3	GOL	3-F	403	-	5,5,5	0.34	0	5,5,5	0.42	0
3	GOL	3-F	404	-	5,5,5	0.41	0	5,5,5	0.44	0
3	GOL	3-F	405	-	5,5,5	0.27	0	5,5,5	0.84	0
3	GOL	3-F	406	-	5,5,5	0.37	0	5,5,5	0.30	0
5	FMT	3-F	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	3-G	401	-	12,12,12	1.53	1 (8%)	14,16,16	2.07	5 (35%)
3	GOL	3-G	402	-	5,5,5	0.41	0	5,5,5	0.40	0
3	GOL	3-G	403	-	5,5,5	0.30	0	5,5,5	0.63	0
3	GOL	3-G	404	-	5,5,5	0.34	0	5,5,5	0.32	0
5	GOL	3-G	405	-	5,5,5	0.28	0	5,5,5	0.37	0
4	FMT	3-G	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	3-H	401	-	12,12,12	2.42	1 (8%)	14,16,16	3.97	7 (50%)
3	GOL	3-H	402	-	5,5,5	0.37	0	5,5,5	0.44	0
3	GOL	3-H	403	-	5,5,5	0.39	0	5,5,5	0.32	0
2	MES	4-A	401	-	12,12,12	2.09	1 (8%)	14,16,16	2.60	6 (42%)
3	GOL	4-A	402	-	5,5,5	0.31	0	5,5,5	0.31	0
3	GOL	4-A	403	-	5,5,5	0.34	0	5,5,5	0.53	0
3	GOL	4-A	404	-	5,5,5	0.38	0	5,5,5	0.53	0
2	MES	4-B	401	-	12,12,12	1.88	1 (8%)	14,16,16	2.49	7 (50%)
3	GOL	4-B	402	-	5,5,5	0.35	0	5,5,5	0.39	0
3	GOL	4-B	403	-	5,5,5	0.50	0	5,5,5	0.79	0
3	GOL	4-B	404	-	5,5,5	0.34	0	5,5,5	0.26	0
3	GOL	4-B	405	-	5,5,5	0.35	0	5,5,5	0.32	0
3	GOL	4-B	406	-	5,5,5	0.34	0	5,5,5	0.50	0
3	GOL	4-B	407	-	5,5,5	0.45	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MES	4-C	401	-	12,12,12	2.56	1 (8%)	14,16,16	3.96	4 (28%)
3	GOL	4-C	402	-	5,5,5	0.37	0	5,5,5	0.25	0
3	GOL	4-C	403	-	5,5,5	0.38	0	5,5,5	0.30	0
5	GOL	4-C	404	-	5,5,5	0.43	0	5,5,5	0.63	0
4	FMT	4-C	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	4-D	401	-	12,12,12	2.04	1 (8%)	14,16,16	2.97	6 (42%)
3	GOL	4-D	402	-	5,5,5	0.35	0	5,5,5	0.39	0
3	GOL	4-D	403	-	5,5,5	0.27	0	5,5,5	0.49	0
2	MES	4-E	401	-	12,12,12	1.33	1 (8%)	14,16,16	2.12	5 (35%)
3	GOL	4-E	402	-	5,5,5	0.28	0	5,5,5	0.33	0
3	GOL	4-E	403	-	5,5,5	0.44	0	5,5,5	0.57	0
4	GOL	4-E	404	-	5,5,5	0.57	0	5,5,5	0.41	0
2	MES	4-F	401	-	12,12,12	1.86	1 (8%)	14,16,16	2.48	6 (42%)
3	GOL	4-F	402	-	5,5,5	0.37	0	5,5,5	0.37	0
3	GOL	4-F	403	-	5,5,5	0.42	0	5,5,5	0.22	0
3	GOL	4-F	404	-	5,5,5	0.28	0	5,5,5	0.61	0
3	FMT	4-F	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	4-G	401	-	12,12,12	2.04	1 (8%)	14,16,16	2.95	4 (28%)
3	GOL	4-G	402	-	5,5,5	0.38	0	5,5,5	0.26	0
3	GOL	4-G	403	-	5,5,5	0.35	0	5,5,5	0.37	0
3	GOL	4-G	404	-	5,5,5	0.39	0	5,5,5	0.60	0
5	GOL	4-G	405	-	5,5,5	0.44	0	5,5,5	0.29	0
4	GOL	4-G	406	-	5,5,5	0.38	0	5,5,5	0.22	0
4	FMT	4-G	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	4-H	401	-	12,12,12	1.98	1 (8%)	14,16,16	2.40	7 (50%)
3	GOL	4-H	402	-	5,5,5	0.44	0	5,5,5	0.27	0
3	GOL	4-H	403	-	5,5,5	0.31	0	5,5,5	0.41	0
3	GOL	4-H	404	-	5,5,5	0.32	0	5,5,5	0.24	0
2	MES	5-A	401	-	12,12,12	1.78	1 (8%)	14,16,16	2.55	7 (50%)
3	GOL	5-A	402	-	5,5,5	0.28	0	5,5,5	0.33	0
3	GOL	5-A	403	-	5,5,5	0.39	0	5,5,5	0.46	0
3	GOL	5-A	404	-	5,5,5	0.36	0	5,5,5	0.43	0
4	GOL	5-A	405	-	5,5,5	0.35	0	5,5,5	0.32	0
2	MES	5-B	401	-	12,12,12	2.05	2 (16%)	14,16,16	2.87	8 (57%)
3	GOL	5-B	402	-	5,5,5	0.34	0	5,5,5	0.34	0
3	GOL	5-B	403	-	5,5,5	0.39	0	5,5,5	0.32	0
3	GOL	5-B	404	-	5,5,5	0.33	0	5,5,5	0.45	0
3	GOL	5-B	405	-	5,5,5	0.46	0	5,5,5	0.55	0
3	GOL	5-B	406	-	5,5,5	0.43	0	5,5,5	0.23	0
3	GOL	5-B	407	-	5,5,5	0.20	0	5,5,5	0.45	0
2	MES	5-C	401	-	12,12,12	2.03	1 (8%)	14,16,16	2.42	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	5-C	402	-	5,5,5	0.31	0	5,5,5	0.29	0
3	FMT	5-C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	5-D	401	-	12,12,12	2.07	1 (8%)	14,16,16	3.78	5 (35%)
3	GOL	5-D	402	-	5,5,5	0.31	0	5,5,5	0.35	0
3	GOL	5-D	403	-	5,5,5	0.34	0	5,5,5	0.54	0
3	GOL	5-D	404	-	5,5,5	0.37	0	5,5,5	0.61	0
2	MES	5-E	401	-	12,12,12	2.08	1 (8%)	14,16,16	3.07	9 (64%)
3	GOL	5-E	402	-	5,5,5	0.47	0	5,5,5	0.25	0
3	GOL	5-E	403	-	5,5,5	0.35	0	5,5,5	0.25	0
4	GOL	5-E	404	-	5,5,5	0.36	0	5,5,5	0.27	0
2	MES	5-F	401	-	12,12,12	1.95	1 (8%)	14,16,16	2.76	5 (35%)
3	GOL	5-F	402	-	5,5,5	0.39	0	5,5,5	0.30	0
3	GOL	5-F	403	-	5,5,5	0.47	0	5,5,5	0.09	0
3	GOL	5-F	404	-	5,5,5	0.33	0	5,5,5	0.40	0
3	FMT	5-F	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	5-G	401	-	12,12,12	2.42	1 (8%)	14,16,16	4.11	11 (78%)
3	GOL	5-G	402	-	5,5,5	0.28	0	5,5,5	0.66	0
3	GOL	5-G	403	-	5,5,5	0.42	0	5,5,5	0.22	0
3	GOL	5-G	404	-	5,5,5	0.42	0	5,5,5	0.38	0
5	GOL	5-G	405	-	5,5,5	0.38	0	5,5,5	0.31	0
4	FMT	5-G	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	5-H	401	-	12,12,12	1.95	1 (8%)	14,16,16	3.37	5 (35%)
3	GOL	5-H	402	-	5,5,5	0.41	0	5,5,5	0.19	0
3	GOL	5-H	403	-	5,5,5	0.51	0	5,5,5	0.41	0
3	GOL	5-H	404	-	5,5,5	0.39	0	5,5,5	0.42	0
2	MES	6-A	401	-	12,12,12	1.43	1 (8%)	14,16,16	2.86	7 (50%)
3	GOL	6-A	402	-	5,5,5	0.32	0	5,5,5	0.35	0
3	GOL	6-A	403	-	5,5,5	0.39	0	5,5,5	0.67	0
3	GOL	6-A	404	-	5,5,5	0.34	0	5,5,5	0.34	0
4	GOL	6-A	405	-	5,5,5	0.40	0	5,5,5	0.21	0
2	MES	6-B	401	-	12,12,12	2.15	1 (8%)	14,16,16	2.26	7 (50%)
3	GOL	6-B	402	-	5,5,5	0.32	0	5,5,5	0.27	0
3	GOL	6-B	403	-	5,5,5	0.32	0	5,5,5	0.41	0
3	GOL	6-B	404	-	5,5,5	0.26	0	5,5,5	0.44	0
3	GOL	6-B	405	-	5,5,5	0.40	0	5,5,5	0.33	0
3	GOL	6-B	406	-	5,5,5	0.36	0	5,5,5	0.36	0
3	GOL	6-B	407	-	5,5,5	0.36	0	5,5,5	0.21	0
2	MES	6-C	401	-	12,12,12	2.74	1 (8%)	14,16,16	3.28	8 (57%)
3	GOL	6-C	402	-	5,5,5	0.27	0	5,5,5	0.42	0
3	FMT	6-C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	6-D	401	-	12,12,12	1.91	1 (8%)	14,16,16	3.17	7 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	6-D	402	-	5,5,5	0.42	0	5,5,5	0.48	0
3	GOL	6-D	403	-	5,5,5	0.23	0	5,5,5	0.61	0
3	GOL	6-D	404	-	5,5,5	0.36	0	5,5,5	0.40	0
2	MES	6-E	401	-	12,12,12	1.85	1 (8%)	14,16,16	4.05	8 (57%)
3	GOL	6-E	402	-	5,5,5	0.39	0	5,5,5	0.33	0
3	GOL	6-E	403	-	5,5,5	0.36	0	5,5,5	0.20	0
4	GOL	6-E	404	-	5,5,5	0.45	0	5,5,5	0.21	0
2	MES	6-F	401	-	12,12,12	1.76	1 (8%)	14,16,16	2.42	6 (42%)
3	GOL	6-F	402	-	5,5,5	0.41	0	5,5,5	0.33	0
3	GOL	6-F	403	-	5,5,5	0.38	0	5,5,5	0.50	0
3	GOL	6-F	404	-	5,5,5	0.24	0	5,5,5	0.52	0
3	GOL	6-F	405	-	5,5,5	0.36	0	5,5,5	0.27	0
3	GOL	6-F	406	-	5,5,5	0.33	0	5,5,5	0.25	0
5	FMT	6-F	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	6-G	401	-	12,12,12	1.83	1 (8%)	14,16,16	2.89	6 (42%)
3	GOL	6-G	402	-	5,5,5	0.46	0	5,5,5	0.26	0
3	GOL	6-G	403	-	5,5,5	0.35	0	5,5,5	0.56	0
3	FMT	6-G	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	6-H	401	-	12,12,12	2.30	1 (8%)	14,16,16	2.79	5 (35%)
3	GOL	6-H	402	-	5,5,5	0.85	0	5,5,5	0.37	0
3	GOL	6-H	403	-	5,5,5	0.40	0	5,5,5	0.90	0
3	GOL	6-H	404	-	5,5,5	0.28	0	5,5,5	0.44	0
3	GOL	6-H	405	-	5,5,5	0.53	0	5,5,5	0.26	0
2	MES	7-A	401	-	12,12,12	1.85	1 (8%)	14,16,16	2.27	4 (28%)
3	GOL	7-A	402	-	5,5,5	0.34	0	5,5,5	0.20	0
3	GOL	7-A	403	-	5,5,5	0.34	0	5,5,5	0.23	0
3	GOL	7-A	404	-	5,5,5	0.32	0	5,5,5	0.33	0
4	GOL	7-A	405	-	5,5,5	0.36	0	5,5,5	0.30	0
2	MES	7-B	401	-	12,12,12	1.93	1 (8%)	14,16,16	2.65	6 (42%)
3	GOL	7-B	402	-	5,5,5	0.40	0	5,5,5	0.32	0
3	GOL	7-B	403	-	5,5,5	0.34	0	5,5,5	0.42	0
3	GOL	7-B	404	-	5,5,5	0.29	0	5,5,5	0.69	0
3	GOL	7-B	405	-	5,5,5	0.48	0	5,5,5	0.08	0
3	GOL	7-B	406	-	5,5,5	0.38	0	5,5,5	0.28	0
3	GOL	7-B	407	-	5,5,5	0.35	0	5,5,5	0.23	0
2	MES	7-C	401	-	12,12,12	1.90	1 (8%)	14,16,16	2.34	4 (28%)
3	GOL	7-C	402	-	5,5,5	0.30	0	5,5,5	0.54	0
3	FMT	7-C	403	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	7-D	401	-	12,12,12	2.58	1 (8%)	14,16,16	2.95	6 (42%)
3	GOL	7-D	402	-	5,5,5	0.33	0	5,5,5	0.69	0
3	GOL	7-D	403	-	5,5,5	0.44	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	7-D	404	-	5,5,5	0.26	0	5,5,5	0.83	0
2	MES	7-E	401	-	12,12,12	1.83	1 (8%)	14,16,16	3.20	6 (42%)
3	GOL	7-E	402	-	5,5,5	0.68	0	5,5,5	0.62	0
3	GOL	7-E	403	-	5,5,5	0.41	0	5,5,5	0.56	0
4	GOL	7-E	404	-	5,5,5	0.55	0	5,5,5	0.28	0
2	MES	7-F	401	-	12,12,12	1.86	1 (8%)	14,16,16	2.52	5 (35%)
3	GOL	7-F	402	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	7-F	403	-	5,5,5	0.45	0	5,5,5	0.63	0
3	GOL	7-F	404	-	5,5,5	0.43	0	5,5,5	0.36	0
3	GOL	7-F	405	-	5,5,5	0.33	0	5,5,5	0.29	0
3	GOL	7-F	406	-	5,5,5	0.37	0	5,5,5	0.18	0
5	FMT	7-F	407	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	7-G	401	-	12,12,12	2.02	1 (8%)	14,16,16	3.18	8 (57%)
3	GOL	7-G	402	-	5,5,5	0.42	0	5,5,5	0.35	0
3	GOL	7-G	403	-	5,5,5	0.28	0	5,5,5	0.50	0
3	GOL	7-G	404	-	5,5,5	0.40	0	5,5,5	0.30	0
5	FMT	7-G	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	7-H	401	-	12,12,12	2.28	1 (8%)	14,16,16	2.41	6 (42%)
3	GOL	7-H	402	-	5,5,5	0.44	0	5,5,5	0.26	0
3	GOL	7-H	403	-	5,5,5	0.38	0	5,5,5	0.41	0
3	GOL	7-H	404	-	5,5,5	0.32	0	5,5,5	0.25	0
2	MES	8-A	401	-	12,12,12	2.16	1 (8%)	14,16,16	2.38	6 (42%)
3	GOL	8-A	402	-	5,5,5	0.32	0	5,5,5	0.27	0
3	GOL	8-A	403	-	5,5,5	0.28	0	5,5,5	0.26	0
3	GOL	8-A	404	-	5,5,5	0.40	0	5,5,5	0.26	0
2	MES	8-B	401	-	12,12,12	2.17	1 (8%)	14,16,16	2.68	4 (28%)
3	GOL	8-B	402	-	5,5,5	0.38	0	5,5,5	0.36	0
3	GOL	8-B	403	-	5,5,5	0.29	0	5,5,5	0.46	0
3	GOL	8-B	404	-	5,5,5	0.32	0	5,5,5	0.60	0
3	GOL	8-B	405	-	5,5,5	0.39	0	5,5,5	0.57	0
3	GOL	8-B	406	-	5,5,5	0.39	0	5,5,5	0.33	0
3	GOL	8-B	407	-	5,5,5	0.69	0	5,5,5	0.64	0
4	GOL	8-B	408	-	5,5,5	0.42	0	5,5,5	0.38	0
2	MES	8-C	401	-	12,12,12	2.20	1 (8%)	14,16,16	3.04	7 (50%)
3	GOL	8-C	402	-	5,5,5	0.36	0	5,5,5	0.31	0
3	GOL	8-C	403	-	5,5,5	0.38	0	5,5,5	0.27	0
5	FMT	8-C	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	8-D	401	-	12,12,12	2.37	2 (16%)	14,16,16	2.75	8 (57%)
3	GOL	8-D	402	-	5,5,5	0.39	0	5,5,5	0.39	0
3	GOL	8-D	403	-	5,5,5	0.41	0	5,5,5	0.32	0
2	MES	8-E	401	-	12,12,12	2.43	1 (8%)	14,16,16	3.25	6 (42%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	8-E	402	-	5,5,5	0.92	0	5,5,5	1.22	1 (20%)
3	GOL	8-E	403	-	5,5,5	0.61	0	5,5,5	0.84	0
4	GOL	8-E	404	-	5,5,5	0.34	0	5,5,5	0.48	0
2	MES	8-F	401	-	12,12,12	2.07	1 (8%)	14,16,16	2.53	5 (35%)
3	GOL	8-F	402	-	5,5,5	0.32	0	5,5,5	0.84	0
3	GOL	8-F	403	-	5,5,5	0.47	0	5,5,5	0.28	0
3	GOL	8-F	404	-	5,5,5	0.41	0	5,5,5	0.23	0
3	GOL	8-F	405	-	5,5,5	0.33	0	5,5,5	0.41	0
3	FMT	8-F	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	8-G	401	-	12,12,12	2.30	1 (8%)	14,16,16	2.91	7 (50%)
3	GOL	8-G	402	-	5,5,5	0.48	0	5,5,5	0.24	0
3	GOL	8-G	403	-	5,5,5	0.38	0	5,5,5	0.21	0
3	GOL	8-G	404	-	5,5,5	0.32	0	5,5,5	0.36	0
5	GOL	8-G	405	-	5,5,5	0.36	0	5,5,5	0.56	0
4	FMT	8-G	406	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	8-H	401	-	12,12,12	1.57	1 (8%)	14,16,16	3.23	6 (42%)
3	GOL	8-H	402	-	5,5,5	0.41	0	5,5,5	0.37	0
3	GOL	8-H	403	-	5,5,5	0.36	0	5,5,5	0.36	0
3	GOL	8-H	404	-	5,5,5	0.26	0	5,5,5	0.73	0
2	MES	9-A	401	-	12,12,12	1.67	1 (8%)	14,16,16	3.66	10 (71%)
3	GOL	9-A	402	-	5,5,5	0.28	0	5,5,5	0.18	0
3	GOL	9-A	403	-	5,5,5	0.51	0	5,5,5	0.51	0
3	GOL	9-A	404	-	5,5,5	0.35	0	5,5,5	0.43	0
4	GOL	9-A	405	-	5,5,5	0.30	0	5,5,5	0.36	0
2	MES	9-B	401	-	12,12,12	2.03	1 (8%)	14,16,16	2.19	4 (28%)
3	GOL	9-B	402	-	5,5,5	0.36	0	5,5,5	0.24	0
3	GOL	9-B	403	-	5,5,5	0.41	0	5,5,5	0.39	0
3	GOL	9-B	404	-	5,5,5	0.35	0	5,5,5	0.51	0
3	GOL	9-B	405	-	5,5,5	0.33	0	5,5,5	0.50	0
3	GOL	9-B	406	-	5,5,5	0.33	0	5,5,5	0.25	0
2	MES	9-C	401	-	12,12,12	2.25	1 (8%)	14,16,16	3.39	4 (28%)
3	GOL	9-C	402	-	5,5,5	0.35	0	5,5,5	0.21	0
3	GOL	9-C	403	-	5,5,5	0.36	0	5,5,5	0.60	0
5	FMT	9-C	404	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	9-D	401	-	12,12,12	2.45	1 (8%)	14,16,16	2.24	6 (42%)
3	GOL	9-D	402	-	5,5,5	0.47	0	5,5,5	0.53	0
3	GOL	9-D	403	-	5,5,5	0.75	0	5,5,5	0.75	0
3	GOL	9-D	404	-	5,5,5	0.30	0	5,5,5	0.36	0
2	MES	9-E	401	-	12,12,12	1.87	1 (8%)	14,16,16	2.30	5 (35%)
3	GOL	9-E	402	-	5,5,5	0.31	0	5,5,5	0.43	0
3	GOL	9-E	403	-	5,5,5	0.79	0	5,5,5	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	9-E	404	-	5,5,5	0.41	0	5,5,5	0.35	0
2	MES	9-F	401	-	12,12,12	1.89	1 (8%)	14,16,16	2.72	5 (35%)
3	GOL	9-F	402	-	5,5,5	0.28	0	5,5,5	0.46	0
3	GOL	9-F	403	-	5,5,5	0.37	0	5,5,5	0.32	0
3	GOL	9-F	404	-	5,5,5	0.33	0	5,5,5	0.37	0
3	FMT	9-F	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	9-G	401	-	12,12,12	1.98	1 (8%)	14,16,16	3.13	7 (50%)
3	GOL	9-G	402	-	5,5,5	0.49	0	5,5,5	0.66	0
3	GOL	9-G	403	-	5,5,5	0.37	0	5,5,5	0.28	0
3	GOL	9-G	404	-	5,5,5	0.41	0	5,5,5	0.13	0
5	FMT	9-G	405	-	0,2,2	0.00	-	0,1,1	0.00	-
2	MES	9-H	401	-	12,12,12	2.12	1 (8%)	14,16,16	2.36	5 (35%)
3	GOL	9-H	402	-	5,5,5	0.37	0	5,5,5	0.34	0
3	GOL	9-H	403	-	5,5,5	0.38	0	5,5,5	0.36	0
3	GOL	9-H	404	-	5,5,5	0.41	0	5,5,5	0.42	0
3	GOL	9-H	405	-	5,5,5	0.37	0	5,5,5	0.35	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
2	MES	1-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	1-A	404	-	-	0/4/4/4	0/0/0/0
2	MES	1-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	1-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	1-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	1-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	1-B	407	-	-	0/4/4/4	0/0/0/0
4	GOL	1-B	408	-	-	0/4/4/4	0/0/0/0
2	MES	1-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-C	402	-	-	0/4/4/4	0/0/0/0
3	FMT	1-C	403	-	-	0/0/0/0	0/0/0/0
2	MES	1-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	1-D	404	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	1-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-E	403	-	-	0/4/4/4	0/0/0/0
2	MES	1-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	1-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	1-F	405	-	-	0/4/4/4	0/0/0/0
3	GOL	1-F	406	-	-	0/4/4/4	0/0/0/0
5	GOL	1-F	407	-	-	0/4/4/4	0/0/0/0
4	FMT	1-F	408	-	-	0/0/0/0	0/0/0/0
2	MES	1-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	1-G	404	-	-	0/4/4/4	0/0/0/0
5	GOL	1-G	405	-	-	0/4/4/4	0/0/0/0
4	FMT	1-G	406	-	-	0/0/0/0	0/0/0/0
2	MES	1-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	1-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	1-H	403	-	-	0/4/4/4	0/0/0/0
2	MES	10-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	10-A	404	-	-	0/4/4/4	0/0/0/0
2	MES	10-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	10-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	10-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	10-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	10-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	10-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-C	403	-	-	0/4/4/4	0/0/0/0
5	FMT	10-C	404	-	-	0/0/0/0	0/0/0/0
2	MES	10-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	10-D	404	-	-	0/4/4/4	0/0/0/0
2	MES	10-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-E	403	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	10-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	10-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	10-F	405	-	-	0/4/4/4	0/0/0/0
3	GOL	10-F	406	-	-	0/4/4/4	0/0/0/0
5	FMT	10-F	407	-	-	0/0/0/0	0/0/0/0
2	MES	10-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	10-G	404	-	-	0/4/4/4	0/0/0/0
5	FMT	10-G	405	-	-	0/0/0/0	0/0/0/0
2	MES	10-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	10-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	10-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	10-H	404	-	-	0/4/4/4	0/0/0/0
3	GOL	10-H	405	-	-	0/4/4/4	0/0/0/0
2	MES	2-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	2-A	404	-	-	0/4/4/4	0/0/0/0
2	MES	2-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	2-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	2-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	2-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	2-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	2-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-C	403	-	-	0/4/4/4	0/0/0/0
5	GOL	2-C	404	-	-	0/4/4/4	0/0/0/0
4	FMT	2-C	405	-	-	0/0/0/0	0/0/0/0
2	MES	2-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-D	403	-	-	0/4/4/4	0/0/0/0
2	MES	2-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	2-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	2-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-F	402	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	2-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	2-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	2-F	405	-	-	0/4/4/4	0/0/0/0
3	FMT	2-F	406	-	-	0/0/0/0	0/0/0/0
2	MES	2-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	2-G	404	-	-	0/4/4/4	0/0/0/0
5	FMT	2-G	405	-	-	0/0/0/0	0/0/0/0
2	MES	2-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	2-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	2-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	2-H	404	-	-	0/4/4/4	0/0/0/0
2	MES	3-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	3-A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	3-A	405	-	-	0/4/4/4	0/0/0/0
2	MES	3-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	3-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	3-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	3-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	3-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	3-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-C	403	-	-	0/4/4/4	0/0/0/0
5	FMT	3-C	404	-	-	0/0/0/0	0/0/0/0
2	MES	3-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-D	403	-	-	0/4/4/4	0/0/0/0
2	MES	3-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	3-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	3-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	3-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	3-F	405	-	-	0/4/4/4	0/0/0/0
3	GOL	3-F	406	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FMT	3-F	407	-	-	0/0/0/0	0/0/0/0
2	MES	3-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	3-G	404	-	-	0/4/4/4	0/0/0/0
5	GOL	3-G	405	-	-	0/4/4/4	0/0/0/0
4	FMT	3-G	406	-	-	0/0/0/0	0/0/0/0
2	MES	3-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	3-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	3-H	403	-	-	0/4/4/4	0/0/0/0
2	MES	4-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	4-A	404	-	-	0/4/4/4	0/0/0/0
2	MES	4-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	4-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	4-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	4-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	4-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	4-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-C	403	-	-	0/4/4/4	0/0/0/0
5	GOL	4-C	404	-	-	0/4/4/4	0/0/0/0
4	FMT	4-C	405	-	-	0/0/0/0	0/0/0/0
2	MES	4-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-D	403	-	-	0/4/4/4	0/0/0/0
2	MES	4-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	4-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	4-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	4-F	404	-	-	0/4/4/4	0/0/0/0
3	FMT	4-F	405	-	-	0/0/0/0	0/0/0/0
2	MES	4-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	4-G	404	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	4-G	405	-	-	0/4/4/4	0/0/0/0
4	GOL	4-G	406	-	-	0/4/4/4	0/0/0/0
4	FMT	4-G	407	-	-	0/0/0/0	0/0/0/0
2	MES	4-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	4-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	4-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	4-H	404	-	-	0/4/4/4	0/0/0/0
2	MES	5-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	5-A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	5-A	405	-	-	0/4/4/4	0/0/0/0
2	MES	5-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	5-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	5-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	5-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	5-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	5-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-C	402	-	-	0/4/4/4	0/0/0/0
3	FMT	5-C	403	-	-	0/0/0/0	0/0/0/0
2	MES	5-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	5-D	404	-	-	0/4/4/4	0/0/0/0
2	MES	5-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	5-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	5-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	5-F	404	-	-	0/4/4/4	0/0/0/0
3	FMT	5-F	405	-	-	0/0/0/0	0/0/0/0
2	MES	5-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	5-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	5-G	404	-	-	0/4/4/4	0/0/0/0
5	GOL	5-G	405	-	-	0/4/4/4	0/0/0/0
4	FMT	5-G	406	-	-	0/0/0/0	0/0/0/0
2	MES	5-H	401	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	5-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	5-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	5-H	404	-	-	0/4/4/4	0/0/0/0
2	MES	6-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	6-A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	6-A	405	-	-	0/4/4/4	0/0/0/0
2	MES	6-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	6-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	6-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	6-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	6-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	6-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-C	402	-	-	0/4/4/4	0/0/0/0
3	FMT	6-C	403	-	-	0/0/0/0	0/0/0/0
2	MES	6-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	6-D	404	-	-	0/4/4/4	0/0/0/0
2	MES	6-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	6-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	6-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	6-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	6-F	405	-	-	0/4/4/4	0/0/0/0
3	GOL	6-F	406	-	-	0/4/4/4	0/0/0/0
5	FMT	6-F	407	-	-	0/0/0/0	0/0/0/0
2	MES	6-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-G	403	-	-	0/4/4/4	0/0/0/0
3	FMT	6-G	404	-	-	0/0/0/0	0/0/0/0
2	MES	6-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	6-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	6-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	6-H	404	-	-	0/4/4/4	0/0/0/0
3	GOL	6-H	405	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	7-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	7-A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	7-A	405	-	-	0/4/4/4	0/0/0/0
2	MES	7-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	7-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	7-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	7-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	7-B	407	-	-	0/4/4/4	0/0/0/0
2	MES	7-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-C	402	-	-	0/4/4/4	0/0/0/0
3	FMT	7-C	403	-	-	0/0/0/0	0/0/0/0
2	MES	7-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	7-D	404	-	-	0/4/4/4	0/0/0/0
2	MES	7-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	7-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	7-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	7-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	7-F	405	-	-	0/4/4/4	0/0/0/0
3	GOL	7-F	406	-	-	0/4/4/4	0/0/0/0
5	FMT	7-F	407	-	-	0/0/0/0	0/0/0/0
2	MES	7-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	7-G	404	-	-	0/4/4/4	0/0/0/0
5	FMT	7-G	405	-	-	0/0/0/0	0/0/0/0
2	MES	7-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	7-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	7-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	7-H	404	-	-	0/4/4/4	0/0/0/0
2	MES	8-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-A	403	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	8-A	404	-	-	0/4/4/4	0/0/0/0
2	MES	8-B	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	8-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	8-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	8-B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	8-B	407	-	-	0/4/4/4	0/0/0/0
4	GOL	8-B	408	-	-	0/4/4/4	0/0/0/0
2	MES	8-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-C	403	-	-	0/4/4/4	0/0/0/0
5	FMT	8-C	404	-	-	0/0/0/0	0/0/0/0
2	MES	8-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-D	403	-	-	0/4/4/4	0/0/0/0
2	MES	8-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	8-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	8-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	8-F	404	-	-	0/4/4/4	0/0/0/0
3	GOL	8-F	405	-	-	0/4/4/4	0/0/0/0
3	FMT	8-F	406	-	-	0/0/0/0	0/0/0/0
2	MES	8-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	8-G	404	-	-	0/4/4/4	0/0/0/0
5	GOL	8-G	405	-	-	0/4/4/4	0/0/0/0
4	FMT	8-G	406	-	-	0/0/0/0	0/0/0/0
2	MES	8-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	8-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	8-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	8-H	404	-	-	0/4/4/4	0/0/0/0
2	MES	9-A	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	9-A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	9-A	405	-	-	0/4/4/4	0/0/0/0
2	MES	9-B	401	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	9-B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	9-B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	9-B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	9-B	406	-	-	0/4/4/4	0/0/0/0
2	MES	9-C	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-C	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-C	403	-	-	0/4/4/4	0/0/0/0
5	FMT	9-C	404	-	-	0/0/0/0	0/0/0/0
2	MES	9-D	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-D	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	9-D	404	-	-	0/4/4/4	0/0/0/0
2	MES	9-E	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-E	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-E	403	-	-	0/4/4/4	0/0/0/0
4	GOL	9-E	404	-	-	0/4/4/4	0/0/0/0
2	MES	9-F	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-F	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-F	403	-	-	0/4/4/4	0/0/0/0
3	GOL	9-F	404	-	-	0/4/4/4	0/0/0/0
3	FMT	9-F	405	-	-	0/0/0/0	0/0/0/0
2	MES	9-G	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-G	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-G	403	-	-	0/4/4/4	0/0/0/0
3	GOL	9-G	404	-	-	0/4/4/4	0/0/0/0
5	FMT	9-G	405	-	-	0/0/0/0	0/0/0/0
2	MES	9-H	401	-	-	0/6/14/14	0/1/1/1
3	GOL	9-H	402	-	-	0/4/4/4	0/0/0/0
3	GOL	9-H	403	-	-	0/4/4/4	0/0/0/0
3	GOL	9-H	404	-	-	0/4/4/4	0/0/0/0
3	GOL	9-H	405	-	-	0/4/4/4	0/0/0/0

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-C	401	MES	C8-S	-9.17	1.63	1.77
2	4-C	401	MES	C8-S	-8.62	1.64	1.77
2	7-D	401	MES	C8-S	-8.53	1.64	1.77
2	2-H	401	MES	C8-S	-8.52	1.64	1.77
2	3-H	401	MES	C8-S	-8.16	1.65	1.77
2	8-E	401	MES	C8-S	-8.06	1.65	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9-D	401	MES	C8-S	-8.04	1.65	1.77
2	5-G	401	MES	C8-S	-8.01	1.65	1.77
2	8-D	401	MES	C8-S	-7.75	1.65	1.77
2	8-G	401	MES	C8-S	-7.71	1.66	1.77
2	10-F	401	MES	C8-S	-7.70	1.66	1.77
2	6-H	401	MES	C8-S	-7.60	1.66	1.77
2	7-H	401	MES	C8-S	-7.55	1.66	1.77
2	9-C	401	MES	C8-S	-7.49	1.66	1.77
2	8-C	401	MES	C8-S	-7.21	1.66	1.77
2	6-B	401	MES	C8-S	-7.20	1.66	1.77
2	1-C	401	MES	C8-S	-7.20	1.66	1.77
2	8-B	401	MES	C8-S	-7.14	1.66	1.77
2	3-B	401	MES	C8-S	-7.05	1.66	1.77
2	8-A	401	MES	C8-S	-7.00	1.67	1.77
2	1-A	401	MES	C8-S	-6.98	1.67	1.77
2	10-A	401	MES	C8-S	-6.96	1.67	1.77
2	2-G	401	MES	C8-S	-6.96	1.67	1.77
2	9-H	401	MES	C8-S	-6.96	1.67	1.77
2	10-H	401	MES	C8-S	-6.95	1.67	1.77
2	1-D	401	MES	C8-S	-6.92	1.67	1.77
2	4-A	401	MES	C8-S	-6.92	1.67	1.77
2	5-D	401	MES	C8-S	-6.91	1.67	1.77
2	4-G	401	MES	C8-S	-6.73	1.67	1.77
2	8-F	401	MES	C8-S	-6.69	1.67	1.77
2	1-G	401	MES	C8-S	-6.63	1.67	1.77
2	7-G	401	MES	C8-S	-6.62	1.67	1.77
2	4-D	401	MES	C8-S	-6.61	1.67	1.77
2	9-B	401	MES	C8-S	-6.60	1.67	1.77
2	5-E	401	MES	C8-S	-6.57	1.67	1.77
2	4-H	401	MES	C8-S	-6.52	1.67	1.77
2	9-G	401	MES	C8-S	-6.48	1.67	1.77
2	1-E	401	MES	C8-S	-6.47	1.67	1.77
2	5-B	401	MES	C8-S	-6.43	1.67	1.77
2	5-H	401	MES	C8-S	-6.42	1.67	1.77
2	2-A	401	MES	C8-S	-6.39	1.67	1.77
2	3-C	401	MES	C8-S	-6.39	1.67	1.77
2	5-C	401	MES	C8-S	-6.39	1.67	1.77
2	2-B	401	MES	C8-S	-6.39	1.67	1.77
2	5-F	401	MES	C8-S	-6.36	1.68	1.77
2	7-B	401	MES	C8-S	-6.35	1.68	1.77
2	2-D	401	MES	C8-S	-6.24	1.68	1.77
2	10-D	401	MES	C8-S	-6.17	1.68	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7-C	401	MES	C8-S	-6.13	1.68	1.77
2	10-E	401	MES	C8-S	-6.13	1.68	1.77
2	6-D	401	MES	C8-S	-6.13	1.68	1.77
2	9-E	401	MES	C8-S	-6.04	1.68	1.77
2	7-F	401	MES	C8-S	-6.02	1.68	1.77
2	3-E	401	MES	C8-S	-6.02	1.68	1.77
2	4-B	401	MES	C8-S	-5.99	1.68	1.77
2	10-G	401	MES	C8-S	-5.99	1.68	1.77
2	7-E	401	MES	C8-S	-5.98	1.68	1.77
2	10-B	401	MES	C8-S	-5.98	1.68	1.77
2	9-F	401	MES	C8-S	-5.96	1.68	1.77
2	7-A	401	MES	C8-S	-5.95	1.68	1.77
2	3-F	401	MES	C8-S	-5.92	1.68	1.77
2	1-B	401	MES	C8-S	-5.91	1.68	1.77
2	6-E	401	MES	C8-S	-5.90	1.68	1.77
2	6-G	401	MES	C8-S	-5.86	1.68	1.77
2	4-F	401	MES	C8-S	-5.86	1.68	1.77
2	5-A	401	MES	C8-S	-5.82	1.68	1.77
2	2-E	401	MES	C8-S	-5.71	1.68	1.77
2	2-F	401	MES	C8-S	-5.68	1.69	1.77
2	3-D	401	MES	C8-S	-5.64	1.69	1.77
2	1-H	401	MES	C8-S	-5.63	1.69	1.77
2	6-F	401	MES	C8-S	-5.59	1.69	1.77
2	2-C	401	MES	C8-S	-5.49	1.69	1.77
2	1-F	401	MES	C8-S	-5.42	1.69	1.77
2	9-A	401	MES	C8-S	-5.39	1.69	1.77
2	8-H	401	MES	C8-S	-4.83	1.70	1.77
2	3-G	401	MES	C8-S	-4.83	1.70	1.77
2	10-C	401	MES	C8-S	-4.82	1.70	1.77
2	3-A	401	MES	C8-S	-4.81	1.70	1.77
2	6-A	401	MES	C8-S	-4.37	1.70	1.77
2	4-E	401	MES	C8-S	-3.92	1.71	1.77
3	1-F	406	GOL	O2-C2	-3.05	1.34	1.43
3	2-H	403	GOL	C3-C2	-2.19	1.44	1.52
2	5-B	401	MES	O1S-S	2.10	1.51	1.45
2	8-D	401	MES	O2S-S	2.18	1.51	1.45

All (505) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-B	401	MES	O2S-S-C8	-9.07	99.00	106.79
2	5-G	401	MES	O1S-S-C8	-8.18	99.77	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-H	401	MES	O2S-S-C8	-7.21	100.60	106.79
2	6-C	401	MES	C2-C3-N4	-6.42	101.11	110.11
2	6-E	401	MES	O2S-S-C8	-6.30	101.38	106.79
2	10-C	401	MES	O2S-S-C8	-5.91	101.71	106.79
2	7-H	401	MES	C2-C3-N4	-5.78	102.00	110.11
2	8-C	401	MES	C6-C5-N4	-5.65	102.20	110.11
2	10-C	401	MES	C6-C5-N4	-5.58	102.28	110.11
2	3-E	401	MES	C6-C5-N4	-5.39	102.55	110.11
2	8-G	401	MES	C6-C5-N4	-5.19	102.84	110.11
2	5-H	401	MES	O2S-S-C8	-5.13	102.38	106.79
2	7-D	401	MES	C6-C5-N4	-5.01	103.09	110.11
2	10-F	401	MES	C6-C5-N4	-4.97	103.14	110.11
2	5-G	401	MES	C2-C3-N4	-4.83	103.34	110.11
2	3-E	401	MES	O2S-S-C8	-4.75	102.72	106.79
2	10-G	401	MES	C6-C5-N4	-4.53	103.76	110.11
2	7-D	401	MES	O1-C6-C5	-4.19	102.46	111.83
2	8-C	401	MES	C2-C3-N4	-4.01	104.48	110.11
2	9-A	401	MES	O3S-S-O1S	-3.98	102.24	111.37
2	1-H	401	MES	C6-C5-N4	-3.88	104.67	110.11
2	3-C	401	MES	O3S-S-O2S	-3.80	102.66	111.37
2	6-C	401	MES	C6-C5-N4	-3.78	104.81	110.11
2	3-D	401	MES	O2S-S-O1S	-3.70	101.04	113.86
2	7-D	401	MES	C2-C3-N4	-3.69	104.93	110.11
2	10-H	401	MES	C6-C5-N4	-3.69	104.94	110.11
2	1-C	401	MES	C6-C5-N4	-3.63	105.02	110.11
2	1-A	401	MES	C6-C5-N4	-3.62	105.04	110.11
2	2-D	401	MES	O3S-S-O1S	-3.61	103.08	111.37
2	4-A	401	MES	C6-C5-N4	-3.59	105.08	110.11
2	5-C	401	MES	C6-C5-N4	-3.57	105.11	110.11
2	1-G	401	MES	C6-C5-N4	-3.55	105.13	110.11
2	4-C	401	MES	O2S-S-O1S	-3.52	101.66	113.86
2	6-H	401	MES	C6-C5-N4	-3.49	105.21	110.11
2	8-A	401	MES	C2-C3-N4	-3.48	105.23	110.11
2	1-D	401	MES	C2-C3-N4	-3.45	105.28	110.11
2	6-G	401	MES	C6-C5-N4	-3.36	105.40	110.11
2	4-B	401	MES	C6-C5-N4	-3.30	105.48	110.11
2	10-E	401	MES	C6-C5-N4	-3.23	105.58	110.11
2	7-E	401	MES	C6-C5-N4	-3.22	105.60	110.11
2	1-H	401	MES	O3S-S-O2S	-3.22	104.00	111.37
2	3-E	401	MES	O2S-S-O1S	-3.21	102.74	113.86
2	2-D	401	MES	C6-C5-N4	-3.16	105.69	110.11
2	3-E	401	MES	O3S-S-O1S	-3.14	104.16	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-E	401	MES	O1-C6-C5	-3.11	104.86	111.83
2	2-H	401	MES	C6-C5-N4	-3.08	105.79	110.11
2	4-C	401	MES	C6-C5-N4	-3.06	105.82	110.11
2	5-F	401	MES	O2S-S-O1S	-3.02	103.38	113.86
2	2-C	401	MES	O2S-S-O1S	-3.02	103.39	113.86
2	9-D	401	MES	C6-C5-N4	-3.01	105.89	110.11
2	9-H	401	MES	O2S-S-C8	-3.01	104.21	106.79
2	5-G	401	MES	C6-C5-N4	-3.01	105.89	110.11
2	1-D	401	MES	O3S-S-O2S	-2.94	104.64	111.37
2	3-H	401	MES	O3S-S-O1S	-2.92	104.69	111.37
2	8-H	401	MES	O3S-S-O1S	-2.91	104.69	111.37
2	1-G	401	MES	O3S-S-O2S	-2.88	104.76	111.37
2	3-G	401	MES	O3S-S-O2S	-2.85	104.84	111.37
2	7-G	401	MES	O2S-S-C8	-2.84	104.35	106.79
2	5-B	401	MES	C6-C5-N4	-2.83	106.14	110.11
2	5-G	401	MES	O1-C6-C5	-2.82	105.52	111.83
2	7-B	401	MES	O2S-S-O1S	-2.82	104.10	113.86
2	2-C	401	MES	C6-C5-N4	-2.82	106.16	110.11
2	1-F	401	MES	O2S-S-O1S	-2.81	104.13	113.86
2	10-F	401	MES	O2S-S-O1S	-2.80	104.14	113.86
2	3-D	401	MES	C6-C5-N4	-2.80	106.19	110.11
2	6-H	401	MES	O1S-S-C8	-2.77	104.41	106.79
2	8-G	401	MES	C2-C3-N4	-2.77	106.22	110.11
2	5-A	401	MES	C2-C3-N4	-2.76	106.23	110.11
2	1-F	401	MES	C6-C5-N4	-2.73	106.28	110.11
2	7-G	401	MES	C6-C5-N4	-2.70	106.33	110.11
2	2-F	401	MES	C6-C5-N4	-2.69	106.34	110.11
2	10-F	401	MES	C2-C3-N4	-2.69	106.34	110.11
2	5-G	401	MES	O3S-S-O1S	-2.68	105.23	111.37
2	7-C	401	MES	C6-C5-N4	-2.66	106.38	110.11
2	7-F	401	MES	C6-C5-N4	-2.61	106.45	110.11
2	8-C	401	MES	O2S-S-O1S	-2.58	104.91	113.86
2	7-G	401	MES	O2S-S-O1S	-2.54	105.07	113.86
2	8-D	401	MES	C6-C5-N4	-2.53	106.57	110.11
2	8-D	401	MES	C2-C3-N4	-2.52	106.58	110.11
2	5-E	401	MES	C2-C3-N4	-2.52	106.58	110.11
2	5-E	401	MES	O2S-S-O1S	-2.51	105.17	113.86
2	4-F	401	MES	C6-C5-N4	-2.51	106.59	110.11
2	5-D	401	MES	O1S-S-C8	-2.46	104.68	106.79
2	9-F	401	MES	C6-C5-N4	-2.46	106.66	110.11
2	6-E	401	MES	C2-C3-N4	-2.45	106.67	110.11
2	4-H	401	MES	C6-C5-N4	-2.44	106.69	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-H	401	MES	C2-C3-N4	-2.42	106.71	110.11
2	6-D	401	MES	O2S-S-O1S	-2.41	105.49	113.86
2	6-D	401	MES	C2-C3-N4	-2.40	106.74	110.11
2	9-A	401	MES	O1-C2-C3	-2.40	106.46	111.83
2	2-H	401	MES	C2-C3-N4	-2.40	106.75	110.11
2	3-C	401	MES	C6-C5-N4	-2.37	106.78	110.11
2	1-C	401	MES	O2S-S-O1S	-2.33	105.78	113.86
3	1-D	403	GOL	C3-C2-C1	-2.32	102.31	111.52
2	10-A	401	MES	C6-C5-N4	-2.32	106.86	110.11
2	1-B	401	MES	O3S-S-O1S	-2.30	106.09	111.37
2	1-D	401	MES	C6-C5-N4	-2.30	106.89	110.11
2	9-A	401	MES	C2-C3-N4	-2.28	106.91	110.11
2	2-E	401	MES	O2S-S-O1S	-2.26	106.01	113.86
2	8-E	401	MES	O1S-S-C8	-2.25	104.86	106.79
2	3-B	401	MES	O2S-S-O1S	-2.24	106.10	113.86
2	5-B	401	MES	O3S-S-O1S	-2.22	106.28	111.37
3	2-B	403	GOL	O3-C3-C2	-2.19	99.04	110.07
2	9-C	401	MES	O1-C2-C3	-2.19	106.94	111.83
2	9-G	401	MES	O3S-S-O2S	-2.18	106.36	111.37
2	6-C	401	MES	O2S-S-O1S	-2.15	106.40	113.86
2	8-D	401	MES	O1-C6-C5	-2.14	107.05	111.83
2	6-F	401	MES	C2-C3-N4	-2.14	107.11	110.11
2	9-B	401	MES	O3S-S-O2S	-2.13	106.49	111.37
2	7-H	401	MES	C6-C5-N4	-2.12	107.13	110.11
2	2-F	401	MES	O3S-S-C8	-2.12	103.45	106.06
2	4-D	401	MES	O2S-S-O1S	-2.12	106.53	113.86
2	5-A	401	MES	C6-C5-N4	-2.11	107.15	110.11
3	8-E	402	GOL	O2-C2-C3	-2.10	98.91	108.84
2	5-B	401	MES	C2-C3-N4	-2.10	107.16	110.11
2	4-B	401	MES	O3S-S-O2S	-2.07	106.62	111.37
2	4-E	401	MES	O3S-S-O1S	-2.07	106.62	111.37
2	10-E	401	MES	O3S-S-O1S	-2.06	106.65	111.37
2	10-C	401	MES	O2S-S-O1S	-2.05	106.77	113.86
2	10-F	401	MES	O1-C6-C5	-2.04	107.26	111.83
2	9-D	401	MES	O1-C6-C5	-2.03	107.28	111.83
2	5-H	401	MES	O3S-S-O2S	-2.02	106.73	111.37
2	5-G	401	MES	O3S-S-O2S	-2.02	106.74	111.37
2	6-E	401	MES	O2S-S-O1S	-2.01	106.91	113.86
2	7-G	401	MES	C2-C3-N4	-2.00	107.30	110.11
2	1-A	401	MES	C2-C3-N4	-2.00	107.30	110.11
2	6-F	401	MES	O1-C6-C5	2.00	116.31	111.83
2	5-C	401	MES	C7-N4-C3	2.00	116.40	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6-B	401	MES	C7-N4-C5	2.02	116.45	111.26
2	6-B	401	MES	C6-O1-C2	2.03	116.76	109.89
2	3-E	401	MES	O1-C2-C3	2.03	116.38	111.83
2	8-F	401	MES	C7-N4-C5	2.03	116.47	111.26
2	2-B	401	MES	C7-N4-C5	2.04	116.48	111.26
2	8-D	401	MES	C7-N4-C5	2.04	116.49	111.26
2	10-G	401	MES	C6-O1-C2	2.06	116.85	109.89
2	4-D	401	MES	C7-N4-C5	2.06	116.53	111.26
2	1-H	401	MES	C7-N4-C3	2.06	116.54	111.26
2	9-E	401	MES	C2-C3-N4	2.07	113.01	110.11
2	3-E	401	MES	O3S-S-O2S	2.10	116.18	111.37
2	3-B	401	MES	O1-C6-C5	2.10	116.53	111.83
2	5-F	401	MES	O3S-S-C8	2.10	108.64	106.06
2	7-H	401	MES	O1-C6-C5	2.11	116.54	111.83
2	6-C	401	MES	C7-N4-C3	2.11	116.67	111.26
2	2-C	401	MES	O2S-S-C8	2.13	108.62	106.79
2	10-B	401	MES	C7-N4-C5	2.14	116.74	111.26
2	8-G	401	MES	C7-N4-C3	2.14	116.75	111.26
2	3-A	401	MES	O1S-S-C8	2.15	108.64	106.79
2	1-F	401	MES	O3S-S-C8	2.16	108.71	106.06
2	9-A	401	MES	C7-N4-C5	2.16	116.79	111.26
2	1-G	401	MES	C7-N4-C5	2.17	116.81	111.26
2	7-A	401	MES	O1S-S-C8	2.17	108.65	106.79
3	1-F	406	GOL	O2-C2-C3	2.17	119.08	108.84
2	1-C	401	MES	O2S-S-C8	2.18	108.67	106.79
2	6-A	401	MES	O1-C2-C3	2.20	116.75	111.83
2	9-A	401	MES	O1-C6-C5	2.21	116.77	111.83
2	3-C	401	MES	C7-N4-C5	2.21	116.93	111.26
2	7-H	401	MES	C7-N4-C5	2.22	116.94	111.26
2	4-H	401	MES	O1S-S-C8	2.22	108.70	106.79
2	10-B	401	MES	O1-C2-C3	2.22	116.80	111.83
2	9-D	401	MES	C7-N4-C3	2.23	116.97	111.26
2	4-D	401	MES	O2S-S-C8	2.23	108.71	106.79
2	6-E	401	MES	C7-N4-C3	2.24	116.99	111.26
2	1-G	401	MES	C7-N4-C3	2.25	117.04	111.26
2	7-A	401	MES	C2-C3-N4	2.26	113.27	110.11
2	3-A	401	MES	O2S-S-C8	2.28	108.75	106.79
2	8-B	401	MES	C7-N4-C3	2.29	117.13	111.26
2	2-D	401	MES	C7-N4-C3	2.29	117.14	111.26
2	10-E	401	MES	O1-C2-C3	2.30	116.97	111.83
2	10-B	401	MES	C6-O1-C2	2.32	117.73	109.89
2	9-F	401	MES	C7-N4-C5	2.33	117.22	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-B	401	MES	O1S-S-C8	2.34	108.81	106.79
2	2-D	401	MES	O3S-S-C8	2.35	108.94	106.06
2	10-B	401	MES	C2-C3-N4	2.36	113.41	110.11
2	1-H	401	MES	C7-N4-C5	2.37	117.32	111.26
2	7-B	401	MES	O2S-S-C8	2.38	108.84	106.79
2	4-G	401	MES	C7-N4-C3	2.38	117.37	111.26
2	8-A	401	MES	O3S-S-C8	2.39	108.99	106.06
2	1-A	401	MES	C7-N4-C5	2.39	117.39	111.26
2	6-F	401	MES	O2S-S-C8	2.39	108.85	106.79
2	1-E	401	MES	C7-N4-C5	2.40	117.41	111.26
2	1-F	401	MES	C7-N4-C3	2.42	117.46	111.26
2	9-E	401	MES	C7-N4-C3	2.42	117.46	111.26
2	4-G	401	MES	O2S-S-C8	2.42	108.87	106.79
2	5-G	401	MES	C7-N4-C3	2.43	117.48	111.26
2	1-A	401	MES	C7-N4-C3	2.43	117.49	111.26
2	5-G	401	MES	C7-N4-C5	2.43	117.50	111.26
2	2-B	401	MES	C7-N4-C3	2.45	117.53	111.26
2	5-A	401	MES	C7-N4-C5	2.45	117.55	111.26
2	10-D	401	MES	C7-N4-C3	2.46	117.55	111.26
2	8-H	401	MES	C7-N4-C3	2.46	117.56	111.26
2	10-D	401	MES	C7-N4-C5	2.46	117.56	111.26
2	6-A	401	MES	C2-C3-N4	2.46	113.56	110.11
2	8-E	401	MES	C2-C3-N4	2.46	113.56	110.11
2	6-C	401	MES	O3S-S-C8	2.49	109.12	106.06
2	5-D	401	MES	C6-C5-N4	2.50	113.61	110.11
2	7-D	401	MES	O2S-S-C8	2.52	108.95	106.79
2	5-A	401	MES	C7-N4-C3	2.53	117.73	111.26
2	5-G	401	MES	O2S-S-C8	2.53	108.97	106.79
2	9-E	401	MES	O3S-S-C8	2.54	109.18	106.06
2	9-H	401	MES	C7-N4-C3	2.55	117.79	111.26
2	1-H	401	MES	O2S-S-C8	2.55	108.98	106.79
2	3-D	401	MES	C7-N4-C3	2.57	117.84	111.26
2	4-E	401	MES	C5-N4-C3	2.57	114.69	108.87
2	6-H	401	MES	C5-N4-C3	2.57	114.69	108.87
2	1-B	401	MES	O2S-S-C8	2.57	109.00	106.79
2	3-G	401	MES	O2S-S-C8	2.60	109.02	106.79
2	8-E	401	MES	C7-N4-C3	2.62	117.97	111.26
2	6-B	401	MES	C7-N4-C3	2.62	117.97	111.26
2	3-F	401	MES	O1-C2-C3	2.63	117.71	111.83
2	10-H	401	MES	C7-N4-C3	2.64	118.03	111.26
2	7-E	401	MES	C7-N4-C5	2.65	118.05	111.26
2	10-G	401	MES	O1-C2-C3	2.67	117.81	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-A	401	MES	C7-N4-C3	2.68	118.12	111.26
2	4-F	401	MES	C7-N4-C5	2.68	118.12	111.26
2	9-C	401	MES	C7-N4-C5	2.68	118.14	111.26
2	10-G	401	MES	C2-C3-N4	2.71	113.90	110.11
2	6-G	401	MES	C7-N4-C3	2.71	118.21	111.26
2	3-G	401	MES	O1S-S-C8	2.72	109.13	106.79
2	1-G	401	MES	O1S-S-C8	2.74	109.14	106.79
2	6-G	401	MES	O3S-S-C8	2.74	109.43	106.06
2	10-D	401	MES	O3S-S-C8	2.74	109.43	106.06
2	9-G	401	MES	C7-N4-C5	2.74	118.29	111.26
2	4-E	401	MES	C7-N4-C5	2.75	118.31	111.26
2	5-B	401	MES	C7-N4-C3	2.75	118.32	111.26
2	3-E	401	MES	C7-N4-C5	2.76	118.34	111.26
2	9-A	401	MES	O3S-S-C8	2.77	109.46	106.06
2	4-F	401	MES	O3S-S-C8	2.77	109.46	106.06
2	3-E	401	MES	C2-C3-N4	2.77	113.99	110.11
2	4-H	401	MES	C7-N4-C3	2.78	118.38	111.26
2	8-A	401	MES	C7-N4-C5	2.78	118.38	111.26
2	5-E	401	MES	C7-N4-C5	2.81	118.47	111.26
2	2-F	401	MES	C7-N4-C3	2.82	118.49	111.26
2	2-G	401	MES	C7-N4-C3	2.82	118.49	111.26
2	7-G	401	MES	C7-N4-C5	2.82	118.50	111.26
2	6-F	401	MES	C7-N4-C5	2.83	118.50	111.26
2	7-C	401	MES	C7-N4-C5	2.84	118.55	111.26
2	9-E	401	MES	C7-N4-C5	2.86	118.58	111.26
2	8-C	401	MES	C7-N4-C3	2.86	118.58	111.26
2	8-H	401	MES	C7-N4-C5	2.87	118.60	111.26
2	10-C	401	MES	C7-N4-C5	2.89	118.67	111.26
2	2-E	401	MES	C7-N4-C3	2.89	118.67	111.26
2	4-A	401	MES	C7-N4-C5	2.90	118.68	111.26
2	6-H	401	MES	C7-N4-C5	2.90	118.69	111.26
2	3-G	401	MES	C7-N4-C3	2.92	118.73	111.26
2	2-D	401	MES	C7-N4-C5	2.93	118.76	111.26
2	1-D	401	MES	C7-N4-C3	2.93	118.76	111.26
2	2-D	401	MES	O2S-S-C8	2.93	109.31	106.79
2	8-A	401	MES	O2S-S-C8	2.94	109.32	106.79
2	7-B	401	MES	C7-N4-C5	2.95	118.83	111.26
2	10-C	401	MES	O3S-S-C8	2.96	109.70	106.06
2	5-D	401	MES	C7-N4-C3	2.96	118.85	111.26
2	6-B	401	MES	O1S-S-C8	2.98	109.35	106.79
2	4-B	401	MES	C7-N4-C3	2.98	118.90	111.26
2	5-H	401	MES	C5-N4-C3	2.99	115.64	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-A	401	MES	O2S-S-C8	3.00	109.37	106.79
2	1-D	401	MES	O1S-S-C8	3.00	109.37	106.79
2	9-G	401	MES	O3S-S-C8	3.00	109.75	106.06
2	7-H	401	MES	O2S-S-C8	3.01	109.37	106.79
2	3-C	401	MES	C7-N4-C3	3.01	118.97	111.26
2	10-F	401	MES	C7-N4-C5	3.03	119.02	111.26
2	4-A	401	MES	C7-N4-C3	3.03	119.03	111.26
2	6-A	401	MES	O1S-S-C8	3.04	109.40	106.79
2	3-H	401	MES	C7-N4-C5	3.06	119.11	111.26
2	7-B	401	MES	C7-N4-C3	3.08	119.16	111.26
2	3-A	401	MES	C7-N4-C5	3.09	119.17	111.26
2	9-H	401	MES	C5-N4-C3	3.09	115.88	108.87
2	5-H	401	MES	C7-N4-C3	3.10	119.21	111.26
2	5-C	401	MES	O1S-S-C8	3.11	109.46	106.79
2	1-H	401	MES	C5-N4-C3	3.11	115.92	108.87
2	8-B	401	MES	C5-N4-C3	3.11	115.92	108.87
2	6-B	401	MES	O3S-S-C8	3.12	109.89	106.06
2	7-E	401	MES	C7-N4-C3	3.14	119.31	111.26
2	2-H	401	MES	C7-N4-C3	3.14	119.31	111.26
2	7-C	401	MES	C5-N4-C3	3.17	116.05	108.87
2	8-G	401	MES	C7-N4-C5	3.17	119.39	111.26
2	1-C	401	MES	C7-N4-C5	3.18	119.41	111.26
2	8-F	401	MES	C7-N4-C3	3.19	119.42	111.26
2	8-E	401	MES	O3S-S-C8	3.19	109.98	106.06
2	4-F	401	MES	C7-N4-C3	3.19	119.44	111.26
2	2-C	401	MES	C7-N4-C5	3.20	119.45	111.26
2	8-H	401	MES	O3S-S-C8	3.20	109.99	106.06
2	3-A	401	MES	C7-N4-C3	3.22	119.50	111.26
2	9-H	401	MES	O3S-S-C8	3.22	110.02	106.06
2	2-C	401	MES	O1S-S-C8	3.23	109.56	106.79
2	10-F	401	MES	O2S-S-C8	3.23	109.57	106.79
2	4-H	401	MES	C7-N4-C5	3.23	119.54	111.26
2	6-A	401	MES	C7-N4-C3	3.24	119.57	111.26
2	10-G	401	MES	C7-N4-C5	3.27	119.63	111.26
2	5-G	401	MES	C5-N4-C3	3.28	116.30	108.87
2	6-A	401	MES	C7-N4-C5	3.29	119.69	111.26
2	9-D	401	MES	O1S-S-C8	3.29	109.62	106.79
2	10-B	401	MES	O3S-S-C8	3.30	110.11	106.06
2	8-F	401	MES	O3S-S-C8	3.32	110.14	106.06
2	3-E	401	MES	C7-N4-C3	3.33	119.78	111.26
2	1-H	401	MES	O1S-S-C8	3.33	109.66	106.79
2	3-C	401	MES	C5-N4-C3	3.34	116.43	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-E	401	MES	O3S-S-C8	3.34	110.17	106.06
2	6-D	401	MES	C7-N4-C3	3.35	119.83	111.26
2	7-H	401	MES	C5-N4-C3	3.35	116.46	108.87
2	9-F	401	MES	O2S-S-C8	3.35	109.67	106.79
2	6-D	401	MES	C7-N4-C5	3.36	119.88	111.26
2	7-F	401	MES	C2-C3-N4	3.37	114.82	110.11
2	9-G	401	MES	C7-N4-C3	3.38	119.91	111.26
2	9-A	401	MES	C6-C5-N4	3.38	114.85	110.11
2	4-B	401	MES	O1S-S-C8	3.39	109.70	106.79
2	8-D	401	MES	C7-N4-C3	3.40	119.98	111.26
2	1-B	401	MES	C7-N4-C3	3.41	120.01	111.26
2	6-G	401	MES	C7-N4-C5	3.42	120.02	111.26
2	7-F	401	MES	O1S-S-C8	3.43	109.74	106.79
2	6-E	401	MES	C5-N4-C3	3.44	116.66	108.87
2	2-F	401	MES	C7-N4-C5	3.44	120.08	111.26
2	1-D	401	MES	C7-N4-C5	3.45	120.10	111.26
2	10-A	401	MES	O2S-S-C8	3.46	109.77	106.79
2	1-F	401	MES	C7-N4-C5	3.48	120.18	111.26
2	4-A	401	MES	O1S-S-C8	3.48	109.78	106.79
2	8-D	401	MES	O2S-S-C8	3.48	109.78	106.79
2	3-C	401	MES	O1S-S-C8	3.49	109.79	106.79
2	9-B	401	MES	O2S-S-C8	3.50	109.80	106.79
2	5-A	401	MES	O2S-S-C8	3.52	109.82	106.79
2	2-E	401	MES	C7-N4-C5	3.53	120.31	111.26
2	6-D	401	MES	C5-N4-C3	3.53	116.88	108.87
2	2-B	401	MES	O2S-S-C8	3.54	109.83	106.79
2	5-A	401	MES	O3S-S-C8	3.57	110.45	106.06
2	7-G	401	MES	O1S-S-C8	3.59	109.88	106.79
2	9-D	401	MES	O2S-S-C8	3.62	109.90	106.79
2	10-D	401	MES	C5-N4-C3	3.63	117.09	108.87
2	3-H	401	MES	C7-N4-C3	3.66	120.65	111.26
2	6-B	401	MES	C5-N4-C3	3.66	117.17	108.87
2	9-G	401	MES	O2S-S-C8	3.67	109.94	106.79
2	6-C	401	MES	C7-N4-C5	3.68	120.69	111.26
2	5-B	401	MES	O2S-S-C8	3.70	109.97	106.79
2	10-C	401	MES	C5-N4-C3	3.72	117.29	108.87
2	3-F	401	MES	C7-N4-C3	3.76	120.89	111.26
2	8-H	401	MES	C5-N4-C3	3.76	117.39	108.87
2	3-E	401	MES	C5-N4-C3	3.76	117.39	108.87
2	4-A	401	MES	O2S-S-C8	3.80	110.05	106.79
2	5-E	401	MES	C5-N4-C3	3.80	117.47	108.87
2	6-B	401	MES	O2S-S-C8	3.82	110.07	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-B	401	MES	C7-N4-C5	3.82	121.04	111.26
2	4-H	401	MES	O2S-S-C8	3.82	110.07	106.79
2	3-D	401	MES	C7-N4-C5	3.82	121.05	111.26
2	6-E	401	MES	C7-N4-C5	3.82	121.06	111.26
2	2-A	401	MES	O2S-S-C8	3.83	110.08	106.79
2	10-E	401	MES	C2-C3-N4	3.84	115.49	110.11
2	5-C	401	MES	C7-N4-C5	3.85	121.12	111.26
2	5-E	401	MES	O1S-S-C8	3.85	110.10	106.79
2	2-G	401	MES	C5-N4-C3	3.85	117.60	108.87
2	2-H	401	MES	C5-N4-C3	3.88	117.65	108.87
2	7-D	401	MES	C7-N4-C3	3.90	121.26	111.26
2	4-F	401	MES	O2S-S-C8	3.92	110.16	106.79
2	5-B	401	MES	C7-N4-C5	3.93	121.32	111.26
2	2-H	401	MES	O3S-S-C8	3.96	110.93	106.06
2	4-B	401	MES	O3S-S-C8	3.96	110.93	106.06
2	4-D	401	MES	C7-N4-C3	3.97	121.42	111.26
2	10-H	401	MES	O3S-S-C8	3.97	110.94	106.06
2	5-C	401	MES	O2S-S-C8	3.98	110.21	106.79
2	4-E	401	MES	O1S-S-C8	3.99	110.22	106.79
2	3-D	401	MES	O1S-S-C8	4.01	110.23	106.79
2	9-B	401	MES	C5-N4-C3	4.02	117.98	108.87
2	2-F	401	MES	C5-N4-C3	4.05	118.05	108.87
2	4-G	401	MES	C5-N4-C3	4.09	118.12	108.87
2	8-C	401	MES	C5-N4-C3	4.09	118.13	108.87
2	3-D	401	MES	O3S-S-C8	4.10	111.09	106.06
2	9-F	401	MES	C5-N4-C3	4.10	118.15	108.87
2	3-H	401	MES	C5-N4-C3	4.17	118.32	108.87
2	8-C	401	MES	O2S-S-C8	4.18	110.38	106.79
2	4-B	401	MES	C5-N4-C3	4.18	118.33	108.87
2	2-A	401	MES	C5-N4-C3	4.18	118.34	108.87
2	4-C	401	MES	C5-N4-C3	4.18	118.35	108.87
2	1-E	401	MES	C7-N4-C3	4.20	122.02	111.26
2	5-C	401	MES	C5-N4-C3	4.21	118.42	108.87
2	10-A	401	MES	C5-N4-C3	4.24	118.47	108.87
2	7-E	401	MES	O3S-S-C8	4.24	111.27	106.06
2	10-F	401	MES	O1S-S-C8	4.27	110.46	106.79
2	1-B	401	MES	C5-N4-C3	4.29	118.58	108.87
2	10-A	401	MES	O3S-S-C8	4.29	111.33	106.06
2	5-E	401	MES	C7-N4-C3	4.30	122.29	111.26
2	10-H	401	MES	C5-N4-C3	4.32	118.67	108.87
2	5-E	401	MES	O2S-S-C8	4.33	110.51	106.79
2	1-C	401	MES	O1S-S-C8	4.34	110.52	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-B	403	GOL	C3-C2-C1	4.36	128.83	111.52
2	4-E	401	MES	O3S-S-C8	4.36	111.41	106.06
2	10-D	401	MES	O2S-S-C8	4.38	110.56	106.79
2	2-B	401	MES	O3S-S-C8	4.38	111.45	106.06
2	3-G	401	MES	C5-N4-C3	4.39	118.82	108.87
2	2-A	401	MES	O3S-S-C8	4.40	111.47	106.06
2	2-D	401	MES	C5-N4-C3	4.41	118.85	108.87
2	6-C	401	MES	C5-N4-C3	4.42	118.87	108.87
2	2-C	401	MES	C5-N4-C3	4.44	118.93	108.87
2	1-G	401	MES	O3S-S-C8	4.44	111.52	106.06
2	3-H	401	MES	O3S-S-C8	4.46	111.54	106.06
2	8-G	401	MES	O3S-S-C8	4.46	111.55	106.06
2	8-G	401	MES	O1S-S-C8	4.49	110.65	106.79
2	10-G	401	MES	C5-N4-C3	4.51	119.08	108.87
2	8-G	401	MES	C5-N4-C3	4.52	119.11	108.87
2	3-D	401	MES	C5-N4-C3	4.53	119.13	108.87
2	1-C	401	MES	O3S-S-C8	4.58	111.68	106.06
2	10-B	401	MES	C5-N4-C3	4.59	119.28	108.87
2	3-F	401	MES	C5-N4-C3	4.60	119.28	108.87
2	3-B	401	MES	C5-N4-C3	4.60	119.29	108.87
2	8-B	401	MES	O2S-S-C8	4.61	110.75	106.79
2	9-D	401	MES	C5-N4-C3	4.62	119.33	108.87
2	1-E	401	MES	C5-N4-C3	4.75	119.63	108.87
2	1-F	401	MES	C5-N4-C3	4.75	119.63	108.87
2	7-F	401	MES	C5-N4-C3	4.79	119.72	108.87
2	6-D	401	MES	O3S-S-C8	4.84	112.01	106.06
2	4-A	401	MES	C5-N4-C3	4.84	119.84	108.87
2	6-F	401	MES	C5-N4-C3	4.85	119.85	108.87
2	7-B	401	MES	O3S-S-C8	4.87	112.05	106.06
2	8-C	401	MES	O1S-S-C8	4.88	110.98	106.79
2	4-H	401	MES	C5-N4-C3	4.90	119.98	108.87
2	7-A	401	MES	C5-N4-C3	4.91	119.99	108.87
2	5-B	401	MES	C5-N4-C3	4.92	120.03	108.87
2	1-F	401	MES	O1S-S-C8	4.93	111.03	106.79
2	2-B	401	MES	C5-N4-C3	4.93	120.05	108.87
2	10-B	401	MES	O2S-S-C8	4.95	111.04	106.79
2	3-A	401	MES	O3S-S-C8	4.96	112.15	106.06
2	8-D	401	MES	C5-N4-C3	4.96	120.10	108.87
2	2-C	401	MES	O3S-S-C8	4.98	112.18	106.06
2	8-F	401	MES	O1S-S-C8	4.98	111.07	106.79
2	1-G	401	MES	C5-N4-C3	4.99	120.18	108.87
2	10-E	401	MES	C5-N4-C3	5.02	120.25	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6-A	401	MES	C5-N4-C3	5.03	120.26	108.87
2	6-F	401	MES	O1S-S-C8	5.04	111.12	106.79
2	9-B	401	MES	O3S-S-C8	5.04	112.26	106.06
2	5-F	401	MES	O1S-S-C8	5.10	111.17	106.79
2	9-A	401	MES	O1S-S-C8	5.11	111.18	106.79
2	7-E	401	MES	C5-N4-C3	5.17	120.58	108.87
2	2-E	401	MES	C5-N4-C3	5.18	120.61	108.87
2	1-D	401	MES	C5-N4-C3	5.18	120.61	108.87
2	10-G	401	MES	O2S-S-C8	5.18	111.24	106.79
2	9-A	401	MES	C5-N4-C3	5.19	120.62	108.87
2	7-A	401	MES	O3S-S-C8	5.19	112.44	106.06
2	4-F	401	MES	C5-N4-C3	5.24	120.74	108.87
2	5-F	401	MES	O2S-S-C8	5.24	111.30	106.79
2	8-A	401	MES	C5-N4-C3	5.25	120.75	108.87
2	6-G	401	MES	C5-N4-C3	5.29	120.85	108.87
2	10-E	401	MES	O2S-S-C8	5.32	111.36	106.79
2	4-D	401	MES	C5-N4-C3	5.33	120.95	108.87
2	8-D	401	MES	O3S-S-C8	5.35	112.64	106.06
2	9-G	401	MES	C5-N4-C3	5.37	121.02	108.87
2	8-F	401	MES	C5-N4-C3	5.38	121.06	108.87
2	5-A	401	MES	C5-N4-C3	5.38	121.07	108.87
2	7-F	401	MES	O2S-S-C8	5.40	111.43	106.79
2	3-B	401	MES	C7-N4-C5	5.42	125.14	111.26
2	10-G	401	MES	O1S-S-C8	5.42	111.45	106.79
2	1-C	401	MES	C5-N4-C3	5.42	121.15	108.87
2	5-E	401	MES	O3S-S-C8	5.44	112.74	106.06
2	3-A	401	MES	C5-N4-C3	5.48	121.28	108.87
2	9-E	401	MES	C5-N4-C3	5.53	121.39	108.87
2	1-B	401	MES	O3S-S-C8	5.59	112.94	106.06
2	1-E	401	MES	O1S-S-C8	5.66	111.65	106.79
2	7-B	401	MES	C5-N4-C3	5.67	121.72	108.87
2	5-B	401	MES	O3S-S-C8	5.70	113.06	106.06
2	10-F	401	MES	C5-N4-C3	5.74	121.86	108.87
2	5-F	401	MES	C5-N4-C3	5.76	121.92	108.87
2	2-F	401	MES	O2S-S-C8	5.90	111.86	106.79
2	6-A	401	MES	O3S-S-C8	5.93	113.35	106.06
2	10-H	401	MES	O2S-S-C8	5.95	111.90	106.79
2	7-D	401	MES	C5-N4-C3	6.00	122.45	108.87
2	9-C	401	MES	C5-N4-C3	6.00	122.47	108.87
2	1-D	401	MES	O3S-S-C8	6.03	113.47	106.06
2	1-A	401	MES	C5-N4-C3	6.06	122.60	108.87
2	7-G	401	MES	C5-N4-C3	6.07	122.61	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9-H	401	MES	O1S-S-C8	6.07	112.01	106.79
2	1-H	401	MES	O3S-S-C8	6.12	113.59	106.06
2	7-C	401	MES	O1S-S-C8	6.30	112.21	106.79
2	3-E	401	MES	O3S-S-C8	6.39	113.92	106.06
2	6-G	401	MES	O1S-S-C8	6.48	112.36	106.79
2	6-C	401	MES	O2S-S-C8	6.53	112.40	106.79
2	5-D	401	MES	C5-N4-C3	6.73	124.11	108.87
2	8-E	401	MES	C5-N4-C3	6.73	124.12	108.87
2	9-F	401	MES	O1S-S-C8	6.94	112.76	106.79
2	3-D	401	MES	O2S-S-C8	6.97	112.78	106.79
2	1-F	401	MES	O2S-S-C8	7.04	112.84	106.79
2	7-G	401	MES	O3S-S-C8	7.11	114.80	106.06
2	3-B	401	MES	O3S-S-C8	7.21	114.92	106.06
2	9-G	401	MES	O1S-S-C8	7.21	112.99	106.79
2	6-E	401	MES	O3S-S-C8	7.23	114.95	106.06
2	3-F	401	MES	O2S-S-C8	7.26	113.03	106.79
2	2-F	401	MES	O1S-S-C8	7.35	113.10	106.79
2	3-F	401	MES	O1S-S-C8	7.35	113.11	106.79
2	8-B	401	MES	O1S-S-C8	7.46	113.20	106.79
2	4-D	401	MES	O1S-S-C8	7.48	113.22	106.79
2	2-D	401	MES	O1S-S-C8	7.51	113.24	106.79
2	7-E	401	MES	O2S-S-C8	7.62	113.34	106.79
2	8-E	401	MES	O2S-S-C8	7.71	113.41	106.79
2	2-G	401	MES	O1S-S-C8	7.74	113.44	106.79
2	6-D	401	MES	O1S-S-C8	7.87	113.55	106.79
2	6-H	401	MES	O3S-S-C8	8.22	116.17	106.06
2	9-A	401	MES	O2S-S-C8	8.52	114.11	106.79
2	2-E	401	MES	O2S-S-C8	8.61	114.19	106.79
2	4-G	401	MES	O1S-S-C8	9.02	114.54	106.79
2	5-G	401	MES	O3S-S-C8	9.28	117.47	106.06
2	6-E	401	MES	O1S-S-C8	9.44	114.90	106.79
2	8-H	401	MES	O1S-S-C8	9.47	114.93	106.79
2	3-H	401	MES	O1S-S-C8	9.54	114.98	106.79
2	5-H	401	MES	O1S-S-C8	10.13	115.49	106.79
2	9-C	401	MES	O1S-S-C8	10.20	115.55	106.79
2	5-D	401	MES	O2S-S-C8	11.01	116.25	106.79
2	3-E	401	MES	O1S-S-C8	11.98	117.08	106.79
2	3-B	401	MES	O1S-S-C8	12.41	117.45	106.79
2	10-C	401	MES	O1S-S-C8	12.51	117.54	106.79
2	4-C	401	MES	O2S-S-C8	12.76	117.75	106.79
2	3-C	401	MES	O2S-S-C8	15.74	120.31	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

213 monomers are involved in 426 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1-A	401	MES	1	0
3	1-A	404	GOL	2	0
3	1-B	402	GOL	2	0
3	1-B	405	GOL	1	0
3	1-B	406	GOL	2	0
2	1-C	401	MES	1	0
2	1-D	401	MES	3	0
2	1-E	401	MES	2	0
3	1-E	402	GOL	1	0
3	1-E	403	GOL	1	0
2	1-F	401	MES	2	0
3	1-F	404	GOL	1	0
3	1-F	405	GOL	2	0
2	1-G	401	MES	2	0
3	1-G	402	GOL	2	0
3	1-G	403	GOL	2	0
2	1-H	401	MES	2	0
3	1-H	402	GOL	2	0
3	1-H	403	GOL	1	0
2	10-A	401	MES	2	0
3	10-A	403	GOL	4	0
3	10-A	404	GOL	1	0
2	10-B	401	MES	5	0
3	10-B	404	GOL	3	0
2	10-C	401	MES	2	0
3	10-C	402	GOL	1	0
3	10-D	403	GOL	1	0
3	10-D	404	GOL	2	0
2	10-E	401	MES	2	0
3	10-E	402	GOL	1	0
2	10-F	401	MES	5	0
3	10-F	403	GOL	1	0
3	10-F	406	GOL	1	0
5	10-F	407	FMT	1	0
3	10-G	402	GOL	3	0
3	10-G	404	GOL	1	0
2	10-H	401	MES	5	0
3	10-H	402	GOL	1	0
3	10-H	403	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	10-H	404	GOL	1	0
3	10-H	405	GOL	1	0
3	2-A	402	GOL	1	0
3	2-A	404	GOL	1	0
2	2-B	401	MES	3	0
3	2-B	402	GOL	1	0
3	2-B	403	GOL	1	0
2	2-C	401	MES	5	0
3	2-C	403	GOL	2	0
5	2-C	404	GOL	1	0
2	2-D	401	MES	2	0
3	2-D	403	GOL	1	0
2	2-E	401	MES	4	0
3	2-E	402	GOL	1	0
2	2-F	401	MES	3	0
2	2-G	401	MES	2	0
3	2-G	402	GOL	1	0
3	2-G	403	GOL	1	0
2	2-H	401	MES	2	0
3	2-H	402	GOL	2	0
3	2-H	404	GOL	2	0
3	3-A	402	GOL	1	0
3	3-A	403	GOL	1	0
4	3-A	405	GOL	1	0
2	3-B	401	MES	1	0
3	3-B	402	GOL	2	0
3	3-B	404	GOL	1	0
3	3-B	405	GOL	2	0
2	3-C	401	MES	2	0
2	3-D	401	MES	1	0
3	3-D	403	GOL	1	0
2	3-E	401	MES	6	0
3	3-E	402	GOL	3	0
3	3-E	403	GOL	2	0
2	3-F	401	MES	2	0
3	3-F	403	GOL	1	0
3	3-F	405	GOL	2	0
3	3-F	406	GOL	1	0
5	3-F	407	FMT	2	0
2	3-G	401	MES	3	0
3	3-G	402	GOL	1	0
3	3-G	404	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3-G	406	FMT	1	0
2	3-H	401	MES	5	0
3	3-H	402	GOL	1	0
2	4-A	401	MES	4	0
3	4-A	402	GOL	2	0
3	4-A	403	GOL	1	0
2	4-B	401	MES	5	0
3	4-B	404	GOL	2	0
3	4-B	405	GOL	1	0
3	4-B	406	GOL	1	0
2	4-C	401	MES	8	0
3	4-C	402	GOL	1	0
3	4-C	403	GOL	1	0
5	4-C	404	GOL	1	0
2	4-D	401	MES	3	0
3	4-D	403	GOL	3	0
2	4-E	401	MES	4	0
3	4-E	402	GOL	1	0
4	4-E	404	GOL	1	0
2	4-F	401	MES	2	0
3	4-F	403	GOL	1	0
2	4-G	401	MES	1	0
3	4-G	402	GOL	1	0
3	4-G	404	GOL	2	0
4	4-G	407	FMT	1	0
2	4-H	401	MES	2	0
3	4-H	402	GOL	2	0
3	4-H	404	GOL	2	0
3	5-A	402	GOL	2	0
3	5-A	403	GOL	3	0
4	5-A	405	GOL	3	0
2	5-B	401	MES	3	0
3	5-B	402	GOL	1	0
3	5-B	403	GOL	1	0
3	5-B	405	GOL	4	0
3	5-B	406	GOL	1	0
2	5-C	401	MES	3	0
2	5-D	401	MES	2	0
3	5-D	402	GOL	2	0
3	5-D	404	GOL	1	0
2	5-E	401	MES	5	0
3	5-E	402	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	5-F	401	MES	2	0
3	5-F	402	GOL	2	0
2	5-G	401	MES	6	0
3	5-G	402	GOL	2	0
5	5-G	405	GOL	1	0
2	5-H	401	MES	1	0
3	5-H	402	GOL	2	0
3	5-H	404	GOL	2	0
3	6-A	403	GOL	1	0
3	6-A	404	GOL	1	0
4	6-A	405	GOL	1	0
2	6-B	401	MES	3	0
3	6-B	402	GOL	1	0
3	6-B	405	GOL	1	0
2	6-C	401	MES	1	0
3	6-C	402	GOL	1	0
2	6-D	401	MES	3	0
3	6-D	403	GOL	1	0
3	6-D	404	GOL	3	0
2	6-E	401	MES	3	0
3	6-E	402	GOL	2	0
2	6-F	401	MES	8	0
3	6-F	402	GOL	1	0
3	6-F	403	GOL	2	0
3	6-F	404	GOL	3	0
3	6-F	405	GOL	1	0
2	6-G	401	MES	1	0
3	6-G	402	GOL	1	0
3	6-G	403	GOL	1	0
3	6-G	404	FMT	1	0
2	6-H	401	MES	4	0
3	7-A	402	GOL	4	0
3	7-A	403	GOL	1	0
3	7-A	404	GOL	1	0
2	7-B	401	MES	6	0
3	7-B	405	GOL	1	0
2	7-C	401	MES	2	0
2	7-D	401	MES	2	0
3	7-D	404	GOL	2	0
2	7-E	401	MES	2	0
3	7-E	402	GOL	3	0
3	7-E	403	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	7-F	401	MES	1	0
3	7-F	402	GOL	1	0
3	7-F	404	GOL	2	0
3	7-F	405	GOL	2	0
5	7-F	407	FMT	2	0
2	7-G	401	MES	3	0
3	7-G	404	GOL	2	0
2	7-H	401	MES	6	0
3	7-H	404	GOL	1	0
2	8-A	401	MES	2	0
3	8-A	402	GOL	1	0
3	8-A	403	GOL	1	0
2	8-B	401	MES	2	0
3	8-B	404	GOL	1	0
3	8-B	405	GOL	1	0
3	8-B	407	GOL	2	0
2	8-C	401	MES	8	0
3	8-C	402	GOL	1	0
2	8-D	401	MES	3	0
3	8-D	403	GOL	1	0
3	8-E	402	GOL	5	0
3	8-E	403	GOL	1	0
4	8-E	404	GOL	2	0
2	8-F	401	MES	1	0
3	8-F	402	GOL	2	0
3	8-F	403	GOL	1	0
3	8-F	405	GOL	2	0
2	8-G	401	MES	1	0
3	8-G	402	GOL	1	0
3	8-G	403	GOL	1	0
2	8-H	401	MES	2	0
3	8-H	404	GOL	4	0
2	9-A	401	MES	1	0
2	9-B	401	MES	2	0
2	9-C	401	MES	2	0
3	9-C	403	GOL	2	0
2	9-D	401	MES	3	0
3	9-D	402	GOL	2	0
3	9-D	403	GOL	1	0
3	9-D	404	GOL	2	0
2	9-E	401	MES	2	0
3	9-F	403	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	9-G	402	GOL	2	0
3	9-G	404	GOL	1	0
2	9-H	401	MES	3	0
3	9-H	403	GOL	1	0
3	9-H	404	GOL	1	0
3	9-H	405	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.