Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 12:20 pm GMT

PDB ID	:	8QE9
EMDB ID	:	EMD-18346
Title	:	Complex between the 80a-Sak SSAP and the SaPI2 Stl master regulator
Authors	:	Debiasi-Anders, G.; Mir-Sanchis, I.
Deposited on	:	2023-08-30
Resolution	:	3.90 Å(reported)
Based on initial model	:	.

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

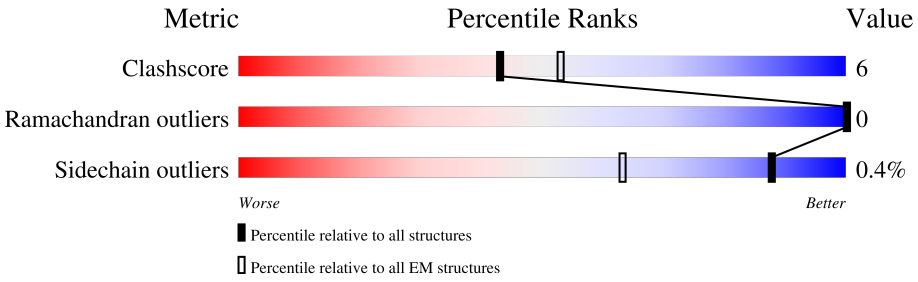
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	1A	206	86% 11% .
1	1B	206	88% 9% .
1	1C	206	77% 21% .
1	1D	206	80% 18% .
1	1E	206	78% 19% .
1	1F	206	84% 11% 5%
1	1G	206	52% 9% 38%
1	1H	206	48% 14% 38%
1	1I	206	80% 17% .

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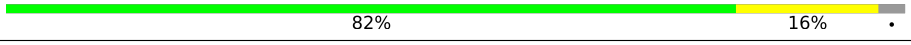
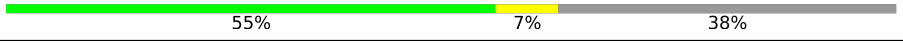
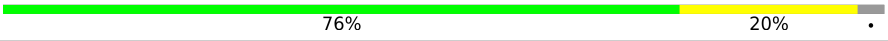
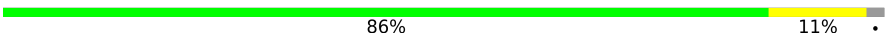
Mol	Chain	Length	Quality of chain
1	1J	206	
1	1K	206	
1	1L	206	
1	1M	206	
1	1N	206	
1	1O	206	
1	1P	206	
1	1Q	206	
1	4A	206	
1	4B	206	
1	4C	206	
1	4D	206	
1	4E	206	
1	4F	206	
1	4G	206	
1	4H	206	
1	4I	206	
1	4J	206	
1	4K	206	
1	4L	206	
1	4M	206	
1	4N	206	
1	4O	206	
1	4P	206	
1	4Q	206	

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Mol	Chain	Length	Quality of chain
2	2A	233	85% 10% 5%
2	2B	233	87% 8% 5%
2	2C	233	86% 9% 5%
2	2D	233	87% 9% 5%
2	2E	233	83% 12% 5%
2	2F	233	82% 13% 5%
2	2G	233	77% 16% 7%
2	2I	233	73% 20% 7%
2	2J	233	77% 16% 7%
2	2L	233	78% 15% 7%
2	2M	233	79% 15% 7%
2	2N	233	68% 25% 7%
2	2O	233	73% 19% 7%
2	2P	233	84% 12% 5%
2	2Q	233	86% 9% 5%
2	3A	233	85% 10% 5%
2	3B	233	87% 8% 5%
2	3C	233	86% 9% 5%
2	3D	233	86% 9% 5%
2	3E	233	82% 13% 5%
2	3F	233	81% 14% 5%
2	3G	233	77% 16% 7%
2	3I	233	74% 19% 7%
2	3J	233	76% 18% 7%
2	3L	233	79% 14% 7%

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Mol	Chain	Length	Quality of chain
2	3M	233	
2	3N	233	
2	3O	233	
2	3P	233	
2	3Q	233	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 104442 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DUF1071 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		
1	1B	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		
1	1C	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		
1	1D	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		
1	1E	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		
1	1F	195	Total	C	N	O	S	0	0
			1580	1002	266	310	2		
1	1G	128	Total	C	N	O	S	0	0
			1043	673	172	197	1		
1	1H	128	Total	C	N	O	S	0	0
			1043	673	172	197	1		
1	1I	200	Total	C	N	O	S	0	0
			1615	1022	275	316	2		
1	1J	200	Total	C	N	O	S	0	0
			1615	1022	275	316	2		
1	1K	128	Total	C	N	O	S	0	0
			1043	673	172	197	1		
1	1L	200	Total	C	N	O	S	0	0
			1615	1022	275	316	2		
1	1M	200	Total	C	N	O	S	0	0
			1615	1022	275	316	2		
1	1N	200	Total	C	N	O	S	0	0
			1615	1022	275	316	2		
1	1O	128	Total	C	N	O	S	0	0
			1043	673	172	197	1		
1	1P	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		
1	1Q	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4A	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		
1	4B	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		
1	4C	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		
1	4D	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		
1	4E	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		
1	4F	195	Total	C	N	O	S	0	0
			1580	1002	266	310	2		
1	4G	128	Total	C	N	O	S	0	0
			1043	673	172	197	1		
1	4H	128	Total	C	N	O	S	0	0
			1043	673	172	197	1		
1	4I	200	Total	C	N	O	S	0	0
			1615	1022	275	316	2		
1	4J	200	Total	C	N	O	S	0	0
			1615	1022	275	316	2		
1	4K	128	Total	C	N	O	S	0	0
			1043	673	172	197	1		
1	4L	200	Total	C	N	O	S	0	0
			1615	1022	275	316	2		
1	4M	200	Total	C	N	O	S	0	0
			1615	1022	275	316	2		
1	4N	200	Total	C	N	O	S	0	0
			1615	1022	275	316	2		
1	4O	128	Total	C	N	O	S	0	0
			1043	673	172	197	1		
1	4P	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		
1	4Q	201	Total	C	N	O	S	0	0
			1624	1027	276	319	2		

- Molecule 2 is a protein called Helix-turn-helix XRE family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2A	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	2B	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	2C	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	2D	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	2E	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	2F	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	2G	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	2I	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	2J	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	2L	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	2M	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	2N	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	2O	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	2P	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	2Q	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	3A	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	3B	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	3C	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	3D	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	3E	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	3F	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	3G	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	3I	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	3J	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	3L	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	3M	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	3N	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	3O	217	Total	C	N	O	S	0	0
			1782	1132	294	353	3		
2	3P	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		
2	3Q	222	Total	C	N	O	S	0	0
			1819	1154	301	361	3		

There are 300 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2A	0	MET	-	initiating methionine	UNP A0FIL5
2A	1	GLY	-	expression tag	UNP A0FIL5
2A	225	GLY	-	expression tag	UNP A0FIL5
2A	226	SER	-	expression tag	UNP A0FIL5
2A	227	HIS	-	expression tag	UNP A0FIL5
2A	228	HIS	-	expression tag	UNP A0FIL5
2A	229	HIS	-	expression tag	UNP A0FIL5
2A	230	HIS	-	expression tag	UNP A0FIL5
2A	231	HIS	-	expression tag	UNP A0FIL5
2A	232	HIS	-	expression tag	UNP A0FIL5
2B	0	MET	-	initiating methionine	UNP A0FIL5
2B	1	GLY	-	expression tag	UNP A0FIL5
2B	225	GLY	-	expression tag	UNP A0FIL5
2B	226	SER	-	expression tag	UNP A0FIL5
2B	227	HIS	-	expression tag	UNP A0FIL5
2B	228	HIS	-	expression tag	UNP A0FIL5
2B	229	HIS	-	expression tag	UNP A0FIL5
2B	230	HIS	-	expression tag	UNP A0FIL5
2B	231	HIS	-	expression tag	UNP A0FIL5
2B	232	HIS	-	expression tag	UNP A0FIL5
2C	0	MET	-	initiating methionine	UNP A0FIL5
2C	1	GLY	-	expression tag	UNP A0FIL5
2C	225	GLY	-	expression tag	UNP A0FIL5
2C	226	SER	-	expression tag	UNP A0FIL5
2C	227	HIS	-	expression tag	UNP A0FIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
2C	228	HIS	-	expression tag	UNP A0FIL5
2C	229	HIS	-	expression tag	UNP A0FIL5
2C	230	HIS	-	expression tag	UNP A0FIL5
2C	231	HIS	-	expression tag	UNP A0FIL5
2C	232	HIS	-	expression tag	UNP A0FIL5
2D	0	MET	-	initiating methionine	UNP A0FIL5
2D	1	GLY	-	expression tag	UNP A0FIL5
2D	225	GLY	-	expression tag	UNP A0FIL5
2D	226	SER	-	expression tag	UNP A0FIL5
2D	227	HIS	-	expression tag	UNP A0FIL5
2D	228	HIS	-	expression tag	UNP A0FIL5
2D	229	HIS	-	expression tag	UNP A0FIL5
2D	230	HIS	-	expression tag	UNP A0FIL5
2D	231	HIS	-	expression tag	UNP A0FIL5
2D	232	HIS	-	expression tag	UNP A0FIL5
2E	0	MET	-	initiating methionine	UNP A0FIL5
2E	1	GLY	-	expression tag	UNP A0FIL5
2E	225	GLY	-	expression tag	UNP A0FIL5
2E	226	SER	-	expression tag	UNP A0FIL5
2E	227	HIS	-	expression tag	UNP A0FIL5
2E	228	HIS	-	expression tag	UNP A0FIL5
2E	229	HIS	-	expression tag	UNP A0FIL5
2E	230	HIS	-	expression tag	UNP A0FIL5
2E	231	HIS	-	expression tag	UNP A0FIL5
2E	232	HIS	-	expression tag	UNP A0FIL5
2F	0	MET	-	initiating methionine	UNP A0FIL5
2F	1	GLY	-	expression tag	UNP A0FIL5
2F	225	GLY	-	expression tag	UNP A0FIL5
2F	226	SER	-	expression tag	UNP A0FIL5
2F	227	HIS	-	expression tag	UNP A0FIL5
2F	228	HIS	-	expression tag	UNP A0FIL5
2F	229	HIS	-	expression tag	UNP A0FIL5
2F	230	HIS	-	expression tag	UNP A0FIL5
2F	231	HIS	-	expression tag	UNP A0FIL5
2F	232	HIS	-	expression tag	UNP A0FIL5
2G	0	MET	-	initiating methionine	UNP A0FIL5
2G	1	GLY	-	expression tag	UNP A0FIL5
2G	225	GLY	-	expression tag	UNP A0FIL5
2G	226	SER	-	expression tag	UNP A0FIL5
2G	227	HIS	-	expression tag	UNP A0FIL5
2G	228	HIS	-	expression tag	UNP A0FIL5
2G	229	HIS	-	expression tag	UNP A0FIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
2G	230	HIS	-	expression tag	UNP A0FIL5
2G	231	HIS	-	expression tag	UNP A0FIL5
2G	232	HIS	-	expression tag	UNP A0FIL5
2I	0	MET	-	initiating methionine	UNP A0FIL5
2I	1	GLY	-	expression tag	UNP A0FIL5
2I	225	GLY	-	expression tag	UNP A0FIL5
2I	226	SER	-	expression tag	UNP A0FIL5
2I	227	HIS	-	expression tag	UNP A0FIL5
2I	228	HIS	-	expression tag	UNP A0FIL5
2I	229	HIS	-	expression tag	UNP A0FIL5
2I	230	HIS	-	expression tag	UNP A0FIL5
2I	231	HIS	-	expression tag	UNP A0FIL5
2I	232	HIS	-	expression tag	UNP A0FIL5
2J	0	MET	-	initiating methionine	UNP A0FIL5
2J	1	GLY	-	expression tag	UNP A0FIL5
2J	225	GLY	-	expression tag	UNP A0FIL5
2J	226	SER	-	expression tag	UNP A0FIL5
2J	227	HIS	-	expression tag	UNP A0FIL5
2J	228	HIS	-	expression tag	UNP A0FIL5
2J	229	HIS	-	expression tag	UNP A0FIL5
2J	230	HIS	-	expression tag	UNP A0FIL5
2J	231	HIS	-	expression tag	UNP A0FIL5
2J	232	HIS	-	expression tag	UNP A0FIL5
2L	0	MET	-	initiating methionine	UNP A0FIL5
2L	1	GLY	-	expression tag	UNP A0FIL5
2L	225	GLY	-	expression tag	UNP A0FIL5
2L	226	SER	-	expression tag	UNP A0FIL5
2L	227	HIS	-	expression tag	UNP A0FIL5
2L	228	HIS	-	expression tag	UNP A0FIL5
2L	229	HIS	-	expression tag	UNP A0FIL5
2L	230	HIS	-	expression tag	UNP A0FIL5
2L	231	HIS	-	expression tag	UNP A0FIL5
2L	232	HIS	-	expression tag	UNP A0FIL5
2M	0	MET	-	initiating methionine	UNP A0FIL5
2M	1	GLY	-	expression tag	UNP A0FIL5
2M	225	GLY	-	expression tag	UNP A0FIL5
2M	226	SER	-	expression tag	UNP A0FIL5
2M	227	HIS	-	expression tag	UNP A0FIL5
2M	228	HIS	-	expression tag	UNP A0FIL5
2M	229	HIS	-	expression tag	UNP A0FIL5
2M	230	HIS	-	expression tag	UNP A0FIL5
2M	231	HIS	-	expression tag	UNP A0FIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
2M	232	HIS	-	expression tag	UNP A0FIL5
2N	0	MET	-	initiating methionine	UNP A0FIL5
2N	1	GLY	-	expression tag	UNP A0FIL5
2N	225	GLY	-	expression tag	UNP A0FIL5
2N	226	SER	-	expression tag	UNP A0FIL5
2N	227	HIS	-	expression tag	UNP A0FIL5
2N	228	HIS	-	expression tag	UNP A0FIL5
2N	229	HIS	-	expression tag	UNP A0FIL5
2N	230	HIS	-	expression tag	UNP A0FIL5
2N	231	HIS	-	expression tag	UNP A0FIL5
2N	232	HIS	-	expression tag	UNP A0FIL5
2O	0	MET	-	initiating methionine	UNP A0FIL5
2O	1	GLY	-	expression tag	UNP A0FIL5
2O	225	GLY	-	expression tag	UNP A0FIL5
2O	226	SER	-	expression tag	UNP A0FIL5
2O	227	HIS	-	expression tag	UNP A0FIL5
2O	228	HIS	-	expression tag	UNP A0FIL5
2O	229	HIS	-	expression tag	UNP A0FIL5
2O	230	HIS	-	expression tag	UNP A0FIL5
2O	231	HIS	-	expression tag	UNP A0FIL5
2O	232	HIS	-	expression tag	UNP A0FIL5
2P	0	MET	-	initiating methionine	UNP A0FIL5
2P	1	GLY	-	expression tag	UNP A0FIL5
2P	225	GLY	-	expression tag	UNP A0FIL5
2P	226	SER	-	expression tag	UNP A0FIL5
2P	227	HIS	-	expression tag	UNP A0FIL5
2P	228	HIS	-	expression tag	UNP A0FIL5
2P	229	HIS	-	expression tag	UNP A0FIL5
2P	230	HIS	-	expression tag	UNP A0FIL5
2P	231	HIS	-	expression tag	UNP A0FIL5
2P	232	HIS	-	expression tag	UNP A0FIL5
2Q	0	MET	-	initiating methionine	UNP A0FIL5
2Q	1	GLY	-	expression tag	UNP A0FIL5
2Q	225	GLY	-	expression tag	UNP A0FIL5
2Q	226	SER	-	expression tag	UNP A0FIL5
2Q	227	HIS	-	expression tag	UNP A0FIL5
2Q	228	HIS	-	expression tag	UNP A0FIL5
2Q	229	HIS	-	expression tag	UNP A0FIL5
2Q	230	HIS	-	expression tag	UNP A0FIL5
2Q	231	HIS	-	expression tag	UNP A0FIL5
2Q	232	HIS	-	expression tag	UNP A0FIL5
3A	0	MET	-	initiating methionine	UNP A0FIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
3A	1	GLY	-	expression tag	UNP A0FIL5
3A	225	GLY	-	expression tag	UNP A0FIL5
3A	226	SER	-	expression tag	UNP A0FIL5
3A	227	HIS	-	expression tag	UNP A0FIL5
3A	228	HIS	-	expression tag	UNP A0FIL5
3A	229	HIS	-	expression tag	UNP A0FIL5
3A	230	HIS	-	expression tag	UNP A0FIL5
3A	231	HIS	-	expression tag	UNP A0FIL5
3A	232	HIS	-	expression tag	UNP A0FIL5
3B	0	MET	-	initiating methionine	UNP A0FIL5
3B	1	GLY	-	expression tag	UNP A0FIL5
3B	225	GLY	-	expression tag	UNP A0FIL5
3B	226	SER	-	expression tag	UNP A0FIL5
3B	227	HIS	-	expression tag	UNP A0FIL5
3B	228	HIS	-	expression tag	UNP A0FIL5
3B	229	HIS	-	expression tag	UNP A0FIL5
3B	230	HIS	-	expression tag	UNP A0FIL5
3B	231	HIS	-	expression tag	UNP A0FIL5
3B	232	HIS	-	expression tag	UNP A0FIL5
3C	0	MET	-	initiating methionine	UNP A0FIL5
3C	1	GLY	-	expression tag	UNP A0FIL5
3C	225	GLY	-	expression tag	UNP A0FIL5
3C	226	SER	-	expression tag	UNP A0FIL5
3C	227	HIS	-	expression tag	UNP A0FIL5
3C	228	HIS	-	expression tag	UNP A0FIL5
3C	229	HIS	-	expression tag	UNP A0FIL5
3C	230	HIS	-	expression tag	UNP A0FIL5
3C	231	HIS	-	expression tag	UNP A0FIL5
3C	232	HIS	-	expression tag	UNP A0FIL5
3D	0	MET	-	initiating methionine	UNP A0FIL5
3D	1	GLY	-	expression tag	UNP A0FIL5
3D	225	GLY	-	expression tag	UNP A0FIL5
3D	226	SER	-	expression tag	UNP A0FIL5
3D	227	HIS	-	expression tag	UNP A0FIL5
3D	228	HIS	-	expression tag	UNP A0FIL5
3D	229	HIS	-	expression tag	UNP A0FIL5
3D	230	HIS	-	expression tag	UNP A0FIL5
3D	231	HIS	-	expression tag	UNP A0FIL5
3D	232	HIS	-	expression tag	UNP A0FIL5
3E	0	MET	-	initiating methionine	UNP A0FIL5
3E	1	GLY	-	expression tag	UNP A0FIL5
3E	225	GLY	-	expression tag	UNP A0FIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
3E	226	SER	-	expression tag	UNP A0FIL5
3E	227	HIS	-	expression tag	UNP A0FIL5
3E	228	HIS	-	expression tag	UNP A0FIL5
3E	229	HIS	-	expression tag	UNP A0FIL5
3E	230	HIS	-	expression tag	UNP A0FIL5
3E	231	HIS	-	expression tag	UNP A0FIL5
3E	232	HIS	-	expression tag	UNP A0FIL5
3F	0	MET	-	initiating methionine	UNP A0FIL5
3F	1	GLY	-	expression tag	UNP A0FIL5
3F	225	GLY	-	expression tag	UNP A0FIL5
3F	226	SER	-	expression tag	UNP A0FIL5
3F	227	HIS	-	expression tag	UNP A0FIL5
3F	228	HIS	-	expression tag	UNP A0FIL5
3F	229	HIS	-	expression tag	UNP A0FIL5
3F	230	HIS	-	expression tag	UNP A0FIL5
3F	231	HIS	-	expression tag	UNP A0FIL5
3F	232	HIS	-	expression tag	UNP A0FIL5
3G	0	MET	-	initiating methionine	UNP A0FIL5
3G	1	GLY	-	expression tag	UNP A0FIL5
3G	225	GLY	-	expression tag	UNP A0FIL5
3G	226	SER	-	expression tag	UNP A0FIL5
3G	227	HIS	-	expression tag	UNP A0FIL5
3G	228	HIS	-	expression tag	UNP A0FIL5
3G	229	HIS	-	expression tag	UNP A0FIL5
3G	230	HIS	-	expression tag	UNP A0FIL5
3G	231	HIS	-	expression tag	UNP A0FIL5
3G	232	HIS	-	expression tag	UNP A0FIL5
3I	0	MET	-	initiating methionine	UNP A0FIL5
3I	1	GLY	-	expression tag	UNP A0FIL5
3I	225	GLY	-	expression tag	UNP A0FIL5
3I	226	SER	-	expression tag	UNP A0FIL5
3I	227	HIS	-	expression tag	UNP A0FIL5
3I	228	HIS	-	expression tag	UNP A0FIL5
3I	229	HIS	-	expression tag	UNP A0FIL5
3I	230	HIS	-	expression tag	UNP A0FIL5
3I	231	HIS	-	expression tag	UNP A0FIL5
3I	232	HIS	-	expression tag	UNP A0FIL5
3J	0	MET	-	initiating methionine	UNP A0FIL5
3J	1	GLY	-	expression tag	UNP A0FIL5
3J	225	GLY	-	expression tag	UNP A0FIL5
3J	226	SER	-	expression tag	UNP A0FIL5
3J	227	HIS	-	expression tag	UNP A0FIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
3J	228	HIS	-	expression tag	UNP A0FIL5
3J	229	HIS	-	expression tag	UNP A0FIL5
3J	230	HIS	-	expression tag	UNP A0FIL5
3J	231	HIS	-	expression tag	UNP A0FIL5
3J	232	HIS	-	expression tag	UNP A0FIL5
3L	0	MET	-	initiating methionine	UNP A0FIL5
3L	1	GLY	-	expression tag	UNP A0FIL5
3L	225	GLY	-	expression tag	UNP A0FIL5
3L	226	SER	-	expression tag	UNP A0FIL5
3L	227	HIS	-	expression tag	UNP A0FIL5
3L	228	HIS	-	expression tag	UNP A0FIL5
3L	229	HIS	-	expression tag	UNP A0FIL5
3L	230	HIS	-	expression tag	UNP A0FIL5
3L	231	HIS	-	expression tag	UNP A0FIL5
3L	232	HIS	-	expression tag	UNP A0FIL5
3M	0	MET	-	initiating methionine	UNP A0FIL5
3M	1	GLY	-	expression tag	UNP A0FIL5
3M	225	GLY	-	expression tag	UNP A0FIL5
3M	226	SER	-	expression tag	UNP A0FIL5
3M	227	HIS	-	expression tag	UNP A0FIL5
3M	228	HIS	-	expression tag	UNP A0FIL5
3M	229	HIS	-	expression tag	UNP A0FIL5
3M	230	HIS	-	expression tag	UNP A0FIL5
3M	231	HIS	-	expression tag	UNP A0FIL5
3M	232	HIS	-	expression tag	UNP A0FIL5
3N	0	MET	-	initiating methionine	UNP A0FIL5
3N	1	GLY	-	expression tag	UNP A0FIL5
3N	225	GLY	-	expression tag	UNP A0FIL5
3N	226	SER	-	expression tag	UNP A0FIL5
3N	227	HIS	-	expression tag	UNP A0FIL5
3N	228	HIS	-	expression tag	UNP A0FIL5
3N	229	HIS	-	expression tag	UNP A0FIL5
3N	230	HIS	-	expression tag	UNP A0FIL5
3N	231	HIS	-	expression tag	UNP A0FIL5
3N	232	HIS	-	expression tag	UNP A0FIL5
3O	0	MET	-	initiating methionine	UNP A0FIL5
3O	1	GLY	-	expression tag	UNP A0FIL5
3O	225	GLY	-	expression tag	UNP A0FIL5
3O	226	SER	-	expression tag	UNP A0FIL5
3O	227	HIS	-	expression tag	UNP A0FIL5
3O	228	HIS	-	expression tag	UNP A0FIL5
3O	229	HIS	-	expression tag	UNP A0FIL5

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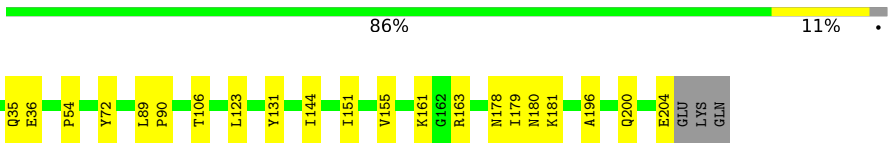
Chain	Residue	Modelled	Actual	Comment	Reference
3O	230	HIS	-	expression tag	UNP A0FIL5
3O	231	HIS	-	expression tag	UNP A0FIL5
3O	232	HIS	-	expression tag	UNP A0FIL5
3P	0	MET	-	initiating methionine	UNP A0FIL5
3P	1	GLY	-	expression tag	UNP A0FIL5
3P	225	GLY	-	expression tag	UNP A0FIL5
3P	226	SER	-	expression tag	UNP A0FIL5
3P	227	HIS	-	expression tag	UNP A0FIL5
3P	228	HIS	-	expression tag	UNP A0FIL5
3P	229	HIS	-	expression tag	UNP A0FIL5
3P	230	HIS	-	expression tag	UNP A0FIL5
3P	231	HIS	-	expression tag	UNP A0FIL5
3P	232	HIS	-	expression tag	UNP A0FIL5
3Q	0	MET	-	initiating methionine	UNP A0FIL5
3Q	1	GLY	-	expression tag	UNP A0FIL5
3Q	225	GLY	-	expression tag	UNP A0FIL5
3Q	226	SER	-	expression tag	UNP A0FIL5
3Q	227	HIS	-	expression tag	UNP A0FIL5
3Q	228	HIS	-	expression tag	UNP A0FIL5
3Q	229	HIS	-	expression tag	UNP A0FIL5
3Q	230	HIS	-	expression tag	UNP A0FIL5
3Q	231	HIS	-	expression tag	UNP A0FIL5
3Q	232	HIS	-	expression tag	UNP A0FIL5

3 Residue-property plots (i)

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

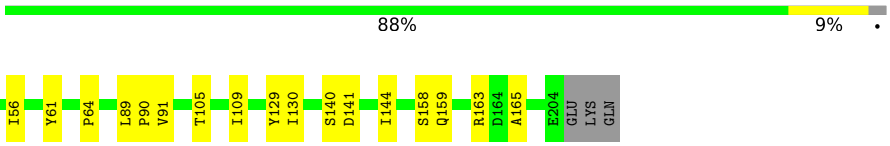
• Molecule 1: DUF1071 domain-containing protein

Chain 1A:



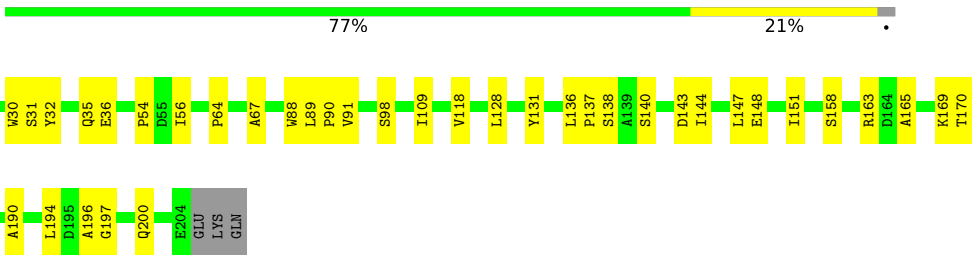
• Molecule 1: DUF1071 domain-containing protein

Chain 1B:



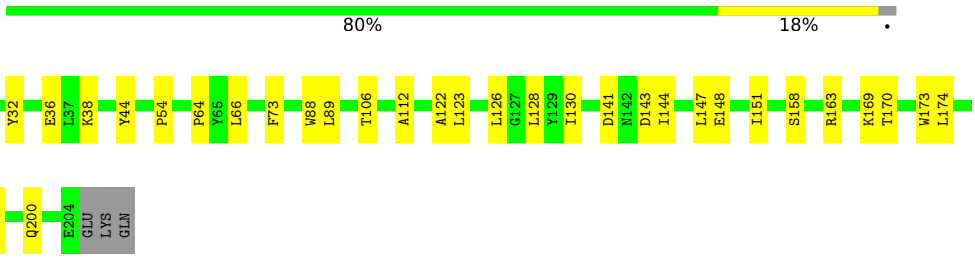
• Molecule 1: DUF1071 domain-containing protein

Chain 1C:



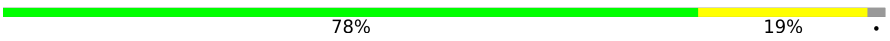
• Molecule 1: DUF1071 domain-containing protein

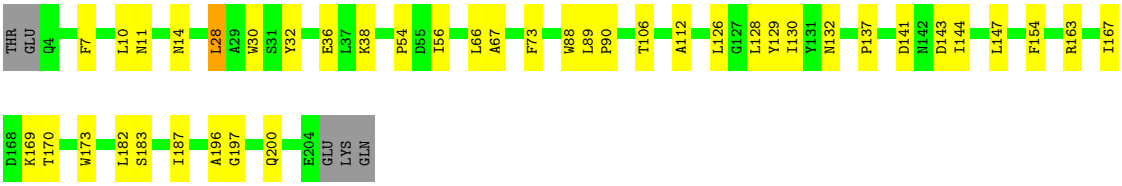
Chain 1D:



• Molecule 1: DUF1071 domain-containing protein

Chain 1E:



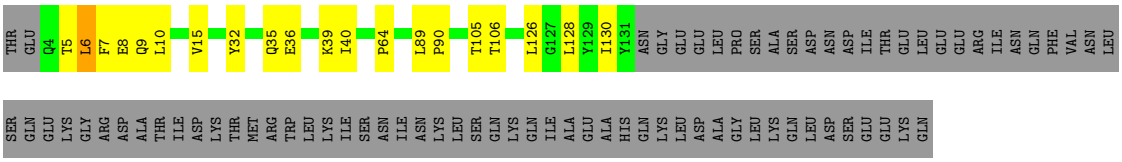


• Molecule 1: DUF1071 domain-containing protein

Chain 1F:

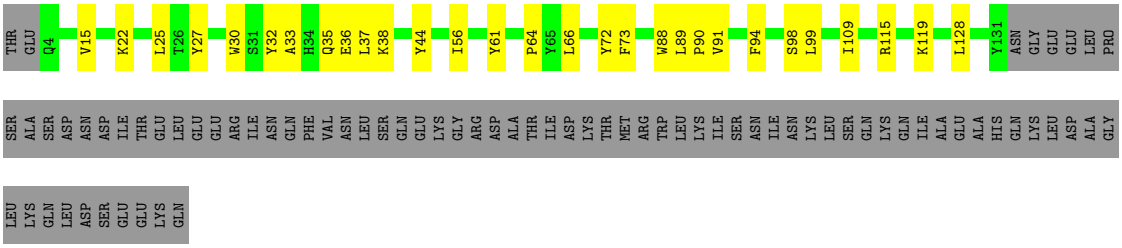
• Molecule 1: DUF1071 domain-containing protein

Chain 1G:



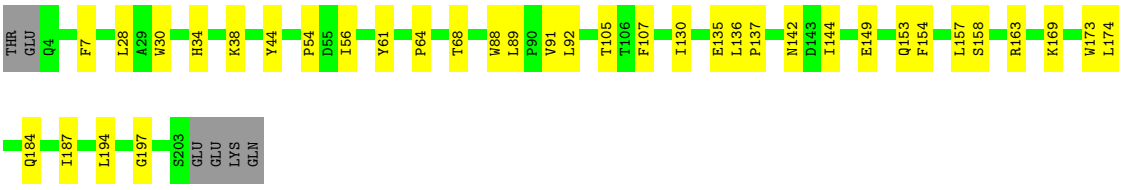
• Molecule 1: DUF1071 domain-containing protein

Chain 1H:



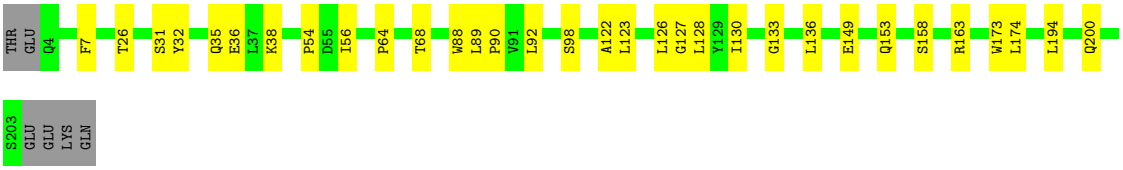
• Molecule 1: DUF1071 domain-containing protein

Chain 1I:



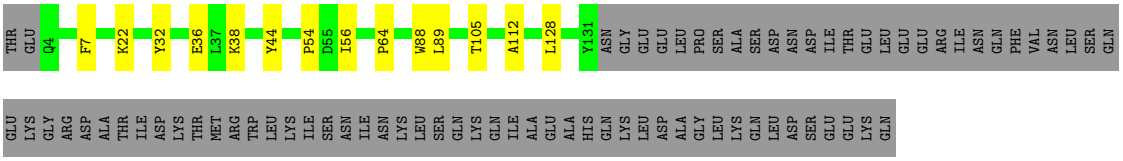
• Molecule 1: DUF1071 domain-containing protein

Chain 1J:



• Molecule 1: DUF1071 domain-containing protein

Chain 1K:

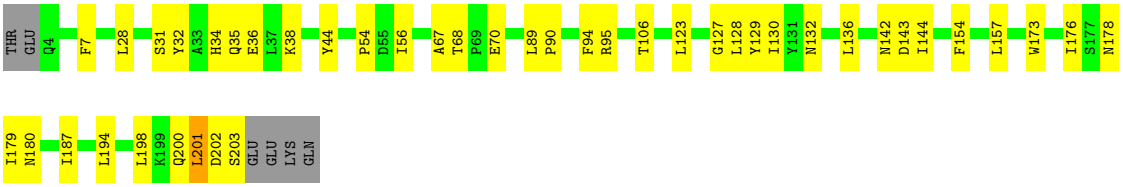


• Molecule 1: DUF1071 domain-containing protein

Chain 1L:

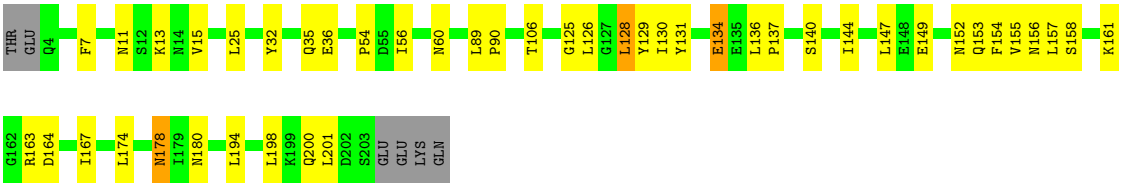
• Molecule 1: DUF1071 domain-containing protein

Chain 1M:



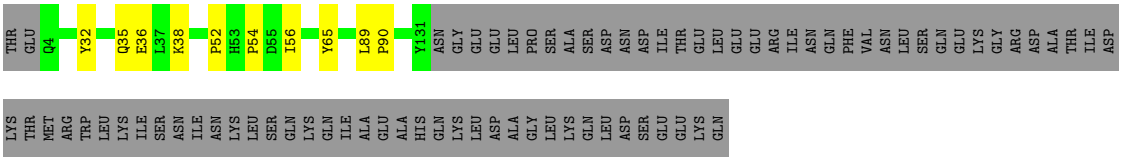
• Molecule 1: DUF1071 domain-containing protein

Chain 1N:



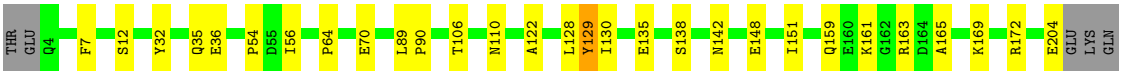
• Molecule 1: DUF1071 domain-containing protein

Chain 1O:



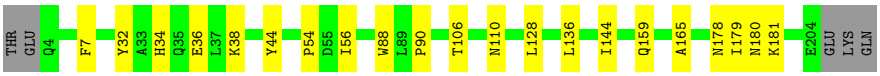
• Molecule 1: DUF1071 domain-containing protein

Chain 1P:



• Molecule 1: DUF1071 domain-containing protein

Chain 1Q:

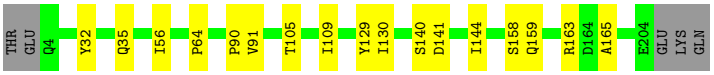


• Molecule 1: DUF1071 domain-containing protein

Chain 4A:

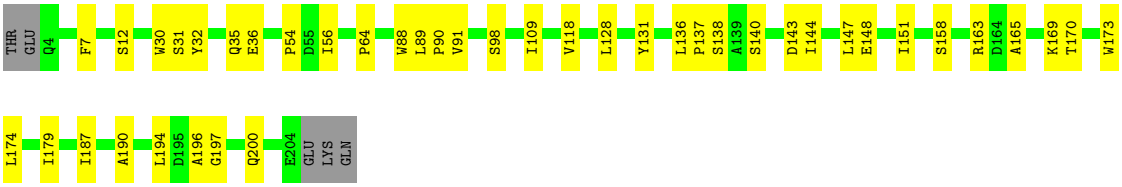
• Molecule 1: DUF1071 domain-containing protein

Chain 4B:



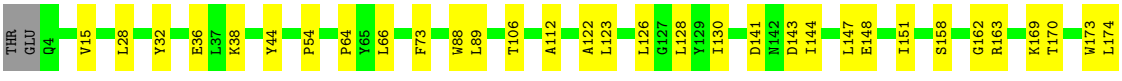
• Molecule 1: DUF1071 domain-containing protein

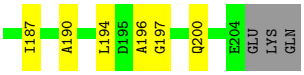
Chain 4C:



• Molecule 1: DUF1071 domain-containing protein

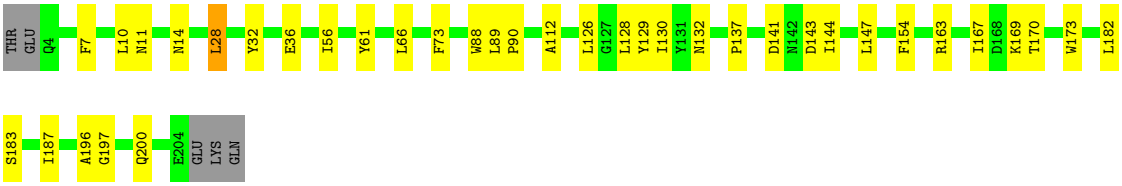
Chain 4D:





• Molecule 1: DUF1071 domain-containing protein

Chain 4E:

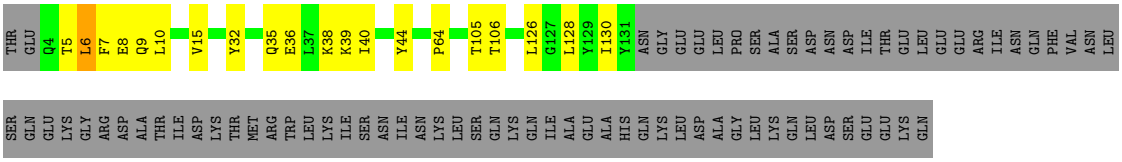


• Molecule 1: DUF1071 domain-containing protein

Chain 4F:

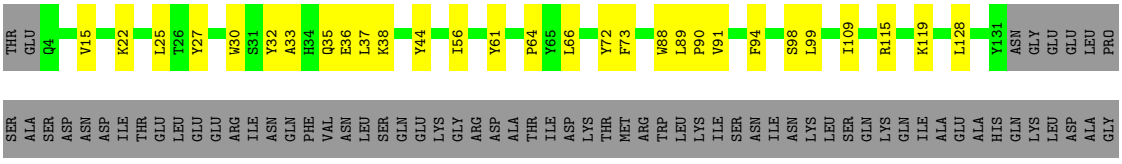
• Molecule 1: DUF1071 domain-containing protein

Chain 4G:



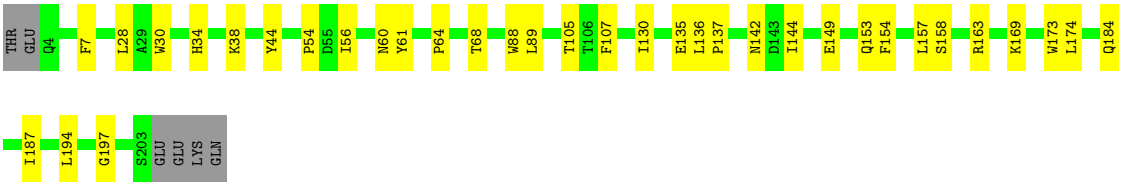
• Molecule 1: DUF1071 domain-containing protein

Chain 4H:



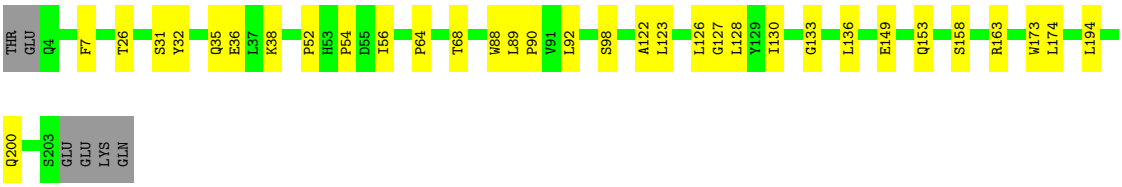
• Molecule 1: DUF1071 domain-containing protein

Chain 4I:



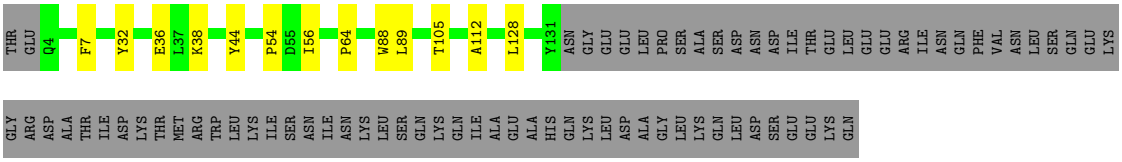
• Molecule 1: DUF1071 domain-containing protein

Chain 4J:



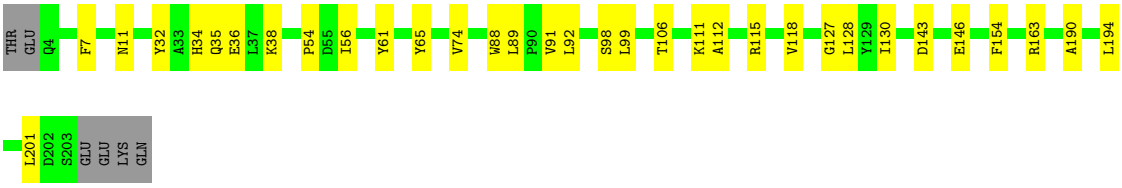
• Molecule 1: DUF1071 domain-containing protein

Chain 4K:



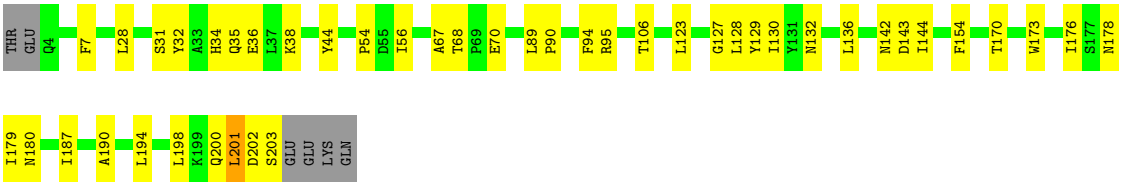
• Molecule 1: DUF1071 domain-containing protein

Chain 4L:



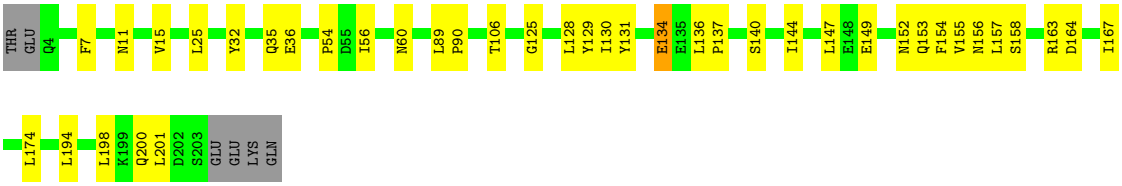
• Molecule 1: DUF1071 domain-containing protein

Chain 4M:



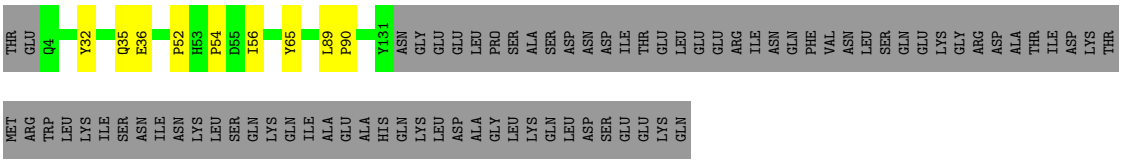
• Molecule 1: DUF1071 domain-containing protein

Chain 4N:



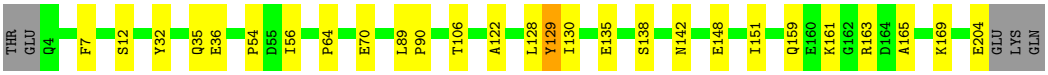
• Molecule 1: DUF1071 domain-containing protein

Chain 4O:



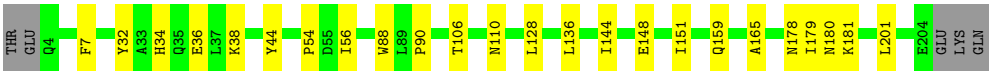
• Molecule 1: DUF1071 domain-containing protein

Chain 4P:



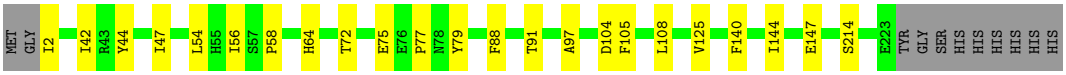
• Molecule 1: DUF1071 domain-containing protein

Chain 4Q:



• Molecule 2: Helix-turn-helix XRE family protein

Chain 2A:



• Molecule 2: Helix-turn-helix XRE family protein

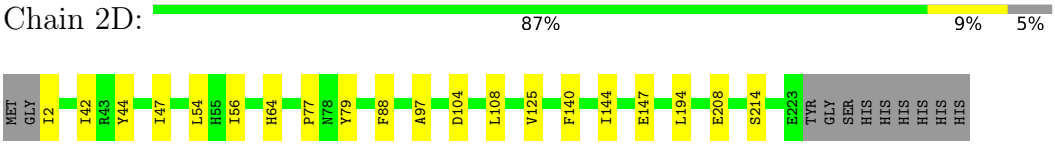
Chain 2B:

• Molecule 2: Helix-turn-helix XRE family protein

Chain 2C:

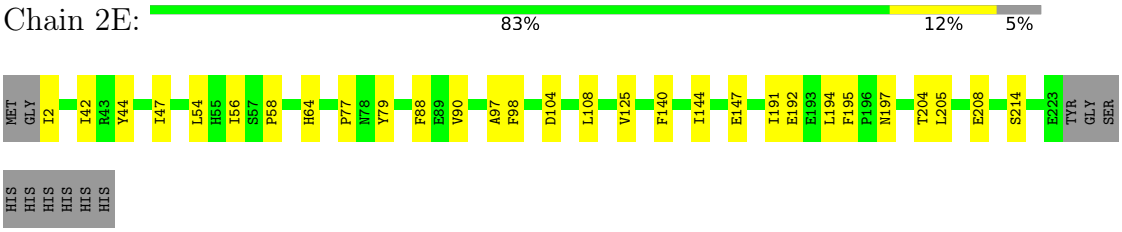
• Molecule 2: Helix-turn-helix XRE family protein

Chain 2D:



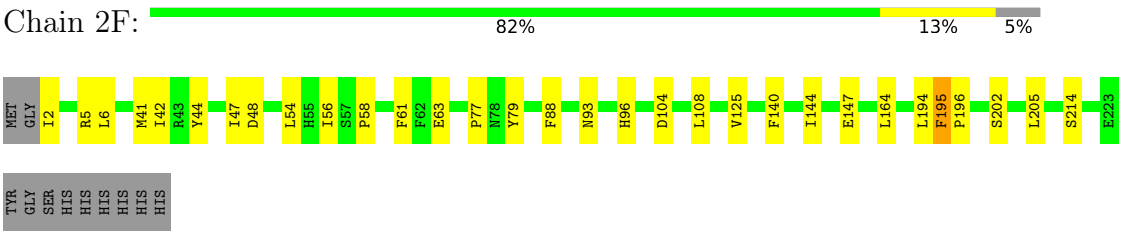
• Molecule 2: Helix-turn-helix XRE family protein

Chain 2E:



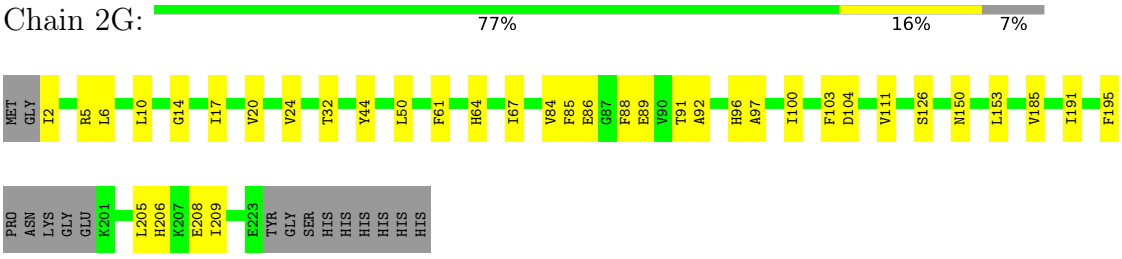
• Molecule 2: Helix-turn-helix XRE family protein

Chain 2F:



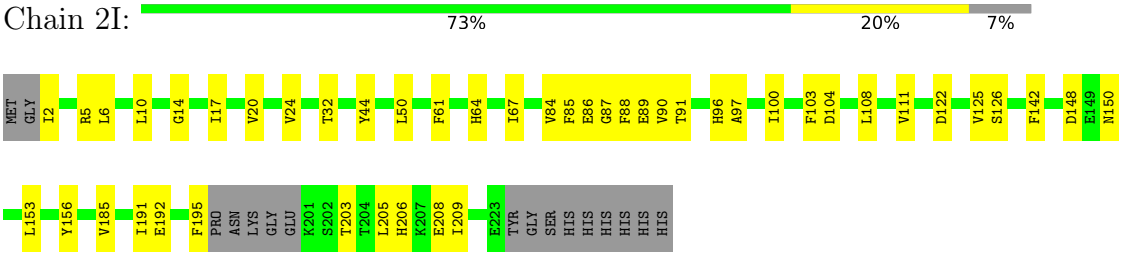
• Molecule 2: Helix-turn-helix XRE family protein

Chain 2G:



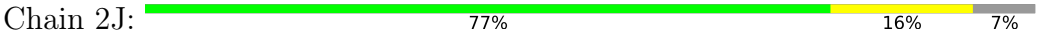
• Molecule 2: Helix-turn-helix XRE family protein

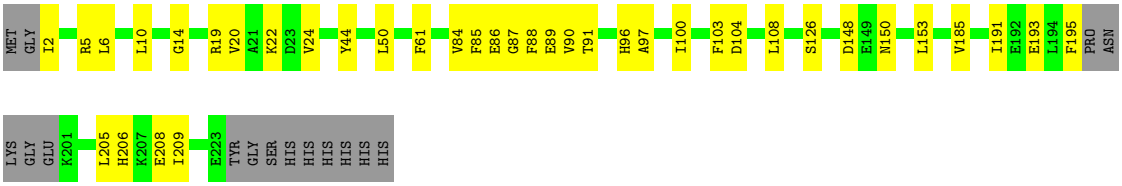
Chain 2I:



• Molecule 2: Helix-turn-helix XRE family protein

Chain 2J:



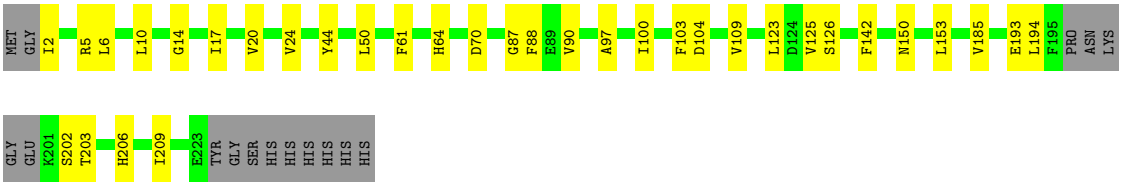


• Molecule 2: Helix-turn-helix XRE family protein

Chain 2L:

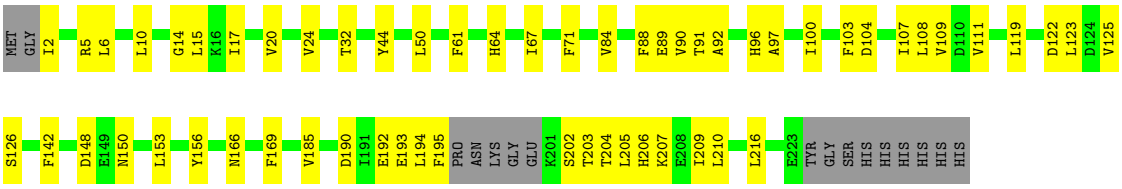
• Molecule 2: Helix-turn-helix XRE family protein

Chain 2M:



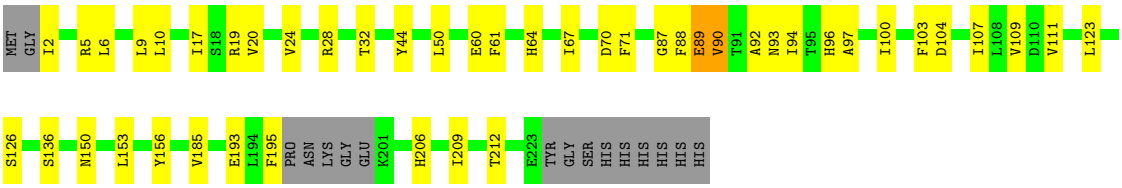
• Molecule 2: Helix-turn-helix XRE family protein

Chain 2N:



• Molecule 2: Helix-turn-helix XRE family protein

Chain 2O:

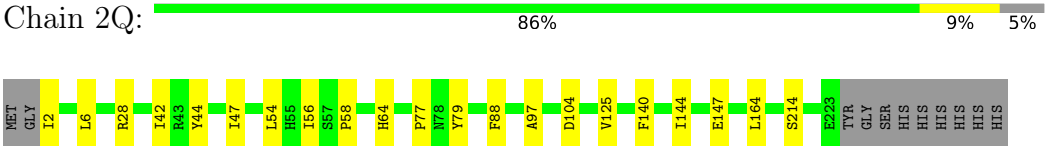


• Molecule 2: Helix-turn-helix XRE family protein

Chain 2P:

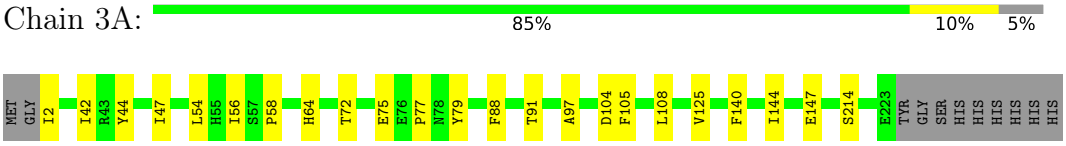
• Molecule 2: Helix-turn-helix XRE family protein

Chain 2Q:



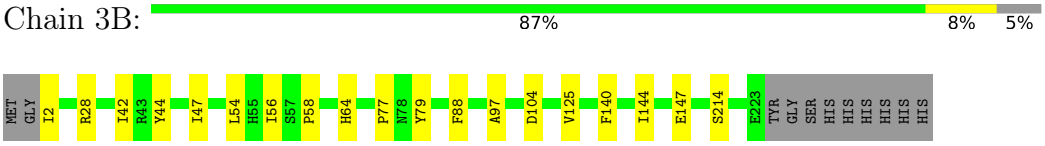
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3A:



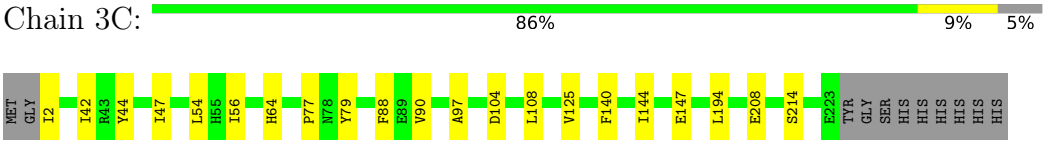
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3B:



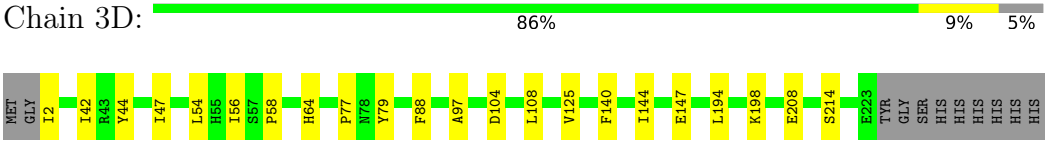
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3C:



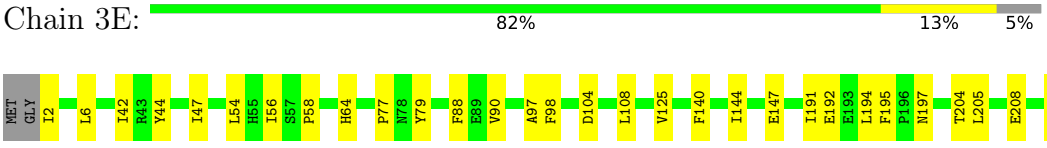
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3D:



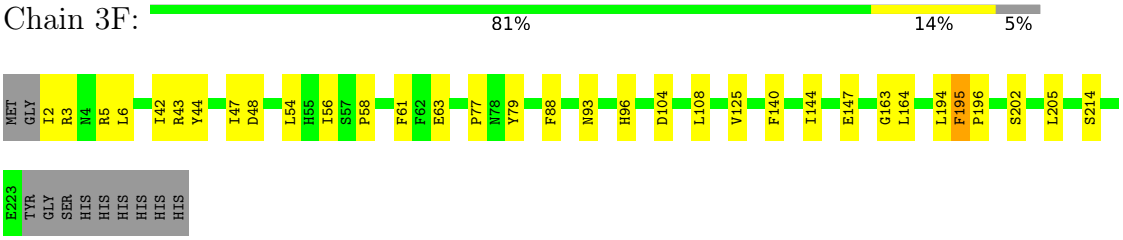
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3E:



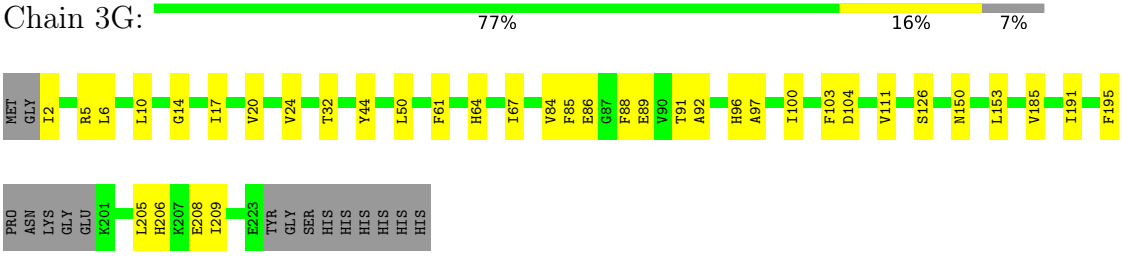
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3F:



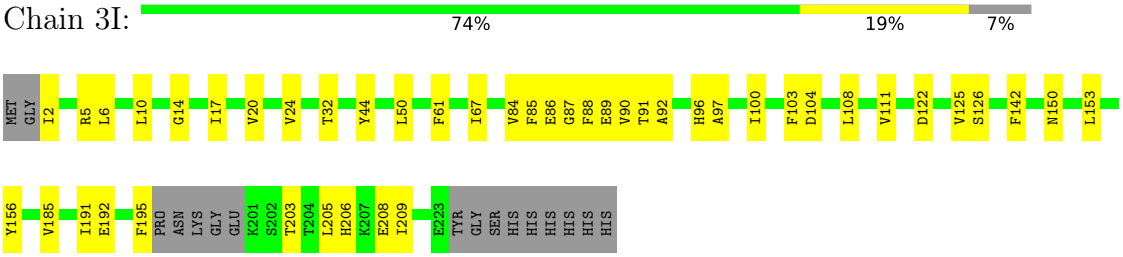
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3G:



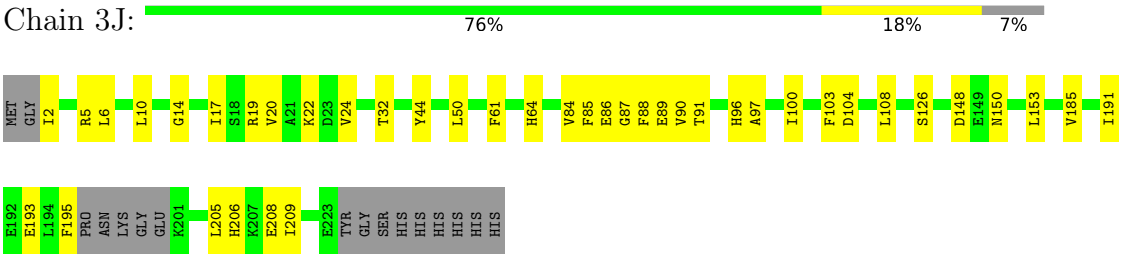
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3I:



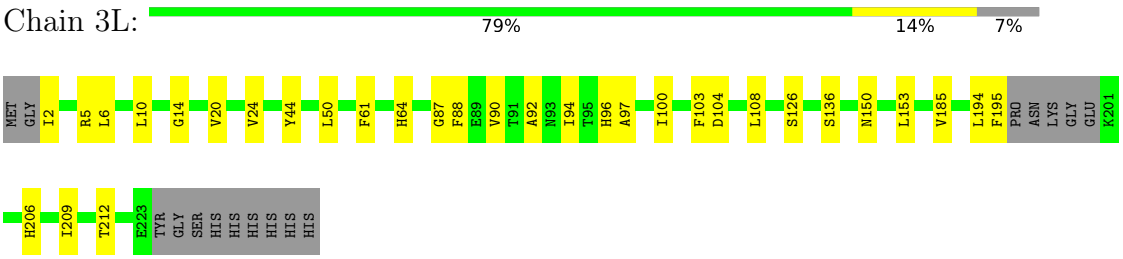
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3J:



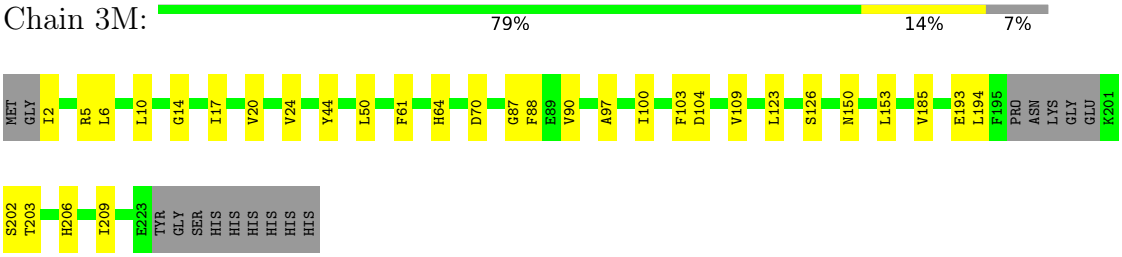
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3L:



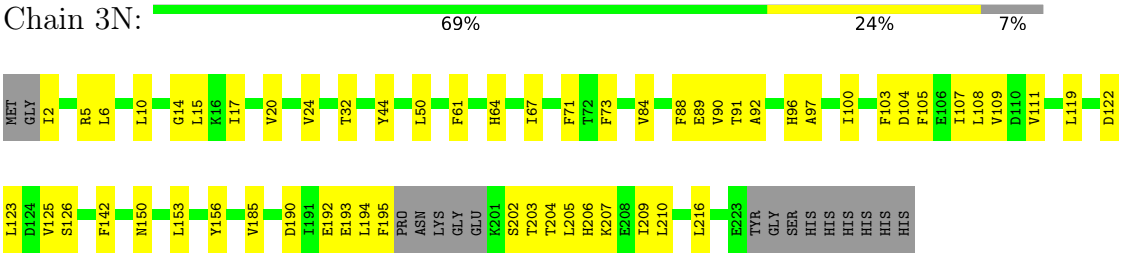
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3M:



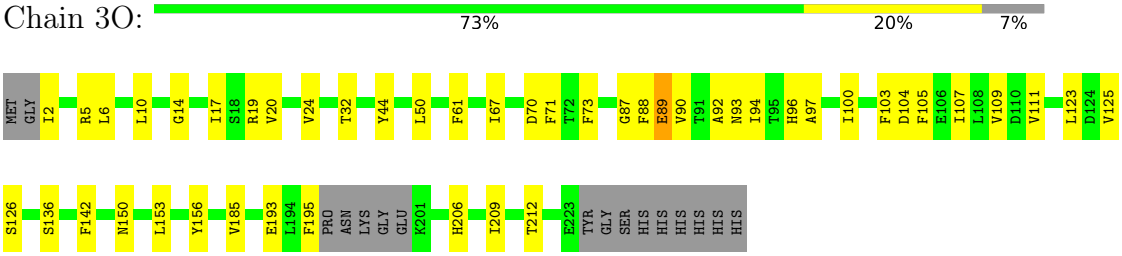
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3N:



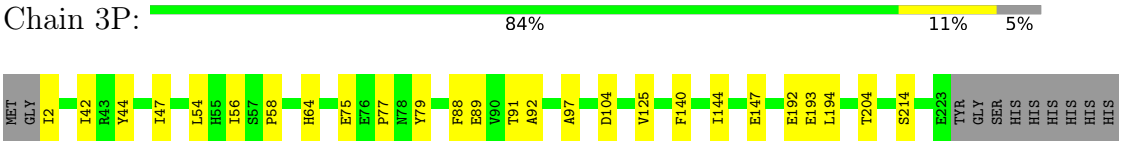
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3O:



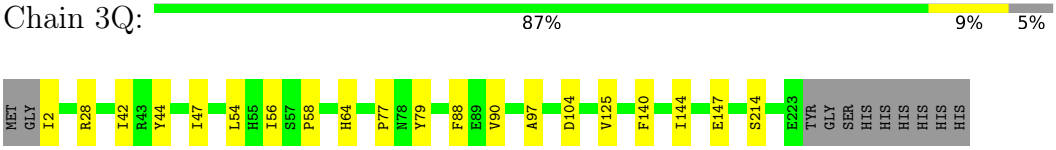
• Molecule 2: Helix-turn-helix XRE family protein

Chain 3P:



• Molecule 2: Helix-turn-helix XRE family protein

Chain 3Q:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208222	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	1A	0.60	0/1658	0.70	0/2246
1	1B	0.60	0/1658	0.69	0/2246
1	1C	0.60	0/1658	0.68	0/2246
1	1D	0.60	0/1658	0.68	0/2246
1	1E	0.60	0/1658	0.67	0/2246
1	1F	0.60	0/1613	0.66	0/2185
1	1G	0.58	0/1072	0.66	0/1459
1	1H	0.58	0/1072	0.65	0/1459
1	1I	0.60	0/1649	0.66	0/2234
1	1J	0.60	0/1649	0.67	0/2234
1	1K	0.59	0/1072	0.67	0/1459
1	1L	0.60	0/1649	0.67	0/2234
1	1M	0.60	0/1649	0.69	0/2234
1	1N	0.60	0/1649	0.67	0/2234
1	1O	0.59	0/1072	0.67	0/1459
1	1P	0.60	0/1658	0.68	0/2246
1	1Q	0.60	0/1658	0.68	0/2246
1	4A	0.60	0/1658	0.70	0/2246
1	4B	0.60	0/1658	0.69	0/2246
1	4C	0.60	0/1658	0.68	0/2246
1	4D	0.60	0/1658	0.68	0/2246
1	4E	0.60	0/1658	0.67	0/2246
1	4F	0.60	0/1613	0.66	0/2185
1	4G	0.58	0/1072	0.66	0/1459
1	4H	0.58	0/1072	0.65	0/1459
1	4I	0.60	0/1649	0.66	0/2234
1	4J	0.60	0/1649	0.67	0/2234
1	4K	0.59	0/1072	0.67	0/1459
1	4L	0.60	0/1649	0.67	0/2234
1	4M	0.60	0/1649	0.69	0/2234
1	4N	0.60	0/1649	0.67	0/2234
1	4O	0.59	0/1072	0.67	0/1459
1	4P	0.60	0/1658	0.68	0/2246
1	4Q	0.60	0/1658	0.68	0/2246

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	2A	0.53	0/1849	0.60	0/2487
2	2B	0.52	0/1849	0.59	0/2487
2	2C	0.52	0/1849	0.59	0/2487
2	2D	0.52	0/1849	0.59	0/2487
2	2E	0.52	0/1849	0.59	0/2487
2	2F	0.53	0/1849	0.59	0/2487
2	2G	0.54	0/1810	0.59	0/2433
2	2I	0.54	0/1810	0.60	0/2433
2	2J	0.54	0/1810	0.59	0/2433
2	2L	0.53	0/1810	0.59	0/2433
2	2M	0.54	0/1810	0.60	0/2433
2	2N	0.54	0/1810	0.60	0/2433
2	2O	0.54	0/1810	0.60	0/2433
2	2P	0.52	0/1849	0.60	0/2487
2	2Q	0.52	0/1849	0.60	0/2487
2	3A	0.53	0/1849	0.60	0/2487
2	3B	0.52	0/1849	0.59	0/2487
2	3C	0.52	0/1849	0.59	0/2487
2	3D	0.52	0/1849	0.59	0/2487
2	3E	0.52	0/1849	0.59	0/2487
2	3F	0.53	0/1849	0.59	0/2487
2	3G	0.54	0/1810	0.59	0/2433
2	3I	0.54	0/1810	0.60	0/2433
2	3J	0.54	0/1810	0.59	0/2433
2	3L	0.53	0/1810	0.59	0/2433
2	3M	0.54	0/1810	0.60	0/2433
2	3N	0.54	0/1810	0.60	0/2433
2	3O	0.54	0/1810	0.59	0/2433
2	3P	0.52	0/1849	0.60	0/2487
2	3Q	0.52	0/1849	0.60	0/2487
All	All	0.56	0/106428	0.63	0/143680

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1A	1624	0	1588	22	0
1	1B	1624	0	1588	18	0
1	1C	1624	0	1588	36	0
1	1D	1624	0	1588	30	0
1	1E	1624	0	1588	35	0
1	1F	1580	0	1542	19	0
1	1G	1043	0	1012	17	0
1	1H	1043	0	1012	26	0
1	1I	1615	0	1582	36	0
1	1J	1615	0	1582	34	0
1	1K	1043	0	1012	16	0
1	1L	1615	0	1582	34	0
1	1M	1615	0	1582	38	0
1	1N	1615	0	1582	47	0
1	1O	1043	0	1012	15	0
1	1P	1624	0	1588	25	0
1	1Q	1624	0	1588	22	0
1	4A	1624	0	1588	22	0
1	4B	1624	0	1588	18	0
1	4C	1624	0	1588	37	0
1	4D	1624	0	1588	32	0
1	4E	1624	0	1588	34	0
1	4F	1580	0	1542	20	0
1	4G	1043	0	1012	17	0
1	4H	1043	0	1012	26	0
1	4I	1615	0	1582	34	0
1	4J	1615	0	1582	35	0
1	4K	1043	0	1012	15	0
1	4L	1615	0	1582	33	0
1	4M	1615	0	1582	45	0
1	4N	1615	0	1582	44	0
1	4O	1043	0	1012	14	0
1	4P	1624	0	1588	22	0
1	4Q	1624	0	1588	24	0
2	2A	1819	0	1797	14	0
2	2B	1819	0	1797	12	0
2	2C	1819	0	1797	14	0
2	2D	1819	0	1797	13	0
2	2E	1819	0	1797	21	0
2	2F	1819	0	1797	24	0
2	2G	1782	0	1761	25	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2I	1782	0	1761	35	0
2	2J	1782	0	1761	31	0
2	2L	1782	0	1761	25	0
2	2M	1782	0	1761	23	0
2	2N	1782	0	1761	44	0
2	2O	1782	0	1761	31	0
2	2P	1819	0	1797	21	0
2	2Q	1819	0	1797	14	0
2	3A	1819	0	1797	15	0
2	3B	1819	0	1797	12	0
2	3C	1819	0	1797	13	0
2	3D	1819	0	1797	15	0
2	3E	1819	0	1797	22	0
2	3F	1819	0	1797	27	0
2	3G	1782	0	1761	25	0
2	3I	1782	0	1761	33	0
2	3J	1782	0	1761	33	0
2	3L	1782	0	1761	22	0
2	3M	1782	0	1761	22	0
2	3N	1782	0	1761	44	0
2	3O	1782	0	1761	29	0
2	3P	1819	0	1797	20	0
2	3Q	1819	0	1797	13	0
All	All	104442	0	102638	1325	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 6.

All (1325) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3N:88:PHE:HB2	2:3N:97:ALA:HB2	1.60	0.83
2:2N:88:PHE:HB2	2:2N:97:ALA:HB2	1.60	0.81
1:1M:200:GLN:HB2	2:2M:90:VAL:HG21	1.63	0.80
2:3M:90:VAL:HG21	1:4M:200:GLN:HB2	1.63	0.79
1:4M:31:SER:O	1:4N:128:LEU:HD21	1.81	0.78
1:1M:34:HIS:HB3	1:1N:128:LEU:HD11	1.66	0.78
1:4M:34:HIS:HB3	1:4N:128:LEU:HD11	1.69	0.74
1:4M:31:SER:O	1:4N:128:LEU:CD2	2.37	0.72
2:2N:190:ASP:HA	2:2N:205:LEU:HB3	1.74	0.70
2:3M:194:LEU:H	2:3M:202:SER:HA	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2M:194:LEU:H	2:2M:202:SER:HA	1.57	0.68
1:4M:154:PHE:HB2	1:4M:198:LEU:HD21	1.76	0.68
1:1M:154:PHE:HB2	1:1M:198:LEU:HD21	1.76	0.68
2:3L:88:PHE:HB2	2:3L:97:ALA:HB2	1.77	0.66
1:4D:141:ASP:HA	1:4D:144:ILE:HG12	1.78	0.66
2:2L:88:PHE:HB2	2:2L:97:ALA:HB2	1.77	0.65
2:3O:88:PHE:HB2	2:3O:97:ALA:HB2	1.77	0.65
2:2O:88:PHE:HB2	2:2O:97:ALA:HB2	1.77	0.65
1:4F:143:ASP:HB3	1:4F:187:ILE:HG21	1.78	0.65
1:1E:141:ASP:HA	1:1E:144:ILE:HG12	1.78	0.65
1:1D:141:ASP:HA	1:1D:144:ILE:HG12	1.78	0.65
2:2I:88:PHE:HB2	2:2I:97:ALA:HB2	1.79	0.65
2:3I:88:PHE:HB2	2:3I:97:ALA:HB2	1.79	0.65
1:1F:143:ASP:HB3	1:1F:187:ILE:HG21	1.78	0.64
2:3N:190:ASP:HA	2:3N:205:LEU:HB3	1.79	0.64
1:1N:56:ILE:HG21	1:1O:54:PRO:HB3	1.79	0.64
1:1N:7:PHE:CE2	1:1N:128:LEU:HD12	2.33	0.64
1:4N:25:LEU:HG	1:4N:140:SER:HB3	1.79	0.64
2:3J:88:PHE:HB2	2:3J:97:ALA:HB2	1.79	0.64
1:4E:141:ASP:HA	1:4E:144:ILE:HG12	1.78	0.64
2:2O:89:GLU:HA	2:2O:193:GLU:HG2	1.80	0.64
1:1F:7:PHE:HZ	1:1F:128:LEU:HD22	1.63	0.64
2:3F:44:TYR:HA	2:3F:47:ILE:HG12	1.80	0.63
1:4F:7:PHE:HZ	1:4F:128:LEU:HD22	1.62	0.63
1:1N:25:LEU:HG	1:1N:140:SER:HB3	1.79	0.63
2:3O:89:GLU:HA	2:3O:193:GLU:HG2	1.80	0.63
1:4N:56:ILE:HG21	1:4O:54:PRO:HB3	1.79	0.63
2:2J:88:PHE:HB2	2:2J:97:ALA:HB2	1.79	0.63
2:2G:88:PHE:HB2	2:2G:97:ALA:HB2	1.79	0.62
1:4N:158:SER:HB3	1:4N:164:ASP:HA	1.82	0.62
2:3G:88:PHE:HB2	2:3G:97:ALA:HB2	1.79	0.62
1:4E:56:ILE:HG21	1:4F:54:PRO:HB3	1.81	0.62
1:1N:158:SER:HB3	1:1N:164:ASP:HA	1.82	0.62
2:3P:194:LEU:HB3	1:4P:169:LYS:HB3	1.82	0.61
1:1C:89:LEU:HD12	1:1C:90:PRO:HD2	1.82	0.61
1:4C:89:LEU:HD12	1:4C:90:PRO:HD2	1.82	0.61
1:1P:169:LYS:HB3	2:2P:194:LEU:HB3	1.82	0.60
1:4B:91:VAL:HG11	1:4B:109:ILE:HD13	1.84	0.60
1:4E:7:PHE:HZ	1:4E:128:LEU:HD22	1.67	0.59
1:1E:7:PHE:HZ	1:1E:128:LEU:HD22	1.67	0.59
1:1J:158:SER:HA	2:2J:195:PHE:HE1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4M:34:HIS:CG	1:4N:128:LEU:HD11	2.38	0.58
2:3J:195:PHE:HE1	1:4J:158:SER:HA	1.67	0.58
1:1N:149:GLU:O	1:1N:153:GLN:HG3	2.03	0.58
1:4L:35:GLN:HB3	1:4M:128:LEU:CD2	2.34	0.58
1:1M:54:PRO:HD2	1:1M:67:ALA:HB3	1.85	0.58
1:4N:149:GLU:O	1:4N:153:GLN:HG3	2.03	0.58
1:1M:194:LEU:O	1:1M:198:LEU:HG	2.04	0.58
1:1L:35:GLN:HB3	1:1M:128:LEU:CD2	2.34	0.58
1:1N:155:VAL:HG21	1:1N:167:ILE:HG12	1.85	0.58
1:4O:56:ILE:HG21	1:4P:54:PRO:HB3	1.85	0.58
1:4N:155:VAL:HG21	1:4N:167:ILE:HG12	1.85	0.58
1:1B:91:VAL:HG11	1:1B:109:ILE:HD13	1.84	0.58
1:1C:56:ILE:HG21	1:1D:54:PRO:HB3	1.86	0.58
1:4A:131:TYR:CD1	1:4A:131:TYR:N	2.72	0.58
1:1O:56:ILE:HG21	1:1P:54:PRO:HB3	1.85	0.57
2:2L:87:GLY:HA3	2:2L:96:HIS:HB3	1.86	0.57
1:1B:105:THR:HB	1:1C:98:SER:CB	2.35	0.57
1:4B:105:THR:HB	1:4C:98:SER:CB	2.35	0.57
1:4C:56:ILE:HG21	1:4D:54:PRO:HB3	1.86	0.57
1:4H:22:LYS:HB2	1:4H:27:TYR:HE2	1.69	0.57
1:1H:38:LYS:HG3	1:1I:7:PHE:CD2	2.40	0.57
1:1I:105:THR:HB	1:1J:98:SER:CB	2.35	0.57
2:3L:87:GLY:HA3	2:3L:96:HIS:HB3	1.86	0.57
1:4M:194:LEU:O	1:4M:198:LEU:HG	2.04	0.57
2:3F:5:ARG:HD2	2:3F:63:GLU:HB2	1.86	0.57
1:1H:22:LYS:HB2	1:1H:27:TYR:HE2	1.69	0.56
1:1N:7:PHE:CZ	1:1N:128:LEU:HD12	2.40	0.56
1:1A:131:TYR:N	1:1A:131:TYR:CD1	2.72	0.56
2:2E:88:PHE:HB3	2:2E:191:ILE:HG21	1.87	0.56
2:3E:88:PHE:HB3	2:3E:191:ILE:HG21	1.87	0.56
2:3F:47:ILE:HG22	2:3F:61:PHE:HE2	1.69	0.56
1:4E:137:PRO:HG3	1:4E:183:SER:HB3	1.87	0.56
1:4H:38:LYS:HG3	1:4I:7:PHE:CD2	2.40	0.56
1:4I:136:LEU:HB3	1:4I:137:PRO:HD3	1.86	0.56
1:1J:64:PRO:HB3	1:1K:88:TRP:CZ2	2.41	0.56
1:1N:60:ASN:CB	1:1O:52:PRO:HG2	2.36	0.56
1:4M:54:PRO:HD2	1:4M:67:ALA:HB3	1.85	0.56
1:4N:154:PHE:HD1	1:4N:198:LEU:HB2	1.70	0.56
1:1E:137:PRO:HG3	1:1E:183:SER:HB3	1.87	0.56
1:4D:64:PRO:HB3	1:4E:88:TRP:CZ2	2.41	0.56
1:4I:105:THR:HB	1:4J:98:SER:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4N:60:ASN:CB	1:4O:52:PRO:HG2	2.36	0.56
1:1I:136:LEU:HB3	1:1I:137:PRO:HD3	1.86	0.56
1:4J:64:PRO:HB3	1:4K:88:TRP:CZ2	2.41	0.56
1:1D:64:PRO:HB3	1:1E:88:TRP:CZ2	2.41	0.56
1:1L:112:ALA:HA	1:1L:115:ARG:HE	1.71	0.56
2:2O:104:ASP:HA	2:2O:126:SER:HA	1.88	0.55
2:3O:107:ILE:HB	2:3O:123:LEU:HD11	1.88	0.55
1:4Q:136:LEU:HD12	1:4Q:181:LYS:HB2	1.88	0.55
1:1N:154:PHE:HD1	1:1N:198:LEU:HB2	1.70	0.55
2:3L:104:ASP:HA	2:3L:126:SER:HA	1.89	0.55
1:4M:34:HIS:CB	1:4N:128:LEU:HD11	2.36	0.55
2:3N:104:ASP:HA	2:3N:126:SER:HA	1.89	0.55
2:3I:104:ASP:HA	2:3I:126:SER:HA	1.89	0.55
2:3M:90:VAL:HG21	1:4M:200:GLN:CB	2.36	0.55
1:1P:56:ILE:HG21	1:1Q:54:PRO:HB3	1.89	0.55
1:4J:127:GLY:O	1:4J:130:ILE:HG22	2.06	0.55
2:2I:104:ASP:HA	2:2I:126:SER:HA	1.89	0.55
1:4F:36:GLU:O	1:4F:40:ILE:HG12	2.07	0.55
1:4N:106:THR:HG23	1:4O:90:PRO:HB2	1.89	0.55
1:4P:56:ILE:HG21	1:4Q:54:PRO:HB3	1.89	0.55
2:3G:104:ASP:HA	2:3G:126:SER:HA	1.89	0.55
1:4A:144:ILE:HG23	1:4A:179:ILE:HG12	1.89	0.55
1:4F:35:GLN:HB3	1:4G:128:LEU:CD2	2.37	0.55
1:4L:112:ALA:HA	1:4L:115:ARG:HE	1.71	0.55
1:4Q:144:ILE:HG23	1:4Q:179:ILE:HG12	1.89	0.55
2:2O:111:VAL:HG21	2:2O:156:TYR:CG	2.41	0.55
2:3J:104:ASP:HA	2:3J:126:SER:HA	1.89	0.55
2:3O:104:ASP:HA	2:3O:126:SER:HA	1.89	0.55
1:4C:91:VAL:HG11	1:4C:109:ILE:HD13	1.89	0.55
2:2P:192:GLU:HA	2:2P:204:THR:HA	1.89	0.55
1:1J:127:GLY:O	1:1J:130:ILE:HG22	2.06	0.54
1:1N:106:THR:HG23	1:1O:90:PRO:HB2	1.89	0.54
2:2F:2:ILE:HG22	2:3F:48:ASP:HB2	1.89	0.54
1:1F:35:GLN:HB3	1:1G:128:LEU:CD2	2.37	0.54
2:3J:90:VAL:HG11	1:4J:200:GLN:HB2	1.89	0.54
2:3M:104:ASP:HA	2:3M:126:SER:HA	1.88	0.54
1:1A:144:ILE:HD13	1:1A:179:ILE:O	2.08	0.54
1:4A:144:ILE:HD13	1:4A:179:ILE:O	2.08	0.54
2:2F:5:ARG:HD2	2:2F:63:GLU:HB2	1.89	0.54
2:2N:104:ASP:HA	2:2N:126:SER:HA	1.89	0.54
1:1B:141:ASP:HA	1:1B:144:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:144:ILE:HG23	1:1A:179:ILE:HG12	1.89	0.54
1:4A:131:TYR:HD1	1:4A:131:TYR:H	1.56	0.54
1:4E:56:ILE:CG2	1:4F:54:PRO:HB3	2.37	0.54
1:4H:56:ILE:HG21	1:4I:54:PRO:HB3	1.90	0.54
1:1E:7:PHE:HE1	1:1E:11:ASN:HD22	1.55	0.54
1:1F:172:ARG:HD2	2:2F:194:LEU:HD11	1.90	0.54
1:1J:200:GLN:HB2	2:2J:90:VAL:HG11	1.89	0.54
2:2F:2:ILE:HG21	2:3F:47:ILE:HG13	1.90	0.54
1:4E:7:PHE:HE1	1:4E:11:ASN:HD22	1.55	0.54
1:1H:30:TRP:HE1	1:1I:135:GLU:HB3	1.73	0.54
1:1J:31:SER:O	1:1K:128:LEU:HD21	2.08	0.54
1:1M:200:GLN:CB	2:2M:90:VAL:HG21	2.36	0.54
2:3P:192:GLU:HA	2:3P:204:THR:HA	1.89	0.54
2:2G:104:ASP:HA	2:2G:126:SER:HA	1.89	0.54
2:2J:104:ASP:HA	2:2J:126:SER:HA	1.89	0.54
1:4H:30:TRP:HE1	1:4I:135:GLU:HB3	1.73	0.54
2:3F:194:LEU:HD11	1:4F:172:ARG:HD2	1.90	0.53
2:3O:71:PHE:HD1	2:3O:109:VAL:HG22	1.73	0.53
1:1Q:144:ILE:HD13	1:1Q:179:ILE:O	2.08	0.53
1:1Q:144:ILE:HG23	1:1Q:179:ILE:HG12	1.89	0.53
2:2M:104:ASP:HA	2:2M:126:SER:HA	1.88	0.53
2:2E:98:PHE:CE2	2:2E:205:LEU:HD21	2.44	0.53
2:2L:104:ASP:HA	2:2L:126:SER:HA	1.89	0.53
2:2O:6:LEU:O	2:2O:10:LEU:HG	2.08	0.53
2:3E:98:PHE:HE2	2:3E:205:LEU:HD21	1.74	0.53
1:4G:10:LEU:HD21	1:4G:40:ILE:HG13	1.90	0.53
1:1I:56:ILE:HG21	1:1J:54:PRO:HB3	1.91	0.53
2:2E:98:PHE:HE2	2:2E:205:LEU:HD21	1.74	0.53
2:2O:5:ARG:HD2	2:2O:60:GLU:O	2.08	0.53
1:1C:91:VAL:HG11	1:1C:109:ILE:HD13	1.89	0.53
1:1I:149:GLU:O	1:1I:153:GLN:HG3	2.09	0.53
2:3N:125:VAL:HB	2:3N:142:PHE:HB3	1.91	0.53
1:4C:7:PHE:HZ	1:4C:128:LEU:HD22	1.74	0.53
1:4Q:144:ILE:HD13	1:4Q:179:ILE:O	2.08	0.53
2:2N:89:GLU:HG2	2:2N:194:LEU:HD23	1.91	0.53
2:2N:111:VAL:HG21	2:2N:156:TYR:CG	2.44	0.53
2:3N:111:VAL:HG21	2:3N:156:TYR:CG	2.44	0.53
1:4D:122:ALA:HA	1:4D:126:LEU:O	2.09	0.53
1:1J:158:SER:HA	2:2J:195:PHE:CE1	2.44	0.53
2:3E:98:PHE:CE2	2:3E:205:LEU:HD21	2.44	0.53
2:3F:44:TYR:HD1	2:3F:47:ILE:HD11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4B:56:ILE:HG21	1:4C:54:PRO:HB3	1.91	0.53
1:4B:141:ASP:HA	1:4B:144:ILE:HG12	1.89	0.53
1:4I:56:ILE:HG21	1:4J:54:PRO:HB3	1.90	0.53
1:4P:122:ALA:O	1:4P:128:LEU:HB2	2.09	0.53
1:1G:10:LEU:HD21	1:1G:40:ILE:HG13	1.90	0.53
1:1Q:136:LEU:HD12	1:1Q:181:LYS:HB2	1.90	0.53
2:3J:195:PHE:CE1	1:4J:158:SER:HA	2.44	0.53
2:3N:89:GLU:HG2	2:3N:194:LEU:HD23	1.91	0.53
1:4J:149:GLU:O	1:4J:153:GLN:HG3	2.09	0.53
1:1H:56:ILE:HG21	1:1I:54:PRO:HB3	1.90	0.52
1:1J:149:GLU:O	1:1J:153:GLN:HG3	2.09	0.52
1:1N:200:GLN:HB2	2:2N:90:VAL:HG11	1.92	0.52
2:2N:206:HIS:O	2:2N:210:LEU:HG	2.10	0.52
1:1G:105:THR:HB	1:1H:98:SER:CB	2.39	0.52
2:2M:87:GLY:HA2	2:2M:90:VAL:HG12	1.91	0.52
2:3N:90:VAL:HG11	1:4N:200:GLN:HB2	1.92	0.52
2:3O:2:ILE:HD12	2:3O:2:ILE:O	2.10	0.52
1:4G:35:GLN:O	1:4G:39:LYS:HG3	2.10	0.52
1:4N:152:ASN:O	1:4N:156:ASN:N	2.40	0.52
1:1A:131:TYR:HD1	1:1A:131:TYR:H	1.56	0.52
1:1A:161:LYS:HE2	1:1A:204:GLU:HG2	1.91	0.52
1:1B:56:ILE:HG21	1:1C:54:PRO:HB3	1.91	0.52
1:1C:7:PHE:HZ	1:1C:128:LEU:HD22	1.74	0.52
2:3J:2:ILE:HD12	2:3J:2:ILE:O	2.10	0.52
1:4G:105:THR:HB	1:4H:98:SER:CB	2.39	0.52
1:4I:149:GLU:O	1:4I:153:GLN:HG3	2.09	0.52
1:1C:158:SER:HB3	1:1C:163:ARG:HB2	1.92	0.52
1:1F:159:GLN:HB2	2:2F:195:PHE:HZ	1.74	0.52
1:1L:61:TYR:OH	1:1M:68:THR:HG22	2.10	0.52
1:1L:163:ARG:HB3	2:2L:195:PHE:HB3	1.91	0.52
2:2N:2:ILE:HD12	2:2N:2:ILE:O	2.10	0.52
2:3A:91:THR:HA	1:4A:163:ARG:HH22	1.75	0.52
1:4J:31:SER:O	1:4K:128:LEU:HD21	2.08	0.52
1:1D:122:ALA:HA	1:1D:126:LEU:O	2.09	0.52
1:1N:152:ASN:O	1:1N:156:ASN:N	2.40	0.52
2:2G:2:ILE:HD12	2:2G:2:ILE:O	2.10	0.52
2:2J:89:GLU:HA	2:2J:193:GLU:HG2	1.92	0.52
2:2M:2:ILE:O	2:2M:2:ILE:HD12	2.09	0.52
2:2N:125:VAL:HB	2:2N:142:PHE:HB3	1.91	0.52
2:3G:20:VAL:O	2:3G:24:VAL:HG22	2.10	0.52
2:3N:67:ILE:HD11	2:3N:111:VAL:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4C:158:SER:HB3	1:4C:163:ARG:HB2	1.92	0.52
1:1G:35:GLN:O	1:1G:39:LYS:HG3	2.10	0.52
2:2N:193:GLU:O	2:2N:202:SER:HA	2.10	0.52
2:3I:2:ILE:HD12	2:3I:2:ILE:O	2.10	0.52
1:4L:61:TYR:OH	1:4M:68:THR:HG22	2.10	0.52
2:3I:203:THR:HG23	1:4I:163:ARG:HH12	1.74	0.52
2:3J:89:GLU:HA	2:3J:193:GLU:HG2	1.92	0.52
2:3N:2:ILE:HD12	2:3N:2:ILE:O	2.10	0.52
1:1A:163:ARG:HH22	2:2A:91:THR:HA	1.75	0.52
1:1E:167:ILE:HA	1:1E:170:THR:HG22	1.92	0.52
2:2N:20:VAL:O	2:2N:24:VAL:HG22	2.10	0.52
2:3F:195:PHE:HZ	1:4F:159:GLN:HB2	1.75	0.52
2:3J:89:GLU:HG3	1:4J:173:TRP:CZ2	2.45	0.52
2:2J:2:ILE:HD12	2:2J:2:ILE:O	2.10	0.52
2:3G:2:ILE:O	2:3G:2:ILE:HD12	2.10	0.52
2:3N:20:VAL:O	2:3N:24:VAL:HG22	2.10	0.52
2:3N:206:HIS:O	2:3N:210:LEU:HG	2.10	0.52
2:3P:140:PHE:HB2	2:3P:214:SER:HB3	1.92	0.52
1:1E:89:LEU:HD22	1:1E:112:ALA:HB1	1.92	0.52
1:1P:163:ARG:HH22	2:2P:91:THR:HA	1.75	0.52
2:2L:2:ILE:HD12	2:2L:2:ILE:O	2.10	0.52
2:2L:20:VAL:O	2:2L:24:VAL:HG22	2.10	0.52
2:2M:20:VAL:O	2:2M:24:VAL:HG22	2.10	0.52
2:3M:87:GLY:HA2	2:3M:90:VAL:HG12	1.91	0.52
2:3P:91:THR:HA	1:4P:163:ARG:HH22	1.75	0.52
1:4A:161:LYS:HE2	1:4A:204:GLU:HG2	1.91	0.52
1:4D:89:LEU:HD22	1:4D:112:ALA:HB1	1.92	0.52
1:4E:89:LEU:HD22	1:4E:112:ALA:HB1	1.92	0.52
1:4E:167:ILE:HA	1:4E:170:THR:HG22	1.92	0.52
1:4H:94:PHE:HE2	1:4I:144:ILE:HG13	1.74	0.52
2:2I:2:ILE:O	2:2I:2:ILE:HD12	2.09	0.51
2:2I:20:VAL:O	2:2I:24:VAL:HG22	2.10	0.51
2:2N:89:GLU:HA	2:2N:193:GLU:HA	1.92	0.51
2:3G:191:ILE:H	2:3G:205:LEU:HB3	1.75	0.51
2:3L:2:ILE:O	2:3L:2:ILE:HD12	2.10	0.51
2:3M:2:ILE:HD12	2:3M:2:ILE:O	2.09	0.51
1:4K:56:ILE:HG21	1:4L:54:PRO:HB3	1.92	0.51
1:4M:31:SER:HA	1:4N:128:LEU:HD21	1.91	0.51
1:4N:131:TYR:HB3	1:4N:134:GLU:OE2	2.11	0.51
1:1B:32:TYR:O	1:1B:35:GLN:HG2	2.10	0.51
1:1C:64:PRO:HB3	1:1D:88:TRP:CZ2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1H:64:PRO:HB3	1:1I:88:TRP:CZ2	2.45	0.51
1:1I:163:ARG:HH12	2:2I:203:THR:HG23	1.74	0.51
1:1N:11:ASN:HA	1:1N:125:GLY:O	2.10	0.51
1:1N:174:LEU:HD11	1:1N:194:LEU:CD2	2.40	0.51
2:2B:140:PHE:HB2	2:2B:214:SER:HB3	1.92	0.51
2:3E:195:PHE:HE1	1:4E:169:LYS:HB2	1.75	0.51
2:3I:185:VAL:HA	2:3I:209:ILE:HD13	1.93	0.51
1:4K:64:PRO:HB3	1:4L:88:TRP:CZ2	2.46	0.51
2:3B:140:PHE:HB2	2:3B:214:SER:HB3	1.92	0.51
2:3F:140:PHE:HB2	2:3F:214:SER:HB3	1.93	0.51
2:3J:185:VAL:HA	2:3J:209:ILE:HD13	1.93	0.51
2:3M:20:VAL:O	2:3M:24:VAL:HG22	2.10	0.51
2:3M:88:PHE:HB2	2:3M:97:ALA:HB2	1.93	0.51
2:3N:193:GLU:O	2:3N:202:SER:HA	2.10	0.51
1:4D:158:SER:HB3	1:4D:163:ARG:HB2	1.92	0.51
1:1H:15:VAL:HG12	1:1H:32:TYR:CE1	2.46	0.51
1:1H:94:PHE:HE2	1:1I:144:ILE:HG13	1.74	0.51
1:1P:122:ALA:O	1:1P:128:LEU:HB2	2.09	0.51
2:2E:140:PHE:HB2	2:2E:214:SER:HB3	1.93	0.51
2:2I:87:GLY:O	2:2I:90:VAL:HG22	2.11	0.51
2:2I:191:ILE:H	2:2I:205:LEU:HB3	1.75	0.51
2:2N:67:ILE:HD11	2:2N:111:VAL:CG2	2.40	0.51
2:2P:140:PHE:HB2	2:2P:214:SER:HB3	1.92	0.51
2:3L:20:VAL:O	2:3L:24:VAL:HG22	2.10	0.51
2:3M:185:VAL:HA	2:3M:209:ILE:HD13	1.93	0.51
1:4H:61:TYR:OH	1:4I:68:THR:HG22	2.11	0.51
1:1I:88:TRP:O	1:1I:89:LEU:HD23	2.11	0.51
1:1N:131:TYR:HB3	1:1N:134:GLU:OE2	2.11	0.51
2:2C:2:ILE:HG13	2:2C:64:HIS:HB2	1.93	0.51
2:2G:20:VAL:O	2:2G:24:VAL:HG22	2.10	0.51
2:3J:85:PHE:HD1	2:3J:191:ILE:HD11	1.76	0.51
2:3J:87:GLY:O	2:3J:90:VAL:HG22	2.11	0.51
2:3L:185:VAL:HA	2:3L:209:ILE:HD13	1.93	0.51
2:3L:195:PHE:HB3	1:4L:163:ARG:HB3	1.91	0.51
2:3N:89:GLU:HA	2:3N:193:GLU:HA	1.92	0.51
1:1C:170:THR:O	1:1C:174:LEU:HD22	2.11	0.51
1:1L:154:PHE:CE2	2:2L:194:LEU:HD12	2.46	0.51
2:3A:2:ILE:HG13	2:3A:64:HIS:HB2	1.93	0.51
2:3I:85:PHE:HD1	2:3I:191:ILE:HD11	1.76	0.51
1:4H:64:PRO:HB3	1:4I:88:TRP:CZ2	2.45	0.51
1:4N:174:LEU:HD11	1:4N:194:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2G:191:ILE:H	2:2G:205:LEU:HB3	1.75	0.51
2:3I:20:VAL:O	2:3I:24:VAL:HG22	2.10	0.51
2:3J:191:ILE:H	2:3J:205:LEU:HB3	1.75	0.51
1:4C:158:SER:HB2	1:4C:165:ALA:HB2	1.92	0.51
1:4I:88:TRP:O	1:4I:89:LEU:HD23	2.11	0.51
1:1B:105:THR:HB	1:1C:98:SER:HB2	1.93	0.51
2:2E:2:ILE:HG13	2:2E:64:HIS:HB2	1.93	0.51
2:3N:185:VAL:HA	2:3N:209:ILE:HD13	1.93	0.51
1:1D:89:LEU:HD22	1:1D:112:ALA:HB1	1.92	0.51
1:1F:35:GLN:HB3	1:1G:128:LEU:HD23	1.93	0.51
1:1K:56:ILE:HG21	1:1L:54:PRO:HB3	1.92	0.51
2:2D:104:ASP:HA	2:2D:125:VAL:O	2.11	0.51
2:2J:20:VAL:O	2:2J:24:VAL:HG22	2.11	0.51
2:3C:140:PHE:HB2	2:3C:214:SER:HB3	1.92	0.51
2:3N:195:PHE:CD1	1:4N:163:ARG:HG2	2.46	0.51
2:3P:88:PHE:CD1	2:3P:97:ALA:HB2	2.46	0.51
1:4C:64:PRO:HB3	1:4D:88:TRP:CZ2	2.45	0.51
1:1B:158:SER:HB3	1:1B:163:ARG:HB2	1.93	0.51
1:1E:169:LYS:HB2	2:2E:195:PHE:HE1	1.75	0.51
1:1H:61:TYR:OH	1:1I:68:THR:HG22	2.11	0.51
1:1J:173:TRP:CZ2	2:2J:89:GLU:HG3	2.45	0.51
1:1N:163:ARG:HG2	2:2N:195:PHE:CD1	2.46	0.51
2:2A:88:PHE:CD1	2:2A:97:ALA:HB2	2.46	0.51
2:2A:104:ASP:HA	2:2A:125:VAL:O	2.11	0.51
2:2A:140:PHE:HB2	2:2A:214:SER:HB3	1.92	0.51
2:2F:47:ILE:HG22	2:2F:61:PHE:HE2	1.76	0.51
2:2O:2:ILE:HD12	2:2O:2:ILE:O	2.10	0.51
2:2O:185:VAL:HA	2:2O:209:ILE:HD13	1.93	0.51
2:2P:88:PHE:CD1	2:2P:97:ALA:HB2	2.46	0.51
2:3D:88:PHE:CD1	2:3D:97:ALA:HB2	2.46	0.51
2:3E:104:ASP:HA	2:3E:125:VAL:O	2.11	0.51
2:3F:104:ASP:HA	2:3F:125:VAL:O	2.11	0.51
2:3G:85:PHE:HD1	2:3G:191:ILE:HD11	1.76	0.51
2:3J:20:VAL:O	2:3J:24:VAL:HG22	2.11	0.51
2:3O:185:VAL:HA	2:3O:209:ILE:HD13	1.93	0.51
1:4H:15:VAL:HG12	1:4H:32:TYR:CE1	2.46	0.51
2:2Q:2:ILE:HG13	2:2Q:64:HIS:HB2	1.93	0.50
2:3B:104:ASP:HA	2:3B:125:VAL:O	2.11	0.50
2:3C:2:ILE:HG13	2:3C:64:HIS:HB2	1.93	0.50
1:4H:72:TYR:HB2	1:4H:91:VAL:HB	1.93	0.50
1:1D:158:SER:HB3	1:1D:163:ARG:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2E:104:ASP:HA	2:2E:125:VAL:O	2.11	0.50
2:2P:2:ILE:HG13	2:2P:64:HIS:HB2	1.93	0.50
2:2Q:104:ASP:HA	2:2Q:125:VAL:O	2.11	0.50
2:3O:111:VAL:HG21	2:3O:156:TYR:CG	2.46	0.50
2:3Q:140:PHE:HB2	2:3Q:214:SER:HB3	1.92	0.50
1:4D:170:THR:O	1:4D:174:LEU:HD22	2.11	0.50
1:4I:184:GLN:HA	1:4I:187:ILE:HG22	1.94	0.50
1:4J:89:LEU:C	1:4J:89:LEU:HD23	2.32	0.50
1:1H:72:TYR:HB2	1:1H:91:VAL:HB	1.93	0.50
1:1J:89:LEU:HD23	1:1J:89:LEU:C	2.32	0.50
1:1K:64:PRO:HB3	1:1L:88:TRP:CZ2	2.46	0.50
2:2C:88:PHE:CD1	2:2C:97:ALA:HB2	2.46	0.50
2:2C:104:ASP:HA	2:2C:125:VAL:O	2.11	0.50
2:2D:2:ILE:HG13	2:2D:64:HIS:HB2	1.93	0.50
2:2F:42:ILE:HD12	2:3F:44:TYR:OH	2.12	0.50
2:2G:85:PHE:HD1	2:2G:191:ILE:HD11	1.76	0.50
2:2J:191:ILE:H	2:2J:205:LEU:HB3	1.75	0.50
2:2Q:88:PHE:CD1	2:2Q:97:ALA:HB2	2.46	0.50
2:3C:88:PHE:CD1	2:3C:97:ALA:HB2	2.46	0.50
2:3F:196:PRO:HA	2:3F:202:SER:HA	1.92	0.50
2:3I:87:GLY:O	2:3I:90:VAL:HG22	2.11	0.50
2:3I:191:ILE:H	2:3I:205:LEU:HB3	1.75	0.50
1:4C:170:THR:O	1:4C:174:LEU:HD22	2.11	0.50
1:4G:35:GLN:HB3	1:4H:128:LEU:CD2	2.41	0.50
1:1C:158:SER:HB2	1:1C:165:ALA:HB2	1.92	0.50
1:1L:38:LYS:HG3	1:1M:7:PHE:CD2	2.47	0.50
2:2I:185:VAL:HA	2:2I:209:ILE:HD13	1.93	0.50
2:3D:104:ASP:HA	2:3D:125:VAL:O	2.11	0.50
2:3E:88:PHE:CD1	2:3E:97:ALA:HB2	2.46	0.50
2:3P:104:ASP:HA	2:3P:125:VAL:O	2.12	0.50
1:4J:122:ALA:HA	1:4J:126:LEU:O	2.12	0.50
1:4K:105:THR:HB	1:4L:98:SER:CB	2.42	0.50
1:4P:12:SER:HA	1:4P:138:SER:HB2	1.93	0.50
1:1D:170:THR:O	1:1D:174:LEU:HD22	2.11	0.50
1:1H:56:ILE:CG2	1:1I:54:PRO:HB3	2.42	0.50
1:1N:174:LEU:HD11	1:1N:194:LEU:HD22	1.93	0.50
2:2F:104:ASP:HA	2:2F:125:VAL:O	2.11	0.50
2:2M:88:PHE:HB2	2:2M:97:ALA:HB2	1.93	0.50
2:2M:123:LEU:HD12	2:2M:123:LEU:O	2.11	0.50
2:3A:140:PHE:HB2	2:3A:214:SER:HB3	1.93	0.50
2:2A:2:ILE:HG13	2:2A:64:HIS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2C:140:PHE:HB2	2:2C:214:SER:HB3	1.93	0.50
2:2D:88:PHE:CD1	2:2D:97:ALA:HB2	2.46	0.50
2:2E:88:PHE:CD1	2:2E:97:ALA:HB2	2.46	0.50
2:2J:85:PHE:HD1	2:2J:191:ILE:HD11	1.76	0.50
2:2J:87:GLY:O	2:2J:90:VAL:HG22	2.11	0.50
2:2N:185:VAL:HA	2:2N:209:ILE:HD13	1.93	0.50
2:2O:17:ILE:HD12	2:2O:32:THR:HB	1.92	0.50
2:3L:194:LEU:HD12	1:4L:154:PHE:CE2	2.46	0.50
2:3P:2:ILE:HG13	2:3P:64:HIS:HB2	1.93	0.50
1:4F:32:TYR:O	1:4F:35:GLN:HG2	2.10	0.50
1:4N:11:ASN:HA	1:4N:125:GLY:O	2.11	0.50
1:1C:140:SER:O	1:1C:144:ILE:HG12	2.12	0.50
1:1I:184:GLN:HA	1:1I:187:ILE:HG22	1.94	0.50
2:2I:85:PHE:HD1	2:2I:191:ILE:HD11	1.76	0.50
2:3A:104:ASP:HA	2:3A:125:VAL:O	2.11	0.50
2:3M:123:LEU:HD12	2:3M:123:LEU:O	2.11	0.50
1:4B:32:TYR:O	1:4B:35:GLN:HG2	2.10	0.50
1:1E:30:TRP:HZ3	1:1F:123:LEU:CD2	2.25	0.50
1:1E:137:PRO:CG	1:1E:183:SER:HB3	2.42	0.50
1:1G:35:GLN:HB3	1:1H:128:LEU:CD2	2.41	0.50
2:2N:122:ASP:OD2	2:2O:19:ARG:HB2	2.12	0.50
2:3D:88:PHE:HZ	2:3D:208:GLU:HG3	1.77	0.50
1:4B:158:SER:HB3	1:4B:163:ARG:HB2	1.93	0.50
1:4J:38:LYS:HG3	1:4K:7:PHE:CD2	2.47	0.50
1:4N:174:LEU:HD11	1:4N:194:LEU:HD22	1.93	0.50
2:2B:88:PHE:CD1	2:2B:97:ALA:HB2	2.46	0.50
2:2B:104:ASP:HA	2:2B:125:VAL:O	2.11	0.50
2:2E:88:PHE:HZ	2:2E:208:GLU:HG3	1.77	0.50
2:2F:44:TYR:HA	2:2F:47:ILE:HG12	1.93	0.50
2:2J:185:VAL:HA	2:2J:209:ILE:HD13	1.93	0.50
2:3O:20:VAL:O	2:3O:24:VAL:HG22	2.12	0.50
2:3Q:88:PHE:CD1	2:3Q:97:ALA:HB2	2.46	0.50
1:1Q:7:PHE:HZ	1:1Q:128:LEU:HD22	1.77	0.49
2:2G:185:VAL:HA	2:2G:209:ILE:HD13	1.93	0.49
2:3B:88:PHE:CD1	2:3B:97:ALA:HB2	2.46	0.49
2:3Q:2:ILE:HG13	2:3Q:64:HIS:HB2	1.93	0.49
1:4E:137:PRO:CG	1:4E:183:SER:HB3	2.42	0.49
1:1L:56:ILE:HD12	1:1M:54:PRO:HB2	1.94	0.49
1:1O:35:GLN:HA	1:1P:7:PHE:CZ	2.46	0.49
2:3E:197:ASN:HA	1:4E:163:ARG:HG2	1.93	0.49
1:4B:105:THR:HB	1:4C:98:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4H:56:ILE:CG2	1:4I:54:PRO:HB3	2.42	0.49
2:2F:41:MET:HG2	2:3F:43:ARG:HG2	1.94	0.49
2:2O:67:ILE:HD11	2:2O:111:VAL:CG2	2.41	0.49
2:2P:104:ASP:HA	2:2P:125:VAL:O	2.12	0.49
2:2Q:140:PHE:HB2	2:2Q:214:SER:HB3	1.92	0.49
2:3B:2:ILE:HG13	2:3B:64:HIS:HB2	1.93	0.49
2:3D:2:ILE:HG13	2:3D:64:HIS:HB2	1.93	0.49
2:3D:140:PHE:HB2	2:3D:214:SER:HB3	1.93	0.49
2:3E:90:VAL:HG23	1:4E:154:PHE:HZ	1.77	0.49
2:3G:185:VAL:HA	2:3G:209:ILE:HD13	1.93	0.49
1:4L:38:LYS:HG3	1:4M:7:PHE:CD2	2.47	0.49
2:2D:140:PHE:HB2	2:2D:214:SER:HB3	1.93	0.49
2:3E:2:ILE:HG13	2:3E:64:HIS:HB2	1.93	0.49
2:3Q:104:ASP:HA	2:3Q:125:VAL:O	2.11	0.49
1:4C:140:SER:O	1:4C:144:ILE:HG12	2.12	0.49
1:1A:144:ILE:CG2	1:1A:179:ILE:HG12	2.43	0.49
1:1Q:144:ILE:CG2	1:1Q:179:ILE:HG12	2.43	0.49
2:2B:2:ILE:HG13	2:2B:64:HIS:HB2	1.93	0.49
2:2D:88:PHE:HZ	2:2D:208:GLU:HG3	1.77	0.49
2:2F:140:PHE:HB2	2:2F:214:SER:HB3	1.93	0.49
2:2O:20:VAL:O	2:2O:24:VAL:HG22	2.12	0.49
2:3M:90:VAL:HG11	1:4M:200:GLN:OE1	2.12	0.49
2:3N:122:ASP:OD2	2:3O:19:ARG:HB2	2.12	0.49
1:4O:35:GLN:HA	1:4P:7:PHE:CZ	2.48	0.49
1:1P:129:TYR:HD1	1:1P:130:ILE:H	1.61	0.49
2:2C:88:PHE:HZ	2:2C:208:GLU:HG3	1.77	0.49
2:3A:72:THR:HB	2:3A:108:LEU:HB2	1.94	0.49
1:1E:163:ARG:HG2	2:2E:197:ASN:HA	1.93	0.49
1:1N:60:ASN:O	1:1O:52:PRO:HD2	2.13	0.49
2:2L:185:VAL:HA	2:2L:209:ILE:HD13	1.93	0.49
2:3E:88:PHE:HZ	2:3E:208:GLU:HG3	1.77	0.49
1:1J:38:LYS:HG3	1:1K:7:PHE:CD2	2.47	0.49
1:1J:122:ALA:HA	1:1J:126:LEU:O	2.12	0.49
2:2A:72:THR:HB	2:2A:108:LEU:HB2	1.94	0.49
2:3C:104:ASP:HA	2:3C:125:VAL:O	2.11	0.49
2:3E:140:PHE:HB2	2:3E:214:SER:HB3	1.93	0.49
2:3O:67:ILE:HD11	2:3O:111:VAL:CG2	2.43	0.49
1:4P:129:TYR:HD1	1:4P:130:ILE:H	1.61	0.49
1:1I:61:TYR:OH	1:1J:68:THR:HG22	2.13	0.49
2:2F:196:PRO:HA	2:2F:202:SER:HA	1.94	0.49
2:2M:185:VAL:HA	2:2M:209:ILE:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3A:88:PHE:CD1	2:3A:97:ALA:HB2	2.46	0.49
2:3F:93:ASN:HB2	2:3F:96:HIS:ND1	2.27	0.49
1:4N:60:ASN:O	1:4O:52:PRO:HD2	2.13	0.49
1:1F:147:LEU:HD12	1:1F:187:ILE:HG13	1.95	0.49
1:1I:30:TRP:NE1	1:1J:133:GLY:HA2	2.28	0.49
1:1K:105:THR:HB	1:1L:98:SER:CB	2.42	0.49
2:2G:84:VAL:HB	2:2G:96:HIS:O	2.13	0.49
2:3N:123:LEU:O	2:3N:123:LEU:HD12	2.13	0.49
1:4C:32:TYR:O	1:4C:35:GLN:HG2	2.13	0.49
1:4Q:7:PHE:HZ	1:4Q:128:LEU:HD22	1.77	0.49
1:1E:28:LEU:H	1:1E:28:LEU:CD1	2.26	0.48
1:1P:12:SER:HA	1:1P:138:SER:HB2	1.93	0.48
2:2F:93:ASN:HB2	2:2F:96:HIS:ND1	2.27	0.48
2:3J:84:VAL:HB	2:3J:96:HIS:O	2.13	0.48
2:3O:87:GLY:HA3	2:3O:96:HIS:HB3	1.96	0.48
1:4G:6:LEU:HD23	1:4G:7:PHE:H	1.78	0.48
1:4E:10:LEU:HB3	1:4E:126:LEU:H	1.79	0.48
1:4I:30:TRP:NE1	1:4J:133:GLY:HA2	2.28	0.48
1:1M:200:GLN:OE1	2:2M:90:VAL:HG11	2.12	0.48
2:3C:88:PHE:HZ	2:3C:208:GLU:HG3	1.77	0.48
1:1C:30:TRP:HZ3	1:1D:123:LEU:CD2	2.26	0.48
1:1E:38:LYS:HG3	1:1F:7:PHE:CD2	2.48	0.48
1:1H:91:VAL:HG11	1:1H:109:ILE:HD13	1.95	0.48
1:4A:32:TYR:O	1:4A:35:GLN:HG2	2.13	0.48
1:4C:30:TRP:HZ3	1:4D:123:LEU:CD2	2.26	0.48
1:4I:34:HIS:CE1	1:4J:123:LEU:O	2.66	0.48
2:3G:84:VAL:HB	2:3G:96:HIS:O	2.13	0.48
1:4L:56:ILE:HD12	1:4M:54:PRO:HB2	1.94	0.48
1:4M:54:PRO:CD	1:4M:67:ALA:HB3	2.43	0.48
1:4N:25:LEU:CG	1:4N:140:SER:HB3	2.42	0.48
1:1I:34:HIS:CE1	1:1J:123:LEU:O	2.66	0.48
2:3I:84:VAL:HB	2:3I:96:HIS:O	2.13	0.48
1:4A:144:ILE:CG2	1:4A:179:ILE:HG12	2.43	0.48
1:4M:32:TYR:O	1:4M:35:GLN:HG2	2.14	0.48
1:1C:136:LEU:HB3	1:1C:137:PRO:HD2	1.96	0.48
1:1E:154:PHE:HZ	2:2E:90:VAL:HG23	1.77	0.48
1:1G:5:THR:O	1:1G:9:GLN:HG3	2.14	0.48
1:4E:28:LEU:H	1:4E:28:LEU:CD1	2.26	0.48
1:4I:61:TYR:OH	1:4J:68:THR:HG22	2.13	0.48
1:1C:32:TYR:O	1:1C:35:GLN:HG2	2.13	0.48
1:1H:33:ALA:O	1:1H:37:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1N:25:LEU:CG	1:1N:140:SER:HB3	2.42	0.48
2:3L:194:LEU:HD12	1:4L:154:PHE:HE2	1.79	0.48
1:4F:132:ASN:OD1	1:4F:134:GLU:HG2	2.14	0.48
1:4Q:144:ILE:CG2	1:4Q:179:ILE:HG12	2.43	0.48
1:1G:6:LEU:HD23	1:1G:7:PHE:H	1.78	0.48
1:1M:32:TYR:O	1:1M:35:GLN:HG2	2.13	0.48
1:1M:136:LEU:HD22	1:1M:136:LEU:H	1.78	0.48
1:4G:5:THR:O	1:4G:9:GLN:HG3	2.14	0.48
1:4M:136:LEU:HD22	1:4M:136:LEU:H	1.78	0.48
1:4O:32:TYR:O	1:4O:35:GLN:HG2	2.13	0.48
1:1E:10:LEU:HB3	1:1E:126:LEU:H	1.79	0.47
1:1J:32:TYR:O	1:1J:35:GLN:HG2	2.13	0.47
1:1L:154:PHE:HE2	2:2L:194:LEU:HD12	1.79	0.47
1:1M:54:PRO:CD	1:1M:67:ALA:HB3	2.43	0.47
2:2I:84:VAL:HB	2:2I:96:HIS:O	2.13	0.47
1:4K:56:ILE:CG2	1:4L:54:PRO:HB3	2.44	0.47
1:4N:32:TYR:O	1:4N:35:GLN:HG2	2.14	0.47
1:1K:56:ILE:CG2	1:1L:54:PRO:HB3	2.44	0.47
1:1N:32:TYR:O	1:1N:35:GLN:HG2	2.13	0.47
1:1O:32:TYR:O	1:1O:35:GLN:HG2	2.13	0.47
1:1P:32:TYR:O	1:1P:35:GLN:HG2	2.15	0.47
2:2N:123:LEU:HD12	2:2N:123:LEU:O	2.13	0.47
2:2O:87:GLY:HA3	2:2O:96:HIS:HB3	1.96	0.47
1:4E:182:LEU:HD23	1:4E:187:ILE:HD12	1.96	0.47
1:4H:91:VAL:HG11	1:4H:109:ILE:HD13	1.95	0.47
1:1A:32:TYR:O	1:1A:35:GLN:HG2	2.13	0.47
1:1E:106:THR:HA	1:1F:73:PHE:CZ	2.49	0.47
1:4P:32:TYR:O	1:4P:35:GLN:HG2	2.15	0.47
1:1I:174:LEU:HD11	1:1I:194:LEU:CD2	2.45	0.47
1:1M:56:ILE:HG21	1:1N:54:PRO:HB3	1.97	0.47
2:2P:75:GLU:HB2	2:2Q:28:ARG:HE	1.80	0.47
1:4A:106:THR:HG23	1:4B:90:PRO:HB2	1.97	0.47
1:4H:33:ALA:O	1:4H:37:LEU:HG	2.14	0.47
1:4K:89:LEU:HD22	1:4K:112:ALA:HB1	1.96	0.47
1:1A:106:THR:HG23	1:1B:90:PRO:HB2	1.97	0.47
1:1K:89:LEU:HD22	1:1K:112:ALA:HB1	1.96	0.47
1:1M:31:SER:HB2	1:1N:129:TYR:HA	1.95	0.47
1:1N:7:PHE:HE2	1:1N:128:LEU:HD12	1.78	0.47
2:2J:84:VAL:HB	2:2J:96:HIS:O	2.13	0.47
1:4N:157:LEU:CD1	1:4N:198:LEU:HD12	2.45	0.47
1:1E:182:LEU:HD23	1:1E:187:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1F:132:ASN:OD1	1:1F:134:GLU:HG2	2.14	0.47
1:1I:174:LEU:HD11	1:1I:194:LEU:HD22	1.97	0.47
1:1L:34:HIS:CE1	1:1M:123:LEU:O	2.67	0.47
1:1M:178:ASN:OD1	1:1M:180:ASN:HB2	2.15	0.47
2:2N:71:PHE:HD1	2:2N:109:VAL:HG22	1.79	0.47
2:3O:17:ILE:HD12	2:3O:32:THR:HB	1.94	0.47
2:3P:75:GLU:HB2	2:3Q:28:ARG:HE	1.80	0.47
1:4A:90:PRO:HD3	1:4Q:110:ASN:CB	2.45	0.47
1:4B:140:SER:O	1:4B:144:ILE:HG23	2.14	0.47
1:4E:7:PHE:CZ	1:4E:128:LEU:HD22	2.49	0.47
1:4J:32:TYR:O	1:4J:35:GLN:HG2	2.13	0.47
1:4J:136:LEU:H	1:4J:136:LEU:HD22	1.80	0.47
1:4J:174:LEU:HD11	1:4J:194:LEU:HD22	1.97	0.47
1:4N:136:LEU:H	1:4N:136:LEU:HD22	1.80	0.47
1:1A:90:PRO:HD3	1:1Q:110:ASN:CB	2.45	0.47
1:1B:140:SER:O	1:1B:144:ILE:HG23	2.14	0.47
1:1I:64:PRO:HB3	1:1J:88:TRP:CZ2	2.50	0.47
1:1N:157:LEU:CD1	1:1N:198:LEU:HD12	2.45	0.47
1:4C:147:LEU:HD23	1:4C:179:ILE:HG13	1.96	0.47
1:4L:34:HIS:CE1	1:4M:123:LEU:O	2.68	0.47
1:1C:144:ILE:HD12	1:1C:179:ILE:O	2.15	0.47
2:3N:71:PHE:HA	2:3N:108:LEU:O	2.14	0.47
1:4F:147:LEU:HD12	1:4F:187:ILE:HG13	1.95	0.47
1:4H:88:TRP:O	1:4H:89:LEU:HD23	2.15	0.47
1:4I:107:PHE:HB2	1:4J:92:LEU:HD21	1.97	0.47
1:1H:88:TRP:O	1:1H:89:LEU:HD23	2.15	0.47
1:1H:91:VAL:HG12	1:1H:99:LEU:HD12	1.96	0.47
1:1N:60:ASN:HB2	1:1O:52:PRO:HG2	1.97	0.47
1:1N:134:GLU:O	1:1N:137:PRO:HD2	2.15	0.47
2:2N:71:PHE:HA	2:2N:108:LEU:O	2.14	0.47
2:3P:89:GLU:HB2	2:3P:194:LEU:HD23	1.97	0.47
1:4M:127:GLY:O	1:4M:130:ILE:HG22	2.15	0.47
1:1D:190:ALA:O	1:1D:194:LEU:HD22	2.16	0.46
2:3P:89:GLU:HA	2:3P:193:GLU:HA	1.98	0.46
1:4C:136:LEU:HB3	1:4C:137:PRO:HD2	1.96	0.46
1:1D:106:THR:HG23	1:1E:90:PRO:HB2	1.97	0.46
2:2M:193:GLU:CD	2:2M:203:THR:HB	2.36	0.46
2:3M:193:GLU:CD	2:3M:203:THR:HB	2.36	0.46
2:3P:92:ALA:HB2	2:3P:193:GLU:CD	2.36	0.46
1:4I:64:PRO:HB3	1:4J:88:TRP:CZ2	2.50	0.46
1:4I:174:LEU:HD11	1:4I:194:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:123:LEU:O	1:1Q:34:HIS:CE1	2.68	0.46
1:1I:38:LYS:HE2	1:1I:44:TYR:CE1	2.51	0.46
1:1J:89:LEU:HD23	1:1J:90:PRO:N	2.31	0.46
1:1J:174:LEU:HD11	1:1J:194:LEU:CD2	2.45	0.46
2:2A:54:LEU:O	2:2A:56:ILE:HG23	2.16	0.46
2:2N:193:GLU:HB3	2:2N:203:THR:H	1.81	0.46
2:2P:89:GLU:HA	2:2P:193:GLU:HA	1.97	0.46
1:1I:107:PHE:HB2	1:1J:92:LEU:HD21	1.97	0.46
1:1J:7:PHE:HZ	1:1J:128:LEU:HG	1.81	0.46
2:3C:54:LEU:O	2:3C:56:ILE:HG23	2.16	0.46
2:3J:50:LEU:HD13	2:3J:61:PHE:HE2	1.81	0.46
2:3N:50:LEU:HD13	2:3N:61:PHE:HE2	1.81	0.46
2:3N:84:VAL:HB	2:3N:96:HIS:O	2.15	0.46
2:3Q:54:LEU:O	2:3Q:56:ILE:HG23	2.16	0.46
1:4H:91:VAL:HG12	1:4H:99:LEU:HD12	1.96	0.46
1:4J:174:LEU:HD11	1:4J:194:LEU:CD2	2.45	0.46
1:1N:136:LEU:HD22	1:1N:136:LEU:H	1.80	0.46
2:2E:54:LEU:O	2:2E:56:ILE:HG23	2.16	0.46
2:3A:54:LEU:O	2:3A:56:ILE:HG23	2.16	0.46
2:3L:50:LEU:HD13	2:3L:61:PHE:HE2	1.81	0.46
1:4J:7:PHE:HZ	1:4J:128:LEU:HG	1.81	0.46
1:4L:65:TYR:OH	1:4M:70:GLU:HB2	2.15	0.46
2:2N:84:VAL:HB	2:2N:96:HIS:O	2.15	0.46
2:3M:50:LEU:HD13	2:3M:61:PHE:HE2	1.81	0.46
2:3P:192:GLU:HB3	2:3P:204:THR:HG22	1.98	0.46
1:4G:32:TYR:O	1:4G:36:GLU:HG2	2.16	0.46
1:4N:60:ASN:HB2	1:4O:52:PRO:HG2	1.97	0.46
1:1J:136:LEU:HD22	1:1J:136:LEU:H	1.80	0.46
2:3I:150:ASN:HB3	2:3I:153:LEU:HB2	1.98	0.46
1:4H:66:LEU:HB2	1:4H:73:PHE:HB2	1.98	0.46
1:4I:38:LYS:HE2	1:4I:44:TYR:CE1	2.51	0.46
1:4M:178:ASN:OD1	1:4M:180:ASN:HB2	2.15	0.46
1:4Q:38:LYS:HE2	1:4Q:44:TYR:CE1	2.51	0.46
1:1C:190:ALA:O	1:1C:194:LEU:HD22	2.16	0.46
2:2I:50:LEU:HD13	2:2I:61:PHE:HE2	1.81	0.46
2:2P:92:ALA:HB2	2:2P:193:GLU:CD	2.36	0.46
2:3B:54:LEU:O	2:3B:56:ILE:HG23	2.16	0.46
2:3N:193:GLU:HB3	2:3N:203:THR:H	1.81	0.46
1:4F:35:GLN:HB3	1:4G:128:LEU:HD23	1.97	0.46
1:1M:127:GLY:O	1:1M:130:ILE:HG22	2.15	0.46
2:2J:150:ASN:HB3	2:2J:153:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3E:54:LEU:O	2:3E:56:ILE:HG23	2.16	0.46
2:3G:50:LEU:HD13	2:3G:61:PHE:HE2	1.81	0.46
2:3G:150:ASN:HB3	2:3G:153:LEU:HB2	1.98	0.46
2:3N:150:ASN:HB3	2:3N:153:LEU:HB2	1.98	0.46
1:4C:144:ILE:HD12	1:4C:179:ILE:O	2.15	0.46
1:1C:147:LEU:HD23	1:1C:179:ILE:HG13	1.96	0.46
1:1D:66:LEU:HB2	1:1D:73:PHE:HB2	1.98	0.46
1:1F:7:PHE:CZ	1:1F:128:LEU:HD22	2.49	0.46
1:1Q:38:LYS:HE2	1:1Q:44:TYR:CE1	2.50	0.46
2:2B:54:LEU:O	2:2B:56:ILE:HG23	2.16	0.46
2:2L:150:ASN:HB3	2:2L:153:LEU:HD12	1.98	0.46
2:2N:50:LEU:HD13	2:2N:61:PHE:HE2	1.81	0.46
2:3F:54:LEU:O	2:3F:56:ILE:HG23	2.16	0.46
1:4M:56:ILE:HG21	1:4N:54:PRO:HB3	1.97	0.46
1:4N:134:GLU:O	1:4N:137:PRO:HD2	2.15	0.46
1:1B:159:GLN:HG3	1:1B:165:ALA:HB3	1.97	0.45
1:1C:12:SER:HA	1:1C:138:SER:HB3	1.97	0.45
1:1G:32:TYR:O	1:1G:36:GLU:HG2	2.16	0.45
1:1N:154:PHE:HA	1:1N:198:LEU:HD13	1.98	0.45
2:2G:67:ILE:HD11	2:2G:111:VAL:CG2	2.46	0.45
2:2I:150:ASN:HB3	2:2I:153:LEU:HB2	1.98	0.45
2:2N:150:ASN:HB3	2:2N:153:LEU:HB2	1.98	0.45
2:2N:150:ASN:HB3	2:2N:153:LEU:HD12	1.98	0.45
2:2Q:54:LEU:O	2:2Q:56:ILE:HG23	2.16	0.45
2:3D:54:LEU:O	2:3D:56:ILE:HG23	2.16	0.45
2:3G:67:ILE:HD11	2:3G:111:VAL:CG2	2.46	0.45
2:3I:50:LEU:HD13	2:3I:61:PHE:HE2	1.81	0.45
2:3J:150:ASN:HB3	2:3J:153:LEU:HD12	1.99	0.45
1:4D:190:ALA:O	1:4D:194:LEU:HD22	2.16	0.45
1:4I:174:LEU:HD11	1:4I:194:LEU:CD2	2.45	0.45
2:2F:88:PHE:CE2	2:2F:205:LEU:HB2	2.51	0.45
2:3G:150:ASN:HB3	2:3G:153:LEU:HD12	1.99	0.45
2:3I:150:ASN:HB3	2:3I:153:LEU:HD12	1.99	0.45
2:3N:71:PHE:HD1	2:3N:109:VAL:HG22	1.79	0.45
2:3O:50:LEU:HD13	2:3O:61:PHE:HE2	1.81	0.45
1:4B:159:GLN:HG3	1:4B:165:ALA:HB3	1.97	0.45
1:4N:56:ILE:CG2	1:4O:54:PRO:HB3	2.46	0.45
1:1E:7:PHE:CZ	1:1E:128:LEU:HD22	2.49	0.45
1:1H:66:LEU:HB2	1:1H:73:PHE:HB2	1.98	0.45
2:2P:54:LEU:O	2:2P:56:ILE:HG23	2.16	0.45
2:3E:192:GLU:HA	2:3E:204:THR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1J:174:LEU:HD11	1:1J:194:LEU:HD22	1.97	0.45
1:1M:143:ASP:OD1	1:1M:187:ILE:HG12	2.17	0.45
2:2D:54:LEU:O	2:2D:56:ILE:HG23	2.16	0.45
2:2J:50:LEU:HD13	2:2J:61:PHE:HE2	1.81	0.45
2:3M:70:ASP:O	2:3M:109:VAL:HA	2.17	0.45
2:3P:54:LEU:O	2:3P:56:ILE:HG23	2.16	0.45
1:4D:106:THR:HG23	1:4E:90:PRO:HB2	1.97	0.45
1:4D:147:LEU:HD23	1:4D:151:ILE:HG23	1.99	0.45
1:1C:144:ILE:HG23	1:1C:179:ILE:HG12	1.99	0.45
1:1L:65:TYR:OH	1:1M:70:GLU:HB2	2.15	0.45
2:2F:44:TYR:CZ	2:3F:42:ILE:HB	2.51	0.45
2:2G:50:LEU:HD13	2:2G:61:PHE:HE2	1.81	0.45
2:2L:50:LEU:HD13	2:2L:61:PHE:HE2	1.81	0.45
2:2O:50:LEU:HD13	2:2O:61:PHE:HE2	1.81	0.45
2:3F:88:PHE:CE2	2:3F:205:LEU:HB2	2.51	0.45
1:4A:123:LEU:O	1:4Q:34:HIS:CE1	2.68	0.45
1:4J:89:LEU:HD23	1:4J:90:PRO:N	2.30	0.45
1:1G:5:THR:HG23	1:1G:8:GLU:H	1.81	0.45
2:2G:150:ASN:HB3	2:2G:153:LEU:HD12	1.98	0.45
2:2M:70:ASP:O	2:2M:109:VAL:HA	2.17	0.45
2:3L:150:ASN:HB3	2:3L:153:LEU:HB2	1.98	0.45
1:4D:38:LYS:HE2	1:4D:44:TYR:CE1	2.52	0.45
1:4H:115:ARG:O	1:4H:119:LYS:HG2	2.17	0.45
1:4J:56:ILE:HG21	1:4K:54:PRO:HB3	1.99	0.45
1:1G:32:TYR:O	1:1G:35:GLN:HG2	2.16	0.45
1:1M:106:THR:HG23	1:1N:90:PRO:HB2	1.98	0.45
2:2F:54:LEU:O	2:2F:56:ILE:HG23	2.16	0.45
2:3N:90:VAL:HG23	2:3N:91:THR:N	2.32	0.45
1:4A:178:ASN:OD1	1:4A:181:LYS:HG2	2.17	0.45
1:4D:28:LEU:HD23	1:4D:130:ILE:HG13	1.99	0.45
1:4M:35:GLN:HA	1:4N:7:PHE:CZ	2.52	0.45
1:4M:38:LYS:HE2	1:4M:44:TYR:CE1	2.52	0.45
1:4N:15:VAL:HG22	1:4N:130:ILE:CD1	2.47	0.45
1:1A:178:ASN:OD1	1:1A:181:LYS:HG2	2.17	0.45
1:1D:38:LYS:HE2	1:1D:44:TYR:CE1	2.52	0.45
1:1D:147:LEU:HD23	1:1D:151:ILE:HG23	1.99	0.45
1:1E:28:LEU:H	1:1E:28:LEU:HD13	1.82	0.45
1:1G:64:PRO:HB3	1:1H:88:TRP:CZ2	2.52	0.45
1:1N:56:ILE:CG2	1:1O:54:PRO:HB3	2.47	0.45
1:1O:35:GLN:HB3	1:1P:128:LEU:HD23	1.99	0.45
2:2M:50:LEU:HD13	2:2M:61:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2N:90:VAL:HG23	2:2N:91:THR:N	2.32	0.45
2:2O:71:PHE:HD1	2:2O:109:VAL:HG22	1.82	0.45
2:2O:107:ILE:HB	2:2O:123:LEU:HD11	1.99	0.45
1:4E:173:TRP:HH2	1:4E:197:GLY:HA3	1.82	0.45
1:4Q:178:ASN:OD1	1:4Q:181:LYS:HG2	2.17	0.45
1:1D:28:LEU:HD23	1:1D:130:ILE:HG13	1.99	0.45
2:2I:150:ASN:HB3	2:2I:153:LEU:HD12	1.99	0.45
2:2J:150:ASN:HB3	2:2J:153:LEU:HD12	1.99	0.45
2:2L:150:ASN:HB3	2:2L:153:LEU:HB2	1.98	0.45
2:2O:5:ARG:O	2:2O:9:LEU:HG	2.17	0.45
2:2P:89:GLU:HB2	2:2P:194:LEU:HD23	1.97	0.45
2:2P:192:GLU:HB3	2:2P:204:THR:HG22	1.98	0.45
1:4C:12:SER:HA	1:4C:138:SER:HB3	1.97	0.45
1:4C:148:GLU:HA	1:4C:151:ILE:HG12	1.99	0.45
1:4E:10:LEU:HB3	1:4E:126:LEU:N	2.31	0.45
1:4K:56:ILE:HD12	1:4L:54:PRO:HB2	1.99	0.45
1:4L:111:LYS:O	1:4L:115:ARG:HG3	2.17	0.45
1:1D:169:LYS:O	2:2D:194:LEU:HD11	2.17	0.45
1:1E:10:LEU:HB3	1:1E:126:LEU:N	2.31	0.45
2:2C:54:LEU:O	2:2C:56:ILE:HG23	2.16	0.45
2:2C:77:PRO:HG2	2:2C:79:TYR:CD1	2.53	0.45
2:2I:122:ASP:OD2	2:2J:19:ARG:HB2	2.18	0.45
2:3P:77:PRO:HG2	2:3P:79:TYR:CD1	2.52	0.45
2:3P:192:GLU:CB	2:3P:204:THR:HG22	2.47	0.45
1:4C:190:ALA:O	1:4C:194:LEU:HD22	2.16	0.45
1:4G:64:PRO:HB3	1:4H:88:TRP:CZ2	2.52	0.45
1:4M:106:THR:HG23	1:4N:90:PRO:HB2	1.98	0.45
1:4M:143:ASP:OD1	1:4M:187:ILE:HG12	2.17	0.45
1:4N:154:PHE:HA	1:4N:198:LEU:HD13	1.98	0.45
1:4P:64:PRO:HB3	1:4Q:88:TRP:CZ2	2.52	0.45
1:1M:35:GLN:HA	1:1N:7:PHE:CZ	2.52	0.44
2:2L:195:PHE:HD1	2:2L:195:PHE:H	1.66	0.44
2:3E:77:PRO:HG2	2:3E:79:TYR:CD1	2.52	0.44
2:3O:90:VAL:HA	2:3O:195:PHE:CE1	2.52	0.44
1:4A:18:HIS:ND1	1:4A:32:TYR:HD2	2.15	0.44
1:4C:158:SER:HB2	1:4C:165:ALA:CB	2.48	0.44
1:4G:32:TYR:O	1:4G:35:GLN:HG2	2.16	0.44
1:4I:56:ILE:CG2	1:4J:54:PRO:HB3	2.47	0.44
1:1B:129:TYR:CE1	1:1B:130:ILE:HG12	2.52	0.44
1:1P:64:PRO:HB3	1:1Q:88:TRP:CZ2	2.52	0.44
2:2E:192:GLU:HA	2:2E:204:THR:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2G:150:ASN:HB3	2:2G:153:LEU:HB2	1.98	0.44
2:3I:67:ILE:HD11	2:3I:111:VAL:CG2	2.48	0.44
2:3J:150:ASN:HB3	2:3J:153:LEU:HB2	1.98	0.44
2:3O:150:ASN:HB3	2:3O:153:LEU:HB2	1.98	0.44
2:3O:150:ASN:HB3	2:3O:153:LEU:HD12	1.98	0.44
1:4A:54:PRO:HB3	1:4Q:56:ILE:HG21	1.98	0.44
1:4B:129:TYR:CE1	1:4B:130:ILE:HG12	2.52	0.44
1:4D:66:LEU:HB2	1:4D:73:PHE:HB2	1.98	0.44
1:4I:28:LEU:HD23	1:4I:130:ILE:HG13	1.99	0.44
1:4P:106:THR:HG23	1:4Q:90:PRO:HB2	1.99	0.44
1:1A:18:HIS:ND1	1:1A:32:TYR:HD2	2.15	0.44
1:1C:158:SER:HB2	1:1C:165:ALA:CB	2.48	0.44
1:1D:148:GLU:HA	1:1D:151:ILE:HG12	1.99	0.44
1:1E:173:TRP:HH2	1:1E:197:GLY:HA3	1.82	0.44
1:1L:111:LYS:O	1:1L:115:ARG:HG3	2.17	0.44
1:1P:106:THR:HG23	1:1Q:90:PRO:HB2	1.99	0.44
1:1Q:178:ASN:OD1	1:1Q:181:LYS:HG2	2.17	0.44
2:2O:150:ASN:HB3	2:2O:153:LEU:HD12	1.98	0.44
2:2Q:77:PRO:HG2	2:2Q:79:TYR:CD1	2.52	0.44
2:3B:77:PRO:HG2	2:3B:79:TYR:CD1	2.52	0.44
2:3C:77:PRO:HG2	2:3C:79:TYR:CD1	2.53	0.44
1:1M:38:LYS:HE2	1:1M:44:TYR:CE1	2.52	0.44
1:1M:142:ASN:C	1:1M:144:ILE:N	2.71	0.44
1:1P:129:TYR:CD1	1:1P:129:TYR:N	2.85	0.44
2:2A:144:ILE:HB	2:2A:147:GLU:HB3	2.00	0.44
2:2D:77:PRO:HG2	2:2D:79:TYR:CD1	2.53	0.44
2:2E:144:ILE:HB	2:2E:147:GLU:HB3	2.00	0.44
2:2J:100:ILE:HG12	2:2J:103:PHE:HD2	1.83	0.44
1:4C:144:ILE:HG23	1:4C:179:ILE:HG12	1.99	0.44
1:4E:28:LEU:H	1:4E:28:LEU:HD13	1.82	0.44
1:4G:5:THR:HG23	1:4G:8:GLU:H	1.81	0.44
1:1D:15:VAL:HG23	1:1D:130:ILE:HD11	2.00	0.44
1:1F:141:ASP:O	1:1F:144:ILE:HG12	2.17	0.44
1:1H:115:ARG:O	1:1H:119:LYS:HG2	2.17	0.44
1:1J:163:ARG:HG3	2:2J:195:PHE:HB3	1.99	0.44
1:1L:106:THR:HG23	1:1M:90:PRO:HB2	2.00	0.44
2:2G:84:VAL:HG12	2:2G:86:GLU:HB2	2.00	0.44
2:2G:100:ILE:HG12	2:2G:103:PHE:HD2	1.83	0.44
2:2N:89:GLU:HB2	2:2N:192:GLU:O	2.17	0.44
2:2P:77:PRO:HG2	2:2P:79:TYR:CD1	2.52	0.44
2:3A:144:ILE:HB	2:3A:147:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3G:84:VAL:HG12	2:3G:86:GLU:HB2	2.00	0.44
2:3L:150:ASN:HB3	2:3L:153:LEU:HD12	1.99	0.44
2:3L:195:PHE:HD1	2:3L:195:PHE:H	1.65	0.44
1:4E:14:ASN:HA	1:4E:129:TYR:OH	2.18	0.44
2:2B:77:PRO:HG2	2:2B:79:TYR:CD1	2.52	0.44
2:2I:67:ILE:HD11	2:2I:111:VAL:CG2	2.48	0.44
2:2P:144:ILE:HB	2:2P:147:GLU:HB3	2.00	0.44
2:3I:122:ASP:OD2	2:3J:19:ARG:HB2	2.18	0.44
2:3I:191:ILE:H	2:3I:205:LEU:CB	2.31	0.44
2:3N:150:ASN:HB3	2:3N:153:LEU:HD12	1.98	0.44
1:4E:129:TYR:O	1:4E:132:ASN:HB3	2.18	0.44
1:1A:54:PRO:HB3	1:1Q:56:ILE:HG21	1.98	0.44
1:1B:64:PRO:HB3	1:1C:88:TRP:CZ2	2.53	0.44
1:1L:32:TYR:O	1:1L:35:GLN:HG2	2.18	0.44
2:2F:58:PRO:HA	2:2F:61:PHE:HB3	2.00	0.44
2:2J:84:VAL:HG12	2:2J:86:GLU:HB2	2.00	0.44
2:2O:150:ASN:HB3	2:2O:153:LEU:HB2	1.98	0.44
2:2P:192:GLU:CB	2:2P:204:THR:HG22	2.47	0.44
2:2Q:144:ILE:HB	2:2Q:147:GLU:HB3	2.00	0.44
2:3A:77:PRO:HG2	2:3A:79:TYR:CD1	2.52	0.44
2:3D:144:ILE:HB	2:3D:147:GLU:HB3	2.00	0.44
2:3D:194:LEU:HD11	1:4D:169:LYS:O	2.17	0.44
2:3E:6:LEU:HD23	2:3E:6:LEU:HA	1.86	0.44
2:3F:77:PRO:HG2	2:3F:79:TYR:CD1	2.52	0.44
2:3Q:77:PRO:HG2	2:3Q:79:TYR:CD1	2.52	0.44
1:4D:147:LEU:HD12	1:4D:187:ILE:HG13	2.00	0.44
1:4L:32:TYR:O	1:4L:35:GLN:HG2	2.18	0.44
1:4M:129:TYR:O	1:4M:132:ASN:HB2	2.18	0.44
1:1E:129:TYR:O	1:1E:132:ASN:HB3	2.18	0.44
1:1H:94:PHE:CE2	1:1I:144:ILE:HG13	2.53	0.44
1:1I:38:LYS:HG3	1:1J:7:PHE:CD2	2.52	0.44
1:1K:56:ILE:HD12	1:1L:54:PRO:HB2	1.99	0.44
1:1M:31:SER:HA	1:1N:128:LEU:HD22	2.00	0.44
2:2G:205:LEU:O	2:2G:209:ILE:HG13	2.18	0.44
2:3B:44:TYR:HA	2:3B:47:ILE:HG12	2.00	0.44
1:4E:28:LEU:HD12	1:4E:130:ILE:HG21	2.00	0.44
1:4O:35:GLN:HB3	1:4P:128:LEU:HD23	2.00	0.44
1:4P:129:TYR:N	1:4P:129:TYR:CD1	2.85	0.44
1:1C:56:ILE:CG2	1:1D:54:PRO:HB3	2.48	0.44
1:1E:28:LEU:HD12	1:1E:130:ILE:HG21	2.00	0.44
1:1J:56:ILE:HG21	1:1K:54:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1L:143:ASP:O	1:1L:146:GLU:HB3	2.18	0.44
2:2A:77:PRO:HG2	2:2A:79:TYR:CD1	2.52	0.44
2:2G:205:LEU:O	2:2G:208:GLU:HB3	2.18	0.44
2:2J:205:LEU:O	2:2J:209:ILE:HG13	2.18	0.44
2:2O:28:ARG:O	2:2O:32:THR:HG22	2.18	0.44
2:3G:100:ILE:HG12	2:3G:103:PHE:HD2	1.83	0.44
2:3I:205:LEU:O	2:3I:208:GLU:HB3	2.18	0.44
2:3I:205:LEU:O	2:3I:209:ILE:HG13	2.18	0.44
2:3L:92:ALA:O	2:3L:136:SER:HA	2.18	0.44
2:3O:195:PHE:HD1	2:3O:195:PHE:H	1.66	0.44
2:3P:144:ILE:HB	2:3P:147:GLU:HB3	2.00	0.44
1:4D:148:GLU:HA	1:4D:151:ILE:HG12	1.99	0.44
1:4H:94:PHE:CE2	1:4I:144:ILE:HG13	2.53	0.44
2:2B:44:TYR:HA	2:2B:47:ILE:HG12	2.00	0.43
2:2B:144:ILE:HB	2:2B:147:GLU:HB3	2.00	0.43
2:2D:144:ILE:HB	2:2D:147:GLU:HB3	2.00	0.43
2:2I:100:ILE:HG12	2:2I:103:PHE:HD2	1.83	0.43
2:3I:84:VAL:HG12	2:3I:86:GLU:HB2	2.00	0.43
2:3J:205:LEU:O	2:3J:209:ILE:HG13	2.18	0.43
2:3O:92:ALA:O	2:3O:136:SER:HA	2.18	0.43
1:4P:56:ILE:CG2	1:4Q:54:PRO:HB3	2.48	0.43
1:1C:148:GLU:HA	1:1C:151:ILE:HG12	1.99	0.43
1:1E:14:ASN:HA	1:1E:129:TYR:OH	2.18	0.43
1:1H:25:LEU:HB2	1:1H:27:TYR:CZ	2.54	0.43
1:1J:26:THR:HG22	1:1J:130:ILE:HD11	1.99	0.43
2:2G:89:GLU:O	2:2G:195:PHE:HB2	2.19	0.43
2:2I:84:VAL:HG12	2:2I:86:GLU:HB2	2.00	0.43
2:2P:44:TYR:HA	2:2P:47:ILE:HG12	2.00	0.43
2:2Q:44:TYR:HA	2:2Q:47:ILE:HG12	2.00	0.43
2:3J:195:PHE:HB3	1:4J:163:ARG:HG3	1.99	0.43
2:3L:100:ILE:HG12	2:3L:103:PHE:HD2	1.83	0.43
1:4B:64:PRO:HB3	1:4C:88:TRP:CZ2	2.53	0.43
1:4I:38:LYS:HG3	1:4J:7:PHE:CD2	2.53	0.43
1:1D:147:LEU:HD12	1:1D:187:ILE:HG13	2.00	0.43
1:1F:89:LEU:HD22	1:1F:112:ALA:HB1	2.00	0.43
1:1N:15:VAL:HG22	1:1N:130:ILE:CD1	2.48	0.43
2:2E:77:PRO:HG2	2:2E:79:TYR:CD1	2.52	0.43
2:2F:144:ILE:HB	2:2F:147:GLU:HB3	2.00	0.43
2:2L:100:ILE:HG12	2:2L:103:PHE:HD2	1.83	0.43
2:3D:77:PRO:HG2	2:3D:79:TYR:CD1	2.53	0.43
2:3N:100:ILE:HG12	2:3N:103:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3N:125:VAL:HG11	2:3N:216:LEU:HD22	2.00	0.43
1:4P:159:GLN:HA	1:4P:163:ARG:O	2.19	0.43
1:1C:143:ASP:HB3	1:1C:187:ILE:HG12	2.00	0.43
1:1I:56:ILE:CG2	1:1J:54:PRO:HB3	2.47	0.43
2:2F:77:PRO:HG2	2:2F:79:TYR:CD1	2.52	0.43
2:2G:5:ARG:O	2:2G:6:LEU:C	2.57	0.43
2:2I:191:ILE:H	2:2I:205:LEU:CB	2.31	0.43
2:2J:205:LEU:O	2:2J:208:GLU:HB3	2.18	0.43
2:2M:150:ASN:HB3	2:2M:153:LEU:HD12	2.00	0.43
2:2N:204:THR:HG23	2:2N:207:LYS:HG3	2.01	0.43
2:3B:144:ILE:HB	2:3B:147:GLU:HB3	2.00	0.43
2:3J:84:VAL:HG12	2:3J:86:GLU:HB2	2.00	0.43
2:3J:205:LEU:O	2:3J:208:GLU:HB3	2.18	0.43
1:4C:56:ILE:CG2	1:4D:54:PRO:HB3	2.48	0.43
1:4H:25:LEU:HB2	1:4H:27:TYR:CZ	2.54	0.43
1:4I:154:PHE:HE2	1:4I:173:TRP:HZ3	1.66	0.43
1:4L:143:ASP:O	1:4L:146:GLU:HB3	2.18	0.43
1:1G:15:VAL:HG12	1:1G:32:TYR:CE1	2.54	0.43
1:1I:28:LEU:HD23	1:1I:130:ILE:HG13	1.99	0.43
1:1L:201:LEU:HD12	1:1L:201:LEU:H	1.84	0.43
1:1N:32:TYR:O	1:1N:36:GLU:HG2	2.19	0.43
2:2N:111:VAL:HG13	2:2N:119:LEU:HB2	2.00	0.43
2:2N:125:VAL:HG11	2:2N:216:LEU:HD22	2.00	0.43
2:3E:144:ILE:HB	2:3E:147:GLU:HB3	2.00	0.43
2:3N:67:ILE:HD11	2:3N:111:VAL:HG23	2.01	0.43
2:3N:89:GLU:HB2	2:3N:192:GLU:O	2.17	0.43
1:4C:118:VAL:HG23	1:4C:131:TYR:OH	2.19	0.43
1:4F:141:ASP:O	1:4F:144:ILE:HG12	2.17	0.43
1:4I:30:TRP:CD1	1:4J:133:GLY:HA2	2.53	0.43
1:4P:159:GLN:HG2	1:4P:165:ALA:H	1.83	0.43
1:1L:35:GLN:HA	1:1M:7:PHE:CZ	2.54	0.43
1:1N:13:LYS:HD3	1:1N:126:LEU:HD13	2.00	0.43
2:2F:48:ASP:HB2	2:3F:2:ILE:N	2.34	0.43
2:2N:67:ILE:HD11	2:2N:111:VAL:HG23	2.01	0.43
2:3C:194:LEU:HD11	1:4C:169:LYS:O	2.18	0.43
2:3I:100:ILE:HG12	2:3I:103:PHE:HD2	1.83	0.43
2:3M:100:ILE:HG12	2:3M:103:PHE:HD2	1.83	0.43
1:4B:56:ILE:HD12	1:4C:54:PRO:HB2	2.01	0.43
1:4D:15:VAL:HG23	1:4D:130:ILE:HD11	2.00	0.43
1:4E:32:TYR:O	1:4E:36:GLU:HG2	2.19	0.43
1:4J:26:THR:HG22	1:4J:130:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4L:91:VAL:HG12	1:4L:99:LEU:HD12	2.01	0.43
1:1D:32:TYR:O	1:1D:36:GLU:HG2	2.19	0.43
1:1J:32:TYR:O	1:1J:36:GLU:HG2	2.18	0.43
1:1M:129:TYR:O	1:1M:132:ASN:HB2	2.18	0.43
2:2N:100:ILE:HG12	2:2N:103:PHE:HD2	1.83	0.43
2:3I:5:ARG:O	2:3I:6:LEU:C	2.57	0.43
2:3L:5:ARG:O	2:3L:6:LEU:C	2.57	0.43
2:3N:89:GLU:O	2:3N:194:LEU:HG	2.19	0.43
2:3N:89:GLU:CD	1:4N:154:PHE:HZ	2.22	0.43
2:3N:204:THR:HG23	2:3N:207:LYS:HG3	2.01	0.43
2:3P:44:TYR:HA	2:3P:47:ILE:HG12	2.00	0.43
1:4D:106:THR:HA	1:4E:73:PHE:CZ	2.54	0.43
1:4F:38:LYS:HE2	1:4F:44:TYR:HE1	1.84	0.43
1:4F:89:LEU:HD22	1:4F:112:ALA:HB1	1.99	0.43
1:4K:32:TYR:O	1:4K:36:GLU:HG2	2.19	0.43
1:4Q:38:LYS:HE2	1:4Q:44:TYR:HE1	1.84	0.43
1:1C:169:LYS:O	2:2C:194:LEU:HD11	2.18	0.43
1:1E:147:LEU:HD12	1:1E:187:ILE:HG13	2.00	0.43
1:1F:136:LEU:HD12	1:1F:181:LYS:O	2.19	0.43
1:1L:32:TYR:O	1:1L:36:GLU:HG2	2.19	0.43
2:2C:144:ILE:HB	2:2C:147:GLU:HB3	2.00	0.43
2:2I:205:LEU:O	2:2I:208:GLU:HB3	2.18	0.43
2:3G:205:LEU:O	2:3G:208:GLU:HB3	2.18	0.43
2:3O:5:ARG:O	2:3O:6:LEU:C	2.57	0.43
1:4D:174:LEU:HD11	1:4D:194:LEU:CD2	2.49	0.43
1:1H:32:TYR:O	1:1H:36:GLU:HG2	2.19	0.43
1:1H:64:PRO:HB3	1:1I:88:TRP:CE2	2.54	0.43
1:1I:30:TRP:CD1	1:1J:133:GLY:HA2	2.53	0.43
2:2A:44:TYR:HA	2:2A:47:ILE:HG12	2.00	0.43
2:2E:44:TYR:HA	2:2E:47:ILE:HG12	2.00	0.43
2:2I:89:GLU:O	2:2I:195:PHE:HB2	2.19	0.43
2:2I:205:LEU:O	2:2I:209:ILE:HG13	2.18	0.43
2:2N:5:ARG:O	2:2N:6:LEU:C	2.57	0.43
2:2N:89:GLU:O	2:2N:194:LEU:HG	2.19	0.43
2:2N:91:THR:O	2:2N:92:ALA:C	2.57	0.43
2:2O:195:PHE:HD1	2:2O:195:PHE:H	1.66	0.43
2:3C:144:ILE:HB	2:3C:147:GLU:HB3	2.00	0.43
2:3G:89:GLU:O	2:3G:195:PHE:HB2	2.19	0.43
2:3G:205:LEU:O	2:3G:209:ILE:HG13	2.18	0.43
2:3J:100:ILE:HG12	2:3J:103:PHE:HD2	1.83	0.43
2:3M:153:LEU:HD23	2:3M:153:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3O:100:ILE:HG12	2:3O:103:PHE:HD2	1.83	0.43
2:3Q:144:ILE:HB	2:3Q:147:GLU:HB3	2.00	0.43
1:4A:72:TYR:H	1:4Q:106:THR:HB	1.84	0.43
1:4C:32:TYR:O	1:4C:36:GLU:HG2	2.19	0.43
1:4F:136:LEU:HD12	1:4F:181:LYS:O	2.19	0.43
1:4H:64:PRO:HB3	1:4I:88:TRP:CE2	2.54	0.43
1:1C:118:VAL:HG23	1:1C:131:TYR:OH	2.19	0.43
1:1N:157:LEU:HD13	1:1N:201:LEU:HD12	2.01	0.43
2:2G:191:ILE:H	2:2G:205:LEU:CB	2.31	0.43
2:2L:92:ALA:O	2:2L:136:SER:HA	2.18	0.43
2:2M:5:ARG:O	2:2M:6:LEU:C	2.57	0.43
2:2M:100:ILE:HG12	2:2M:103:PHE:HD2	1.83	0.43
2:2M:153:LEU:HD23	2:2M:153:LEU:HA	1.88	0.43
2:3I:90:VAL:HG12	1:4I:197:GLY:O	2.19	0.43
1:4A:151:ILE:O	1:4A:155:VAL:HG23	2.19	0.43
1:4P:32:TYR:O	1:4P:36:GLU:HG2	2.19	0.43
1:1C:32:TYR:O	1:1C:36:GLU:HG2	2.19	0.42
1:1E:32:TYR:O	1:1E:36:GLU:HG2	2.19	0.42
1:1I:197:GLY:O	2:2I:90:VAL:HG12	2.19	0.42
1:1K:32:TYR:O	1:1K:36:GLU:HG2	2.19	0.42
1:1P:159:GLN:HG2	1:1P:165:ALA:H	1.83	0.42
2:2O:92:ALA:O	2:2O:136:SER:HA	2.18	0.42
2:3F:6:LEU:HD23	2:3F:6:LEU:HA	1.86	0.42
2:3F:144:ILE:HB	2:3F:147:GLU:HB3	2.00	0.42
2:3J:191:ILE:H	2:3J:205:LEU:CB	2.31	0.42
1:4C:143:ASP:HB3	1:4C:187:ILE:HG12	2.00	0.42
1:4G:15:VAL:HG12	1:4G:32:TYR:CE1	2.54	0.42
1:4L:106:THR:HG23	1:4M:90:PRO:HB2	2.00	0.42
1:4M:142:ASN:C	1:4M:144:ILE:N	2.71	0.42
1:4M:154:PHE:CE1	1:4M:201:LEU:HD12	2.54	0.42
1:1N:15:VAL:HG22	1:1N:130:ILE:HD12	1.99	0.42
1:1O:32:TYR:O	1:1O:36:GLU:HG2	2.19	0.42
1:1P:159:GLN:HA	1:1P:163:ARG:O	2.19	0.42
1:1Q:32:TYR:O	1:1Q:36:GLU:HG2	2.19	0.42
2:3C:44:TYR:HA	2:3C:47:ILE:HG12	2.00	0.42
2:3Q:44:TYR:HA	2:3Q:47:ILE:HG12	2.00	0.42
1:4A:90:PRO:HD3	1:4Q:110:ASN:CG	2.40	0.42
1:4C:173:TRP:HH2	1:4C:197:GLY:HA3	1.85	0.42
1:4D:32:TYR:O	1:4D:36:GLU:HG2	2.19	0.42
1:4O:32:TYR:O	1:4O:36:GLU:HG2	2.19	0.42
1:4P:161:LYS:HE2	1:4P:204:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:54:PRO:HB2	1:1Q:56:ILE:HD12	2.01	0.42
1:1B:61:TYR:OH	1:1C:67:ALA:O	2.33	0.42
1:1F:32:TYR:O	1:1F:36:GLU:HG2	2.19	0.42
1:1G:10:LEU:HB3	1:1G:126:LEU:N	2.34	0.42
1:1I:38:LYS:HE2	1:1I:44:TYR:HE1	1.84	0.42
2:2C:44:TYR:HA	2:2C:47:ILE:HG12	2.00	0.42
2:2N:17:ILE:HD12	2:2N:32:THR:HB	2.02	0.42
2:3G:191:ILE:H	2:3G:205:LEU:CB	2.31	0.42
1:4F:184:GLN:HA	1:4F:187:ILE:HD13	2.00	0.42
1:4K:38:LYS:HG3	1:4L:7:PHE:CD2	2.54	0.42
1:1C:173:TRP:HH2	1:1C:197:GLY:HA3	1.85	0.42
1:1J:56:ILE:CG2	1:1K:54:PRO:HB3	2.50	0.42
1:1P:161:LYS:HE2	1:1P:204:GLU:HG2	2.01	0.42
2:2F:6:LEU:HD23	2:2F:6:LEU:HA	1.86	0.42
2:2I:5:ARG:O	2:2I:6:LEU:C	2.57	0.42
2:2J:191:ILE:H	2:2J:205:LEU:CB	2.31	0.42
2:2O:100:ILE:HG12	2:2O:103:PHE:HD2	1.83	0.42
2:3A:44:TYR:HA	2:3A:47:ILE:HG12	2.00	0.42
2:3D:44:TYR:HA	2:3D:47:ILE:HG12	2.00	0.42
2:3E:44:TYR:HA	2:3E:47:ILE:HG12	2.00	0.42
2:3F:3:ARG:NH1	2:3F:163:GLY:HA3	2.34	0.42
1:4C:174:LEU:HD11	1:4C:194:LEU:CD2	2.49	0.42
1:4D:128:LEU:HD13	1:4D:128:LEU:C	2.40	0.42
1:4G:10:LEU:HB3	1:4G:126:LEU:N	2.34	0.42
1:4H:38:LYS:HE2	1:4H:44:TYR:HE1	1.85	0.42
1:4I:38:LYS:HE2	1:4I:44:TYR:HE1	1.84	0.42
1:4J:32:TYR:O	1:4J:36:GLU:HG2	2.18	0.42
1:4L:201:LEU:HD12	1:4L:201:LEU:H	1.84	0.42
1:4M:32:TYR:O	1:4M:36:GLU:HG2	2.19	0.42
1:1A:151:ILE:O	1:1A:155:VAL:HG23	2.19	0.42
1:1F:184:GLN:HA	1:1F:187:ILE:HD13	2.00	0.42
1:1Q:159:GLN:HG3	1:1Q:165:ALA:HB3	2.02	0.42
2:2G:206:HIS:HA	2:2G:209:ILE:HD12	2.02	0.42
2:3G:17:ILE:HD12	2:3G:32:THR:HB	2.02	0.42
2:3I:195:PHE:HA	1:4I:158:SER:HB3	2.02	0.42
2:3L:90:VAL:HG13	1:4L:201:LEU:HG	2.02	0.42
2:3L:206:HIS:HA	2:3L:209:ILE:HD12	2.01	0.42
2:3N:91:THR:O	2:3N:92:ALA:C	2.57	0.42
2:3O:70:ASP:O	2:3O:109:VAL:HA	2.19	0.42
2:3O:206:HIS:HA	2:3O:209:ILE:HD12	2.02	0.42
1:4A:54:PRO:HB2	1:4Q:56:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4D:143:ASP:HB3	1:4D:187:ILE:HG21	2.02	0.42
1:4L:35:GLN:HA	1:4M:7:PHE:CZ	2.54	0.42
1:1A:72:TYR:H	1:1Q:106:THR:HB	1.84	0.42
1:1C:174:LEU:HD11	1:1C:194:LEU:CD2	2.49	0.42
1:1D:106:THR:HA	1:1E:73:PHE:CZ	2.54	0.42
1:1L:127:GLY:O	1:1L:130:ILE:HG22	2.20	0.42
1:1P:56:ILE:CG2	1:1Q:54:PRO:HB3	2.48	0.42
2:3F:44:TYR:O	2:3F:47:ILE:HG12	2.20	0.42
2:3M:5:ARG:O	2:3M:6:LEU:C	2.57	0.42
2:3M:150:ASN:HB3	2:3M:153:LEU:HD12	2.00	0.42
1:4A:32:TYR:O	1:4A:36:GLU:HG2	2.19	0.42
1:4Q:32:TYR:O	1:4Q:36:GLU:HG2	2.19	0.42
1:1A:90:PRO:HD3	1:1Q:110:ASN:CG	2.40	0.42
1:1B:56:ILE:HD12	1:1C:54:PRO:HB2	2.01	0.42
1:1M:32:TYR:O	1:1M:36:GLU:HG2	2.19	0.42
2:2I:108:LEU:HD12	2:2J:22:LYS:HB2	2.01	0.42
2:2Q:164:LEU:HD23	2:2Q:164:LEU:HA	1.90	0.42
2:3L:94:ILE:HG21	2:3L:212:THR:HG21	2.02	0.42
2:3N:5:ARG:O	2:3N:6:LEU:C	2.57	0.42
1:4E:147:LEU:HD12	1:4E:187:ILE:HG13	2.00	0.42
1:4F:38:LYS:HE2	1:4F:44:TYR:CE1	2.54	0.42
1:4G:106:THR:HG23	1:4H:90:PRO:HB2	2.02	0.42
1:4L:91:VAL:O	1:4L:92:LEU:HD23	2.20	0.42
1:4L:115:ARG:O	1:4L:118:VAL:HG22	2.20	0.42
1:1B:129:TYR:CD1	1:1B:130:ILE:HG12	2.55	0.42
1:1D:143:ASP:HB3	1:1D:187:ILE:HG21	2.02	0.42
1:1E:143:ASP:HB3	1:1E:187:ILE:HG21	2.02	0.42
1:1L:91:VAL:HG12	1:1L:99:LEU:HD12	2.01	0.42
1:1L:190:ALA:O	1:1L:194:LEU:HD22	2.19	0.42
1:1O:89:LEU:HG	1:1O:90:PRO:HD2	2.02	0.42
2:2D:44:TYR:HA	2:2D:47:ILE:HG12	2.00	0.42
2:2J:10:LEU:O	2:2J:14:GLY:N	2.53	0.42
2:2L:5:ARG:O	2:2L:6:LEU:C	2.57	0.42
2:2M:206:HIS:HA	2:2M:209:ILE:HD12	2.02	0.42
2:3I:10:LEU:O	2:3I:14:GLY:N	2.53	0.42
2:3J:206:HIS:HA	2:3J:209:ILE:HD12	2.02	0.42
2:3N:111:VAL:HG13	2:3N:119:LEU:HB2	2.00	0.42
1:4E:61:TYR:OH	1:4F:68:THR:HG22	2.20	0.42
1:4K:38:LYS:HE2	1:4K:44:TYR:CE1	2.55	0.42
1:4L:190:ALA:O	1:4L:194:LEU:HD22	2.19	0.42
1:4N:15:VAL:HG22	1:4N:130:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4N:89:LEU:HG	1:4N:90:PRO:HD2	2.02	0.42
1:4P:89:LEU:HG	1:4P:90:PRO:HD2	2.02	0.42
1:1A:178:ASN:OD1	1:1A:180:ASN:HB2	2.20	0.42
1:1A:196:ALA:O	1:1A:200:GLN:HG2	2.19	0.42
1:1D:128:LEU:HD13	1:1D:128:LEU:C	2.40	0.42
1:1D:174:LEU:HD11	1:1D:194:LEU:CD2	2.49	0.42
1:1K:38:LYS:HG3	1:1L:7:PHE:CD2	2.54	0.42
1:1L:201:LEU:HG	2:2L:90:VAL:HG13	2.02	0.42
1:1M:154:PHE:CE1	1:1M:201:LEU:HD12	2.54	0.42
2:2I:44:TYR:OH	2:3D:42:ILE:HD12	2.20	0.42
2:2J:44:TYR:OH	2:3C:42:ILE:HD12	2.20	0.42
2:2N:107:ILE:HB	2:2N:123:LEU:HD11	2.02	0.42
2:2P:42:ILE:HD12	2:3O:44:TYR:OH	2.20	0.42
2:3A:75:GLU:HB2	2:3B:28:ARG:HE	1.85	0.42
2:3N:10:LEU:O	2:3N:14:GLY:N	2.53	0.42
1:4A:196:ALA:O	1:4A:200:GLN:HG2	2.19	0.42
1:4E:143:ASP:HB3	1:4E:187:ILE:HG21	2.02	0.42
1:4J:56:ILE:CG2	1:4K:54:PRO:HB3	2.50	0.42
1:4L:38:LYS:HG3	1:4M:7:PHE:CE2	2.55	0.42
1:4N:32:TYR:O	1:4N:36:GLU:HG2	2.19	0.42
1:1J:128:LEU:C	1:1J:128:LEU:HD13	2.40	0.42
2:2A:79:TYR:CD1	2:2A:79:TYR:N	2.88	0.42
2:2E:58:PRO:HD3	2:3G:64:HIS:HB3	2.02	0.42
2:2L:64:HIS:HB3	2:3B:58:PRO:HD3	2.02	0.42
2:2M:44:TYR:OH	2:3A:42:ILE:HD12	2.20	0.42
2:2O:90:VAL:HA	2:2O:195:PHE:CE1	2.55	0.42
2:3F:58:PRO:HA	2:3F:61:PHE:HB3	2.00	0.42
2:3F:194:LEU:CD1	1:4F:172:ARG:HD2	2.50	0.42
2:3J:17:ILE:HD12	2:3J:32:THR:HB	2.02	0.42
2:3M:10:LEU:O	2:3M:14:GLY:N	2.53	0.42
2:3M:206:HIS:HA	2:3M:209:ILE:HD12	2.02	0.42
2:3N:17:ILE:HD12	2:3N:32:THR:HB	2.02	0.42
1:4A:89:LEU:HG	1:4A:90:PRO:HD2	2.02	0.42
1:4N:60:ASN:HB3	1:4O:52:PRO:HG2	2.02	0.42
1:1E:56:ILE:CG2	1:1F:54:PRO:HB3	2.50	0.41
1:1K:22:LYS:HE2	1:1K:22:LYS:HB3	1.79	0.41
1:1M:89:LEU:HG	1:1M:90:PRO:HD2	2.02	0.41
1:1P:32:TYR:O	1:1P:36:GLU:HG2	2.19	0.41
2:2I:111:VAL:HG21	2:2I:156:TYR:CG	2.55	0.41
2:2J:206:HIS:HA	2:2J:209:ILE:HD12	2.02	0.41
2:2L:44:TYR:OH	2:3B:42:ILE:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2P:79:TYR:CD1	2:2P:79:TYR:N	2.88	0.41
2:3I:89:GLU:O	2:3I:195:PHE:HB2	2.19	0.41
2:3N:90:VAL:HG11	1:4N:200:GLN:CB	2.50	0.41
2:3O:10:LEU:O	2:3O:14:GLY:N	2.53	0.41
1:4B:141:ASP:O	1:4B:144:ILE:HG12	2.20	0.41
1:4D:38:LYS:HE2	1:4D:44:TYR:HE1	1.85	0.41
1:4E:196:ALA:O	1:4E:200:GLN:HG2	2.20	0.41
1:4J:35:GLN:HA	1:4K:7:PHE:CZ	2.55	0.41
1:4J:128:LEU:C	1:4J:128:LEU:HD13	2.40	0.41
1:4L:128:LEU:HD13	1:4L:128:LEU:C	2.41	0.41
1:4Q:178:ASN:OD1	1:4Q:180:ASN:HB2	2.20	0.41
1:1A:32:TYR:O	1:1A:36:GLU:HG2	2.19	0.41
1:1L:91:VAL:O	1:1L:92:LEU:HD23	2.20	0.41
2:2B:79:TYR:CD1	2:2B:79:TYR:N	2.88	0.41
2:2C:58:PRO:HD3	2:3J:64:HIS:HB3	2.02	0.41
2:2D:42:ILE:HD12	2:3I:44:TYR:OH	2.20	0.41
2:2I:64:HIS:HB3	2:3D:58:PRO:HD3	2.02	0.41
2:2J:5:ARG:O	2:2J:6:LEU:C	2.57	0.41
2:2N:10:LEU:O	2:2N:14:GLY:N	2.53	0.41
2:2O:44:TYR:OH	2:3P:42:ILE:HD12	2.20	0.41
2:2O:94:ILE:HG21	2:2O:212:THR:HG21	2.02	0.41
2:2Q:79:TYR:CD1	2:2Q:79:TYR:N	2.88	0.41
2:3A:79:TYR:CD1	2:3A:79:TYR:N	2.88	0.41
2:3E:79:TYR:CD1	2:3E:79:TYR:N	2.88	0.41
2:3E:194:LEU:O	1:4E:169:LYS:HD3	2.20	0.41
2:3E:195:PHE:HZ	1:4E:170:THR:HB	1.85	0.41
2:3F:79:TYR:CD1	2:3F:79:TYR:N	2.88	0.41
2:3G:10:LEU:O	2:3G:14:GLY:N	2.53	0.41
2:3I:108:LEU:HD12	2:3J:22:LYS:HB2	2.01	0.41
2:3J:10:LEU:O	2:3J:14:GLY:N	2.53	0.41
2:3N:153:LEU:HD23	2:3N:153:LEU:HA	1.91	0.41
2:3O:94:ILE:HG21	2:3O:212:THR:HG21	2.02	0.41
2:3Q:90:VAL:HG12	1:4Q:201:LEU:HD21	2.02	0.41
1:4L:74:VAL:HG22	1:4L:89:LEU:O	2.20	0.41
1:4Q:136:LEU:CD1	1:4Q:181:LYS:HB2	2.50	0.41
1:1D:173:TRP:HH2	1:1D:197:GLY:HA3	1.85	0.41
1:1E:66:LEU:HB2	1:1E:73:PHE:HB2	2.02	0.41
1:1I:169:LYS:HB3	2:2I:192:GLU:OE2	2.20	0.41
1:1K:38:LYS:HE2	1:1K:44:TYR:CE1	2.55	0.41
1:1O:65:TYR:OH	1:1P:70:GLU:HB2	2.20	0.41
1:1P:32:TYR:CE1	1:1P:36:GLU:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2C:79:TYR:CD1	2:2C:79:TYR:N	2.88	0.41
2:2M:10:LEU:O	2:2M:14:GLY:N	2.53	0.41
2:2O:70:ASP:O	2:2O:109:VAL:HA	2.19	0.41
2:3G:206:HIS:HA	2:3G:209:ILE:HD12	2.02	0.41
2:3N:10:LEU:HD22	2:3N:15:LEU:HB2	2.02	0.41
2:3N:73:PHE:HD2	2:3N:105:PHE:HE2	1.68	0.41
1:4P:32:TYR:CE1	1:4P:36:GLU:HG3	2.56	0.41
1:1C:173:TRP:CH2	2:2C:90:VAL:HG21	2.55	0.41
1:1F:172:ARG:HD2	2:2F:194:LEU:CD1	2.50	0.41
1:1H:32:TYR:O	1:1H:35:GLN:HG2	2.20	0.41
1:1J:35:GLN:HA	1:1K:7:PHE:CZ	2.55	0.41
1:1L:66:LEU:HB2	1:1L:73:PHE:HB2	2.02	0.41
1:1N:89:LEU:HG	1:1N:90:PRO:HD2	2.02	0.41
1:1N:161:LYS:HB3	1:1N:161:LYS:NZ	2.36	0.41
2:2G:17:ILE:HD12	2:2G:32:THR:HB	2.02	0.41
2:2N:166:ASN:HA	2:2N:169:PHE:HD2	1.85	0.41
2:2Q:42:ILE:HD12	2:3N:44:TYR:OH	2.20	0.41
2:3G:5:ARG:O	2:3G:6:LEU:C	2.57	0.41
1:4B:35:GLN:HA	1:4C:7:PHE:CZ	2.56	0.41
1:4B:129:TYR:CD1	1:4B:130:ILE:HG12	2.55	0.41
1:4C:196:ALA:O	1:4C:200:GLN:HG2	2.20	0.41
1:4H:32:TYR:O	1:4H:35:GLN:HG2	2.20	0.41
1:4Q:159:GLN:HG3	1:4Q:165:ALA:HB3	2.02	0.41
1:1A:89:LEU:HG	1:1A:90:PRO:HD2	2.02	0.41
1:1E:169:LYS:HD3	2:2E:194:LEU:O	2.20	0.41
1:1G:89:LEU:HG	1:1G:90:PRO:HD2	2.02	0.41
1:1G:106:THR:HG23	1:1H:90:PRO:HB2	2.02	0.41
1:1Q:38:LYS:HE2	1:1Q:44:TYR:HE1	1.84	0.41
2:2A:75:GLU:HB2	2:2B:28:ARG:HE	1.85	0.41
2:2F:79:TYR:CD1	2:2F:79:TYR:N	2.88	0.41
2:2G:10:LEU:O	2:2G:14:GLY:N	2.53	0.41
2:3I:206:HIS:HA	2:3I:209:ILE:HD12	2.02	0.41
2:3Q:79:TYR:CD1	2:3Q:79:TYR:N	2.88	0.41
1:4D:173:TRP:HH2	1:4D:197:GLY:HA3	1.85	0.41
1:4H:32:TYR:O	1:4H:36:GLU:HG2	2.19	0.41
1:4M:202:ASP:O	1:4M:203:SER:C	2.59	0.41
1:4O:89:LEU:HG	1:4O:90:PRO:HD2	2.02	0.41
1:4Q:148:GLU:O	1:4Q:151:ILE:HG12	2.21	0.41
1:1C:196:ALA:O	1:1C:200:GLN:HG2	2.20	0.41
1:1E:54:PRO:HD2	1:1E:67:ALA:HB3	2.02	0.41
1:1I:174:LEU:HD22	1:1I:174:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1L:74:VAL:HG22	1:1L:89:LEU:O	2.20	0.41
1:1N:158:SER:CB	1:1N:164:ASP:HA	2.49	0.41
1:1Q:178:ASN:OD1	1:1Q:180:ASN:HB2	2.20	0.41
2:2B:42:ILE:HD12	2:3L:44:TYR:OH	2.20	0.41
2:2L:10:LEU:O	2:2L:14:GLY:N	2.53	0.41
2:2L:206:HIS:HA	2:2L:209:ILE:HD12	2.01	0.41
2:3I:111:VAL:HG21	2:3I:156:TYR:CG	2.55	0.41
2:3I:192:GLU:OE2	1:4I:169:LYS:HB3	2.20	0.41
2:3N:107:ILE:HB	2:3N:123:LEU:HD11	2.02	0.41
1:4B:56:ILE:CG2	1:4C:54:PRO:HB3	2.51	0.41
1:4E:66:LEU:HB2	1:4E:73:PHE:HB2	2.02	0.41
1:4G:15:VAL:HG23	1:4G:130:ILE:HD11	2.02	0.41
1:1B:141:ASP:O	1:1B:144:ILE:HG12	2.20	0.41
1:1G:15:VAL:HG23	1:1G:130:ILE:HD11	2.02	0.41
1:1I:154:PHE:HE2	1:1I:173:TRP:HZ3	1.66	0.41
1:1N:144:ILE:O	1:1N:147:LEU:HB3	2.21	0.41
2:2A:42:ILE:HD12	2:3M:44:TYR:OH	2.20	0.41
2:2B:58:PRO:HD3	2:3L:64:HIS:HB3	2.02	0.41
2:2C:42:ILE:HD12	2:3J:44:TYR:OH	2.20	0.41
2:3B:79:TYR:CD1	2:3B:79:TYR:N	2.88	0.41
1:4L:127:GLY:O	1:4L:130:ILE:HG22	2.20	0.41
1:1E:170:THR:HB	2:2E:195:PHE:HZ	1.85	0.41
1:1L:115:ARG:O	1:1L:118:VAL:HG22	2.20	0.41
1:1N:154:PHE:HZ	2:2N:89:GLU:CD	2.22	0.41
1:1O:38:LYS:HG3	1:1P:7:PHE:CD2	2.56	0.41
2:2D:79:TYR:CD1	2:2D:79:TYR:N	2.88	0.41
2:2E:79:TYR:CD1	2:2E:79:TYR:N	2.88	0.41
2:2G:64:HIS:HB3	2:3E:58:PRO:HD3	2.02	0.41
2:2J:90:VAL:HG23	2:2J:91:THR:N	2.36	0.41
2:2O:206:HIS:HA	2:2O:209:ILE:HD12	2.02	0.41
2:3O:73:PHE:HD2	2:3O:105:PHE:HE2	1.69	0.41
2:3P:79:TYR:CD1	2:3P:79:TYR:N	2.88	0.41
1:4D:196:ALA:O	1:4D:200:GLN:HG2	2.21	0.41
1:4L:32:TYR:O	1:4L:36:GLU:HG2	2.19	0.41
1:4N:157:LEU:HD13	1:4N:201:LEU:HD12	2.01	0.41
1:1B:89:LEU:HG	1:1B:90:PRO:HD2	2.02	0.41
1:1D:173:TRP:HB2	2:2D:194:LEU:CD2	2.51	0.41
1:1E:196:ALA:O	1:1E:200:GLN:HG2	2.21	0.41
1:1I:158:SER:HB3	2:2I:195:PHE:HA	2.02	0.41
1:1L:128:LEU:HD13	1:1L:128:LEU:C	2.41	0.41
1:1M:176:ILE:HD12	1:1M:179:ILE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1N:200:GLN:CB	2:2N:90:VAL:HG11	2.50	0.41
1:1P:89:LEU:HG	1:1P:90:PRO:HD2	2.02	0.41
1:1P:148:GLU:O	1:1P:151:ILE:HG12	2.21	0.41
2:2A:58:PRO:HD3	2:3M:64:HIS:HB3	2.02	0.41
2:2F:164:LEU:HD23	2:2F:164:LEU:HA	1.90	0.41
2:2G:44:TYR:OH	2:3E:42:ILE:HD12	2.20	0.41
2:2G:91:THR:O	2:2G:92:ALA:C	2.60	0.41
2:2I:90:VAL:HG23	2:2I:91:THR:N	2.36	0.41
2:2I:148:ASP:N	2:2I:148:ASP:OD1	2.54	0.41
2:2M:125:VAL:HB	2:2M:142:PHE:HB3	2.03	0.41
2:2N:64:HIS:HB3	2:3Q:58:PRO:HD3	2.02	0.41
2:3C:79:TYR:CD1	2:3C:79:TYR:N	2.88	0.41
2:3C:90:VAL:HG21	1:4C:173:TRP:CH2	2.55	0.41
2:3D:194:LEU:CD2	1:4D:173:TRP:HB2	2.51	0.41
2:3I:17:ILE:HD12	2:3I:32:THR:HB	2.02	0.41
2:3I:91:THR:O	2:3I:92:ALA:C	2.59	0.41
2:3L:10:LEU:O	2:3L:14:GLY:N	2.53	0.41
2:3O:125:VAL:HB	2:3O:142:PHE:HB3	2.03	0.41
1:4A:178:ASN:OD1	1:4A:180:ASN:HB2	2.20	0.41
1:4M:190:ALA:O	1:4M:194:LEU:HD23	2.21	0.41
1:4N:144:ILE:O	1:4N:147:LEU:HB3	2.21	0.41
1:4O:65:TYR:OH	1:4P:70:GLU:HB2	2.20	0.41
1:4P:148:GLU:O	1:4P:151:ILE:HG12	2.21	0.41
1:1H:38:LYS:HE2	1:1H:44:TYR:HE1	1.85	0.41
2:2I:10:LEU:O	2:2I:14:GLY:N	2.53	0.41
2:2I:206:HIS:HA	2:2I:209:ILE:HD12	2.02	0.41
2:3D:79:TYR:CD1	2:3D:79:TYR:N	2.88	0.41
2:3J:5:ARG:O	2:3J:6:LEU:C	2.57	0.41
1:4M:31:SER:HB2	1:4N:129:TYR:HA	2.03	0.41
1:4M:94:PHE:CD1	1:4M:95:ARG:HG3	2.56	0.41
1:1L:7:PHE:HE1	1:1L:11:ASN:HD22	1.67	0.40
1:1M:94:PHE:CD1	1:1M:95:ARG:HG3	2.56	0.40
1:1M:157:LEU:HD13	1:1M:202:ASP:HB2	2.03	0.40
1:1N:60:ASN:HB3	1:1O:52:PRO:HG2	2.02	0.40
1:1P:110:ASN:CB	1:1Q:90:PRO:HD3	2.51	0.40
2:2E:42:ILE:HD12	2:3G:44:TYR:OH	2.20	0.40
2:2I:125:VAL:HB	2:2I:142:PHE:HB3	2.03	0.40
2:2J:148:ASP:OD1	2:2J:148:ASP:N	2.53	0.40
2:2N:148:ASP:N	2:2N:148:ASP:OD1	2.53	0.40
2:2P:164:LEU:HD23	2:2P:164:LEU:HA	1.90	0.40
2:2Q:58:PRO:HD3	2:3N:64:HIS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3I:125:VAL:HB	2:3I:142:PHE:HB3	2.03	0.40
1:4B:35:GLN:CB	1:4C:7:PHE:CZ	3.04	0.40
1:4M:38:LYS:HE2	1:4M:44:TYR:HE1	1.86	0.40
1:1D:38:LYS:HE2	1:1D:44:TYR:HE1	1.85	0.40
1:1D:196:ALA:O	1:1D:200:GLN:HG2	2.21	0.40
1:1I:91:VAL:O	1:1I:92:LEU:HD23	2.21	0.40
1:1M:173:TRP:HZ2	1:1M:194:LEU:CD1	2.34	0.40
1:1M:202:ASP:O	1:1M:203:SER:C	2.59	0.40
2:2N:10:LEU:HD22	2:2N:15:LEU:HB2	2.02	0.40
2:3J:90:VAL:HG23	2:3J:91:THR:N	2.36	0.40
2:3O:93:ASN:HB3	2:3O:96:HIS:CE1	2.56	0.40
1:4M:56:ILE:HD12	1:4N:54:PRO:HB2	2.02	0.40
1:4M:170:THR:HA	1:4M:173:TRP:CD1	2.56	0.40
1:1I:89:LEU:HD23	1:1I:89:LEU:HA	1.92	0.40
1:1N:178:ASN:ND2	1:1N:180:ASN:H	2.19	0.40
1:1P:172:ARG:HD3	2:2P:194:LEU:HD11	2.03	0.40
2:2L:17:ILE:HD12	2:2L:32:THR:HB	2.03	0.40
2:2L:94:ILE:HG21	2:2L:212:THR:HG21	2.02	0.40
2:2L:148:ASP:N	2:2L:148:ASP:OD1	2.53	0.40
2:2O:10:LEU:HD21	2:2O:20:VAL:HG21	2.03	0.40
2:2O:93:ASN:HB3	2:2O:96:HIS:CE1	2.56	0.40
2:3J:148:ASP:N	2:3J:148:ASP:OD1	2.53	0.40
1:4C:31:SER:HB2	1:4D:128:LEU:HD13	2.03	0.40
1:4I:60:ASN:HB2	1:4J:52:PRO:HG2	2.03	0.40
1:4L:7:PHE:HE1	1:4L:11:ASN:HD22	1.67	0.40
1:1C:31:SER:HB2	1:1D:128:LEU:HD13	2.03	0.40
2:2M:64:HIS:HB3	2:3A:58:PRO:HD3	2.02	0.40
2:2N:44:TYR:OH	2:3Q:42:ILE:HD12	2.20	0.40
2:3D:198:LYS:HA	1:4D:162:GLY:O	2.21	0.40
1:4M:173:TRP:HZ2	1:4M:194:LEU:CD1	2.34	0.40
1:1B:35:GLN:HA	1:1C:7:PHE:CZ	2.56	0.40
1:1L:38:LYS:HG3	1:1M:7:PHE:CE2	2.55	0.40
1:1N:154:PHE:CD1	1:1N:198:LEU:HB2	2.54	0.40
2:2I:17:ILE:HD12	2:2I:32:THR:HB	2.02	0.40
2:2L:100:ILE:HG12	2:2L:103:PHE:HB2	2.04	0.40
2:2O:64:HIS:HB3	2:3P:58:PRO:HD3	2.03	0.40
2:2Q:6:LEU:HD23	2:2Q:6:LEU:HA	1.86	0.40
2:3A:88:PHE:HB2	2:3A:97:ALA:HA	2.04	0.40
2:3F:164:LEU:HA	2:3F:164:LEU:HD23	1.90	0.40
2:3G:91:THR:O	2:3G:92:ALA:C	2.59	0.40
1:4D:38:LYS:HG3	1:4E:7:PHE:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4G:38:LYS:HE2	1:4G:44:TYR:CE1	2.56	0.40
1:4M:89:LEU:HG	1:4M:90:PRO:HD2	2.02	0.40
1:4M:176:ILE:HD12	1:4M:179:ILE:HA	2.02	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 PDB entries followed by that with respect to all EM entries.

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	1A	199/206 (97%)	195 (98%)	4 (2%)	0	100	100
1	1B	199/206 (97%)	196 (98%)	3 (2%)	0	100	100
1	1C	199/206 (97%)	196 (98%)	3 (2%)	0	100	100
1	1D	199/206 (97%)	195 (98%)	4 (2%)	0	100	100
1	1E	199/206 (97%)	194 (98%)	5 (2%)	0	100	100
1	1F	191/206 (93%)	189 (99%)	2 (1%)	0	100	100
1	1G	126/206 (61%)	124 (98%)	2 (2%)	0	100	100
1	1H	126/206 (61%)	124 (98%)	2 (2%)	0	100	100
1	1I	198/206 (96%)	194 (98%)	4 (2%)	0	100	100
1	1J	198/206 (96%)	194 (98%)	4 (2%)	0	100	100
1	1K	126/206 (61%)	124 (98%)	2 (2%)	0	100	100
1	1L	198/206 (96%)	195 (98%)	3 (2%)	0	100	100
1	1M	198/206 (96%)	194 (98%)	4 (2%)	0	100	100
1	1N	198/206 (96%)	195 (98%)	3 (2%)	0	100	100
1	1O	126/206 (61%)	124 (98%)	2 (2%)	0	100	100
1	1P	199/206 (97%)	196 (98%)	3 (2%)	0	100	100
1	1Q	199/206 (97%)	195 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4A	199/206 (97%)	195 (98%)	4 (2%)	0	100	100
1	4B	199/206 (97%)	196 (98%)	3 (2%)	0	100	100
1	4C	199/206 (97%)	196 (98%)	3 (2%)	0	100	100
1	4D	199/206 (97%)	195 (98%)	4 (2%)	0	100	100
1	4E	199/206 (97%)	194 (98%)	5 (2%)	0	100	100
1	4F	191/206 (93%)	189 (99%)	2 (1%)	0	100	100
1	4G	126/206 (61%)	124 (98%)	2 (2%)	0	100	100
1	4H	126/206 (61%)	124 (98%)	2 (2%)	0	100	100
1	4I	198/206 (96%)	194 (98%)	4 (2%)	0	100	100
1	4J	198/206 (96%)	194 (98%)	4 (2%)	0	100	100
1	4K	126/206 (61%)	124 (98%)	2 (2%)	0	100	100
1	4L	198/206 (96%)	195 (98%)	3 (2%)	0	100	100
1	4M	198/206 (96%)	194 (98%)	4 (2%)	0	100	100
1	4N	198/206 (96%)	195 (98%)	3 (2%)	0	100	100
1	4O	126/206 (61%)	124 (98%)	2 (2%)	0	100	100
1	4P	199/206 (97%)	196 (98%)	3 (2%)	0	100	100
1	4Q	199/206 (97%)	195 (98%)	4 (2%)	0	100	100
2	2A	220/233 (94%)	216 (98%)	4 (2%)	0	100	100
2	2B	220/233 (94%)	216 (98%)	4 (2%)	0	100	100
2	2C	220/233 (94%)	217 (99%)	3 (1%)	0	100	100
2	2D	220/233 (94%)	216 (98%)	4 (2%)	0	100	100
2	2E	220/233 (94%)	214 (97%)	6 (3%)	0	100	100
2	2F	220/233 (94%)	214 (97%)	6 (3%)	0	100	100
2	2G	213/233 (91%)	208 (98%)	5 (2%)	0	100	100
2	2I	213/233 (91%)	208 (98%)	5 (2%)	0	100	100
2	2J	213/233 (91%)	208 (98%)	5 (2%)	0	100	100
2	2L	213/233 (91%)	208 (98%)	5 (2%)	0	100	100
2	2M	213/233 (91%)	207 (97%)	6 (3%)	0	100	100
2	2N	213/233 (91%)	209 (98%)	4 (2%)	0	100	100
2	2O	213/233 (91%)	209 (98%)	4 (2%)	0	100	100
2	2P	220/233 (94%)	215 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2Q	220/233 (94%)	216 (98%)	4 (2%)	0	100	100
2	3A	220/233 (94%)	216 (98%)	4 (2%)	0	100	100
2	3B	220/233 (94%)	216 (98%)	4 (2%)	0	100	100
2	3C	220/233 (94%)	217 (99%)	3 (1%)	0	100	100
2	3D	220/233 (94%)	216 (98%)	4 (2%)	0	100	100
2	3E	220/233 (94%)	214 (97%)	6 (3%)	0	100	100
2	3F	220/233 (94%)	214 (97%)	6 (3%)	0	100	100
2	3G	213/233 (91%)	208 (98%)	5 (2%)	0	100	100
2	3I	213/233 (91%)	208 (98%)	5 (2%)	0	100	100
2	3J	213/233 (91%)	208 (98%)	5 (2%)	0	100	100
2	3L	213/233 (91%)	208 (98%)	5 (2%)	0	100	100
2	3M	213/233 (91%)	207 (97%)	6 (3%)	0	100	100
2	3N	213/233 (91%)	209 (98%)	4 (2%)	0	100	100
2	3O	213/233 (91%)	209 (98%)	4 (2%)	0	100	100
2	3P	220/233 (94%)	215 (98%)	5 (2%)	0	100	100
2	3Q	220/233 (94%)	216 (98%)	4 (2%)	0	100	100
All	All	12658/13994 (90%)	12410 (98%)	248 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1A	180/185 (97%)	180 (100%)	0	100	100
1	1B	180/185 (97%)	180 (100%)	0	100	100
1	1C	180/185 (97%)	180 (100%)	0	100	100
1	1D	180/185 (97%)	180 (100%)	0	100	100
1	1E	180/185 (97%)	179 (99%)	1 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1F	176/185 (95%)	176 (100%)	0	100 100
1	1G	115/185 (62%)	114 (99%)	1 (1%)	75 83
1	1H	115/185 (62%)	115 (100%)	0	100 100
1	1I	179/185 (97%)	177 (99%)	2 (1%)	70 79
1	1J	179/185 (97%)	179 (100%)	0	100 100
1	1K	115/185 (62%)	115 (100%)	0	100 100
1	1L	179/185 (97%)	179 (100%)	0	100 100
1	1M	179/185 (97%)	177 (99%)	2 (1%)	70 79
1	1N	179/185 (97%)	176 (98%)	3 (2%)	56 72
1	1O	115/185 (62%)	115 (100%)	0	100 100
1	1P	180/185 (97%)	177 (98%)	3 (2%)	56 72
1	1Q	180/185 (97%)	180 (100%)	0	100 100
1	4A	180/185 (97%)	180 (100%)	0	100 100
1	4B	180/185 (97%)	180 (100%)	0	100 100
1	4C	180/185 (97%)	180 (100%)	0	100 100
1	4D	180/185 (97%)	180 (100%)	0	100 100
1	4E	180/185 (97%)	179 (99%)	1 (1%)	84 88
1	4F	176/185 (95%)	176 (100%)	0	100 100
1	4G	115/185 (62%)	114 (99%)	1 (1%)	75 83
1	4H	115/185 (62%)	115 (100%)	0	100 100
1	4I	179/185 (97%)	177 (99%)	2 (1%)	70 79
1	4J	179/185 (97%)	179 (100%)	0	100 100
1	4K	115/185 (62%)	115 (100%)	0	100 100
1	4L	179/185 (97%)	179 (100%)	0	100 100
1	4M	179/185 (97%)	177 (99%)	2 (1%)	70 79
1	4N	179/185 (97%)	178 (99%)	1 (1%)	84 88
1	4O	115/185 (62%)	115 (100%)	0	100 100
1	4P	180/185 (97%)	177 (98%)	3 (2%)	56 72
1	4Q	180/185 (97%)	180 (100%)	0	100 100
2	2A	209/218 (96%)	208 (100%)	1 (0%)	86 90
2	2B	209/218 (96%)	209 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2C	209/218 (96%)	208 (100%)	1 (0%)	86	90
2	2D	209/218 (96%)	208 (100%)	1 (0%)	86	90
2	2E	209/218 (96%)	208 (100%)	1 (0%)	86	90
2	2F	209/218 (96%)	207 (99%)	2 (1%)	73	81
2	2G	205/218 (94%)	205 (100%)	0	100	100
2	2I	205/218 (94%)	205 (100%)	0	100	100
2	2J	205/218 (94%)	204 (100%)	1 (0%)	86	90
2	2L	205/218 (94%)	204 (100%)	1 (0%)	86	90
2	2M	205/218 (94%)	204 (100%)	1 (0%)	86	90
2	2N	205/218 (94%)	205 (100%)	0	100	100
2	2O	205/218 (94%)	203 (99%)	2 (1%)	73	81
2	2P	209/218 (96%)	208 (100%)	1 (0%)	86	90
2	2Q	209/218 (96%)	209 (100%)	0	100	100
2	3A	209/218 (96%)	208 (100%)	1 (0%)	86	90
2	3B	209/218 (96%)	209 (100%)	0	100	100
2	3C	209/218 (96%)	208 (100%)	1 (0%)	86	90
2	3D	209/218 (96%)	208 (100%)	1 (0%)	86	90
2	3E	209/218 (96%)	208 (100%)	1 (0%)	86	90
2	3F	209/218 (96%)	207 (99%)	2 (1%)	73	81
2	3G	205/218 (94%)	205 (100%)	0	100	100
2	3I	205/218 (94%)	205 (100%)	0	100	100
2	3J	205/218 (94%)	204 (100%)	1 (0%)	86	90
2	3L	205/218 (94%)	204 (100%)	1 (0%)	86	90
2	3M	205/218 (94%)	204 (100%)	1 (0%)	86	90
2	3N	205/218 (94%)	205 (100%)	0	100	100
2	3O	205/218 (94%)	204 (100%)	1 (0%)	86	90
2	3P	209/218 (96%)	209 (100%)	0	100	100
2	3Q	209/218 (96%)	209 (100%)	0	100	100
All	All	11796/12830 (92%)	11752 (100%)	44 (0%)	88	91

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1E	28	LEU
1	1G	6	LEU
1	1I	142	ASN
1	1I	157	LEU
1	1M	28	LEU
1	1M	201	LEU
1	1N	128	LEU
1	1N	134	GLU
1	1N	178	ASN
1	1P	129	TYR
1	1P	135	GLU
1	1P	142	ASN
2	2A	105	PHE
2	2C	108	LEU
2	2D	108	LEU
2	2E	108	LEU
2	2F	108	LEU
2	2F	195	PHE
2	2J	108	LEU
2	2L	108	LEU
2	2M	17	ILE
2	2O	89	GLU
2	2O	90	VAL
2	2P	28	ARG
2	3A	105	PHE
2	3C	108	LEU
2	3D	108	LEU
2	3E	108	LEU
2	3F	108	LEU
2	3F	195	PHE
2	3J	108	LEU
2	3L	108	LEU
2	3M	17	ILE
2	3O	89	GLU
1	4E	28	LEU
1	4G	6	LEU
1	4I	142	ASN
1	4I	157	LEU
1	4M	28	LEU
1	4M	201	LEU
1	4N	134	GLU
1	4P	129	TYR
1	4P	135	GLU

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Mol	Chain	Res	Type
1	4P	142	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	4	GLN
1	1A	34	HIS
1	1A	191	HIS
1	1B	4	GLN
1	1B	34	HIS
1	1B	200	GLN
1	1C	4	GLN
1	1D	4	GLN
1	1D	180	ASN
1	1E	4	GLN
1	1E	34	HIS
1	1E	110	ASN
1	1E	132	ASN
1	1E	180	ASN
1	1F	4	GLN
1	1F	34	HIS
1	1F	132	ASN
1	1G	4	GLN
1	1H	4	GLN
1	1H	23	ASN
1	1I	4	GLN
1	1I	34	HIS
1	1I	132	ASN
1	1I	142	ASN
1	1J	4	GLN
1	1J	34	HIS
1	1J	156	ASN
1	1K	4	GLN
1	1K	34	HIS
1	1L	4	GLN
1	1L	34	HIS
1	1M	4	GLN
1	1M	34	HIS
1	1M	191	HIS
1	1N	4	GLN
1	1N	34	HIS
1	1N	178	ASN

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Mol	Chain	Res	Type
1	1N	180	ASN
1	1O	4	GLN
1	1O	34	HIS
1	1P	4	GLN
1	1P	34	HIS
1	1P	132	ASN
1	1P	142	ASN
1	1P	191	HIS
1	1Q	4	GLN
1	1Q	34	HIS
1	1Q	191	HIS
2	2F	55	HIS
2	2G	65	ASN
2	2G	137	GLN
2	2G	138	HIS
2	2I	65	ASN
2	2I	137	GLN
2	2I	138	HIS
2	2J	65	ASN
2	2J	137	GLN
2	2J	138	HIS
2	2L	65	ASN
2	2M	65	ASN
2	2N	65	ASN
2	2O	65	ASN
2	2O	138	HIS
2	3G	65	ASN
2	3G	137	GLN
2	3G	138	HIS
2	3I	65	ASN
2	3I	137	GLN
2	3I	138	HIS
2	3J	65	ASN
2	3J	137	GLN
2	3J	138	HIS
2	3L	65	ASN
2	3M	65	ASN
2	3N	65	ASN
2	3O	65	ASN
1	4A	4	GLN
1	4A	34	HIS
1	4A	191	HIS

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Mol	Chain	Res	Type
1	4B	4	GLN
1	4B	34	HIS
1	4B	200	GLN
1	4C	4	GLN
1	4D	4	GLN
1	4D	180	ASN
1	4E	4	GLN
1	4E	34	HIS
1	4E	132	ASN
1	4E	180	ASN
1	4F	4	GLN
1	4F	132	ASN
1	4G	4	GLN
1	4H	4	GLN
1	4H	23	ASN
1	4I	4	GLN
1	4I	34	HIS
1	4I	132	ASN
1	4I	142	ASN
1	4J	4	GLN
1	4J	34	HIS
1	4J	156	ASN
1	4K	4	GLN
1	4K	34	HIS
1	4L	4	GLN
1	4L	34	HIS
1	4M	4	GLN
1	4M	191	HIS
1	4N	4	GLN
1	4N	34	HIS
1	4O	4	GLN
1	4O	34	HIS
1	4P	4	GLN
1	4P	34	HIS
1	4P	132	ASN
1	4P	142	ASN
1	4P	191	HIS
1	4Q	4	GLN
1	4Q	34	HIS
1	4Q	191	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.