



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:33 PM GMT

PDB ID : 3TXX  
Title : Crystal structure of putrescine transcarbamylase from *Enterococcus faecalis*  
Authors : Shi, D.; Yu, X.; Zhao, G.; Allewell, N.M.; Tuchman, M.  
Deposited on : 2011-09-23  
Resolution : 3.20 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

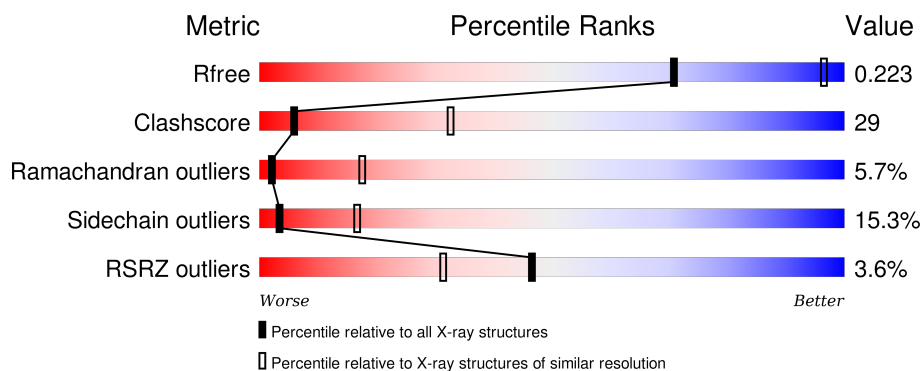
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	359	<div> <div>50%</div> <div>32%</div> <div>12%</div> <div>6%</div> </div>
1	B	359	<div> <div>51%</div> <div>33%</div> <div>13%</div> <div>2%</div> </div>
1	C	359	<div> <div>51%</div> <div>31%</div> <div>12%</div> <div>5%</div> </div>
1	D	359	<div> <div>53%</div> <div>32%</div> <div>11%</div> <div>2%</div> </div>
1	E	359	<div> <div>52%</div> <div>32%</div> <div>11%</div> <div>2%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	359	
1	G	359	
1	H	359	
1	I	359	
1	J	359	
1	K	359	
1	L	359	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	340	-	-	-	X
2	SO4	G	340	-	-	-	X
2	SO4	H	340	-	-	-	X
2	SO4	K	340	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32142 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putrescine carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2642	1660	441	520	21			
1	B	353	Total	C	N	O	S	0	0	0
			2766	1733	470	541	22			
1	C	340	Total	C	N	O	S	0	0	0
			2659	1668	444	525	22			
1	D	347	Total	C	N	O	S	0	0	0
			2707	1698	455	532	22			
1	E	343	Total	C	N	O	S	0	0	0
			2694	1687	457	528	22			
1	F	340	Total	C	N	O	S	0	0	0
			2664	1670	446	526	22			
1	G	341	Total	C	N	O	S	0	0	0
			2660	1665	447	526	22			
1	H	336	Total	C	N	O	S	0	0	0
			2631	1648	441	520	22			
1	I	332	Total	C	N	O	S	0	0	0
			2606	1634	438	512	22			
1	J	341	Total	C	N	O	S	0	0	0
			2651	1662	446	521	22			
1	K	341	Total	C	N	O	S	0	0	0
			2656	1663	446	525	22			
1	L	341	Total	C	N	O	S	0	0	0
			2671	1674	449	526	22			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q837U7
A	-18	GLY	-	EXPRESSION TAG	UNP Q837U7
A	-17	SER	-	EXPRESSION TAG	UNP Q837U7
A	-16	SER	-	EXPRESSION TAG	UNP Q837U7
A	-15	HIS	-	EXPRESSION TAG	UNP Q837U7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	EXPRESSION TAG	UNP Q837U7
A	-13	HIS	-	EXPRESSION TAG	UNP Q837U7
A	-12	HIS	-	EXPRESSION TAG	UNP Q837U7
A	-11	HIS	-	EXPRESSION TAG	UNP Q837U7
A	-10	HIS	-	EXPRESSION TAG	UNP Q837U7
A	-9	SER	-	EXPRESSION TAG	UNP Q837U7
A	-8	SER	-	EXPRESSION TAG	UNP Q837U7
A	-7	GLY	-	EXPRESSION TAG	UNP Q837U7
A	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
A	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
A	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
A	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
A	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
A	-1	SER	-	EXPRESSION TAG	UNP Q837U7
A	0	HIS	-	EXPRESSION TAG	UNP Q837U7
B	-19	MET	-	EXPRESSION TAG	UNP Q837U7
B	-18	GLY	-	EXPRESSION TAG	UNP Q837U7
B	-17	SER	-	EXPRESSION TAG	UNP Q837U7
B	-16	SER	-	EXPRESSION TAG	UNP Q837U7
B	-15	HIS	-	EXPRESSION TAG	UNP Q837U7
B	-14	HIS	-	EXPRESSION TAG	UNP Q837U7
B	-13	HIS	-	EXPRESSION TAG	UNP Q837U7
B	-12	HIS	-	EXPRESSION TAG	UNP Q837U7
B	-11	HIS	-	EXPRESSION TAG	UNP Q837U7
B	-10	HIS	-	EXPRESSION TAG	UNP Q837U7
B	-9	SER	-	EXPRESSION TAG	UNP Q837U7
B	-8	SER	-	EXPRESSION TAG	UNP Q837U7
B	-7	GLY	-	EXPRESSION TAG	UNP Q837U7
B	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
B	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
B	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
B	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
B	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
B	-1	SER	-	EXPRESSION TAG	UNP Q837U7
B	0	HIS	-	EXPRESSION TAG	UNP Q837U7
C	-19	MET	-	EXPRESSION TAG	UNP Q837U7
C	-18	GLY	-	EXPRESSION TAG	UNP Q837U7
C	-17	SER	-	EXPRESSION TAG	UNP Q837U7
C	-16	SER	-	EXPRESSION TAG	UNP Q837U7
C	-15	HIS	-	EXPRESSION TAG	UNP Q837U7
C	-14	HIS	-	EXPRESSION TAG	UNP Q837U7
C	-13	HIS	-	EXPRESSION TAG	UNP Q837U7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	EXPRESSION TAG	UNP Q837U7
C	-11	HIS	-	EXPRESSION TAG	UNP Q837U7
C	-10	HIS	-	EXPRESSION TAG	UNP Q837U7
C	-9	SER	-	EXPRESSION TAG	UNP Q837U7
C	-8	SER	-	EXPRESSION TAG	UNP Q837U7
C	-7	GLY	-	EXPRESSION TAG	UNP Q837U7
C	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
C	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
C	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
C	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
C	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
C	-1	SER	-	EXPRESSION TAG	UNP Q837U7
C	0	HIS	-	EXPRESSION TAG	UNP Q837U7
D	-19	MET	-	EXPRESSION TAG	UNP Q837U7
D	-18	GLY	-	EXPRESSION TAG	UNP Q837U7
D	-17	SER	-	EXPRESSION TAG	UNP Q837U7
D	-16	SER	-	EXPRESSION TAG	UNP Q837U7
D	-15	HIS	-	EXPRESSION TAG	UNP Q837U7
D	-14	HIS	-	EXPRESSION TAG	UNP Q837U7
D	-13	HIS	-	EXPRESSION TAG	UNP Q837U7
D	-12	HIS	-	EXPRESSION TAG	UNP Q837U7
D	-11	HIS	-	EXPRESSION TAG	UNP Q837U7
D	-10	HIS	-	EXPRESSION TAG	UNP Q837U7
D	-9	SER	-	EXPRESSION TAG	UNP Q837U7
D	-8	SER	-	EXPRESSION TAG	UNP Q837U7
D	-7	GLY	-	EXPRESSION TAG	UNP Q837U7
D	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
D	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
D	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
D	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
D	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
D	-1	SER	-	EXPRESSION TAG	UNP Q837U7
D	0	HIS	-	EXPRESSION TAG	UNP Q837U7
E	-19	MET	-	EXPRESSION TAG	UNP Q837U7
E	-18	GLY	-	EXPRESSION TAG	UNP Q837U7
E	-17	SER	-	EXPRESSION TAG	UNP Q837U7
E	-16	SER	-	EXPRESSION TAG	UNP Q837U7
E	-15	HIS	-	EXPRESSION TAG	UNP Q837U7
E	-14	HIS	-	EXPRESSION TAG	UNP Q837U7
E	-13	HIS	-	EXPRESSION TAG	UNP Q837U7
E	-12	HIS	-	EXPRESSION TAG	UNP Q837U7
E	-11	HIS	-	EXPRESSION TAG	UNP Q837U7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	EXPRESSION TAG	UNP Q837U7
E	-9	SER	-	EXPRESSION TAG	UNP Q837U7
E	-8	SER	-	EXPRESSION TAG	UNP Q837U7
E	-7	GLY	-	EXPRESSION TAG	UNP Q837U7
E	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
E	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
E	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
E	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
E	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
E	-1	SER	-	EXPRESSION TAG	UNP Q837U7
E	0	HIS	-	EXPRESSION TAG	UNP Q837U7
F	-19	MET	-	EXPRESSION TAG	UNP Q837U7
F	-18	GLY	-	EXPRESSION TAG	UNP Q837U7
F	-17	SER	-	EXPRESSION TAG	UNP Q837U7
F	-16	SER	-	EXPRESSION TAG	UNP Q837U7
F	-15	HIS	-	EXPRESSION TAG	UNP Q837U7
F	-14	HIS	-	EXPRESSION TAG	UNP Q837U7
F	-13	HIS	-	EXPRESSION TAG	UNP Q837U7
F	-12	HIS	-	EXPRESSION TAG	UNP Q837U7
F	-11	HIS	-	EXPRESSION TAG	UNP Q837U7
F	-10	HIS	-	EXPRESSION TAG	UNP Q837U7
F	-9	SER	-	EXPRESSION TAG	UNP Q837U7
F	-8	SER	-	EXPRESSION TAG	UNP Q837U7
F	-7	GLY	-	EXPRESSION TAG	UNP Q837U7
F	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
F	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
F	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
F	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
F	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
F	-1	SER	-	EXPRESSION TAG	UNP Q837U7
F	0	HIS	-	EXPRESSION TAG	UNP Q837U7
G	-19	MET	-	EXPRESSION TAG	UNP Q837U7
G	-18	GLY	-	EXPRESSION TAG	UNP Q837U7
G	-17	SER	-	EXPRESSION TAG	UNP Q837U7
G	-16	SER	-	EXPRESSION TAG	UNP Q837U7
G	-15	HIS	-	EXPRESSION TAG	UNP Q837U7
G	-14	HIS	-	EXPRESSION TAG	UNP Q837U7
G	-13	HIS	-	EXPRESSION TAG	UNP Q837U7
G	-12	HIS	-	EXPRESSION TAG	UNP Q837U7
G	-11	HIS	-	EXPRESSION TAG	UNP Q837U7
G	-10	HIS	-	EXPRESSION TAG	UNP Q837U7
G	-9	SER	-	EXPRESSION TAG	UNP Q837U7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	EXPRESSION TAG	UNP Q837U7
G	-7	GLY	-	EXPRESSION TAG	UNP Q837U7
G	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
G	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
G	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
G	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
G	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
G	-1	SER	-	EXPRESSION TAG	UNP Q837U7
G	0	HIS	-	EXPRESSION TAG	UNP Q837U7
H	-19	MET	-	EXPRESSION TAG	UNP Q837U7
H	-18	GLY	-	EXPRESSION TAG	UNP Q837U7
H	-17	SER	-	EXPRESSION TAG	UNP Q837U7
H	-16	SER	-	EXPRESSION TAG	UNP Q837U7
H	-15	HIS	-	EXPRESSION TAG	UNP Q837U7
H	-14	HIS	-	EXPRESSION TAG	UNP Q837U7
H	-13	HIS	-	EXPRESSION TAG	UNP Q837U7
H	-12	HIS	-	EXPRESSION TAG	UNP Q837U7
H	-11	HIS	-	EXPRESSION TAG	UNP Q837U7
H	-10	HIS	-	EXPRESSION TAG	UNP Q837U7
H	-9	SER	-	EXPRESSION TAG	UNP Q837U7
H	-8	SER	-	EXPRESSION TAG	UNP Q837U7
H	-7	GLY	-	EXPRESSION TAG	UNP Q837U7
H	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
H	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
H	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
H	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
H	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
H	-1	SER	-	EXPRESSION TAG	UNP Q837U7
H	0	HIS	-	EXPRESSION TAG	UNP Q837U7
I	-19	MET	-	EXPRESSION TAG	UNP Q837U7
I	-18	GLY	-	EXPRESSION TAG	UNP Q837U7
I	-17	SER	-	EXPRESSION TAG	UNP Q837U7
I	-16	SER	-	EXPRESSION TAG	UNP Q837U7
I	-15	HIS	-	EXPRESSION TAG	UNP Q837U7
I	-14	HIS	-	EXPRESSION TAG	UNP Q837U7
I	-13	HIS	-	EXPRESSION TAG	UNP Q837U7
I	-12	HIS	-	EXPRESSION TAG	UNP Q837U7
I	-11	HIS	-	EXPRESSION TAG	UNP Q837U7
I	-10	HIS	-	EXPRESSION TAG	UNP Q837U7
I	-9	SER	-	EXPRESSION TAG	UNP Q837U7
I	-8	SER	-	EXPRESSION TAG	UNP Q837U7
I	-7	GLY	-	EXPRESSION TAG	UNP Q837U7

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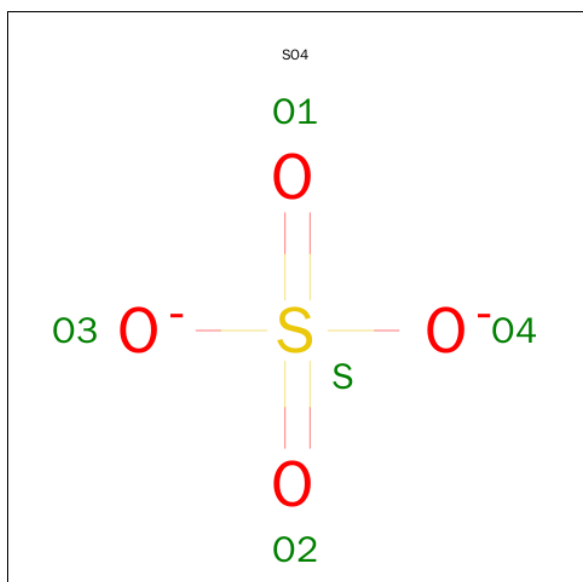
Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
I	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
I	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
I	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
I	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
I	-1	SER	-	EXPRESSION TAG	UNP Q837U7
I	0	HIS	-	EXPRESSION TAG	UNP Q837U7
J	-19	MET	-	EXPRESSION TAG	UNP Q837U7
J	-18	GLY	-	EXPRESSION TAG	UNP Q837U7
J	-17	SER	-	EXPRESSION TAG	UNP Q837U7
J	-16	SER	-	EXPRESSION TAG	UNP Q837U7
J	-15	HIS	-	EXPRESSION TAG	UNP Q837U7
J	-14	HIS	-	EXPRESSION TAG	UNP Q837U7
J	-13	HIS	-	EXPRESSION TAG	UNP Q837U7
J	-12	HIS	-	EXPRESSION TAG	UNP Q837U7
J	-11	HIS	-	EXPRESSION TAG	UNP Q837U7
J	-10	HIS	-	EXPRESSION TAG	UNP Q837U7
J	-9	SER	-	EXPRESSION TAG	UNP Q837U7
J	-8	SER	-	EXPRESSION TAG	UNP Q837U7
J	-7	GLY	-	EXPRESSION TAG	UNP Q837U7
J	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
J	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
J	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
J	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
J	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
J	-1	SER	-	EXPRESSION TAG	UNP Q837U7
J	0	HIS	-	EXPRESSION TAG	UNP Q837U7
K	-19	MET	-	EXPRESSION TAG	UNP Q837U7
K	-18	GLY	-	EXPRESSION TAG	UNP Q837U7
K	-17	SER	-	EXPRESSION TAG	UNP Q837U7
K	-16	SER	-	EXPRESSION TAG	UNP Q837U7
K	-15	HIS	-	EXPRESSION TAG	UNP Q837U7
K	-14	HIS	-	EXPRESSION TAG	UNP Q837U7
K	-13	HIS	-	EXPRESSION TAG	UNP Q837U7
K	-12	HIS	-	EXPRESSION TAG	UNP Q837U7
K	-11	HIS	-	EXPRESSION TAG	UNP Q837U7
K	-10	HIS	-	EXPRESSION TAG	UNP Q837U7
K	-9	SER	-	EXPRESSION TAG	UNP Q837U7
K	-8	SER	-	EXPRESSION TAG	UNP Q837U7
K	-7	GLY	-	EXPRESSION TAG	UNP Q837U7
K	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
K	-5	VAL	-	EXPRESSION TAG	UNP Q837U7

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
K	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
K	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
K	-1	SER	-	EXPRESSION TAG	UNP Q837U7
K	0	HIS	-	EXPRESSION TAG	UNP Q837U7
L	-19	MET	-	EXPRESSION TAG	UNP Q837U7
L	-18	GLY	-	EXPRESSION TAG	UNP Q837U7
L	-17	SER	-	EXPRESSION TAG	UNP Q837U7
L	-16	SER	-	EXPRESSION TAG	UNP Q837U7
L	-15	HIS	-	EXPRESSION TAG	UNP Q837U7
L	-14	HIS	-	EXPRESSION TAG	UNP Q837U7
L	-13	HIS	-	EXPRESSION TAG	UNP Q837U7
L	-12	HIS	-	EXPRESSION TAG	UNP Q837U7
L	-11	HIS	-	EXPRESSION TAG	UNP Q837U7
L	-10	HIS	-	EXPRESSION TAG	UNP Q837U7
L	-9	SER	-	EXPRESSION TAG	UNP Q837U7
L	-8	SER	-	EXPRESSION TAG	UNP Q837U7
L	-7	GLY	-	EXPRESSION TAG	UNP Q837U7
L	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
L	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
L	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
L	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
L	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
L	-1	SER	-	EXPRESSION TAG	UNP Q837U7
L	0	HIS	-	EXPRESSION TAG	UNP Q837U7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	J	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	L	1	Total O S 5 4 1	0	0
2	I	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

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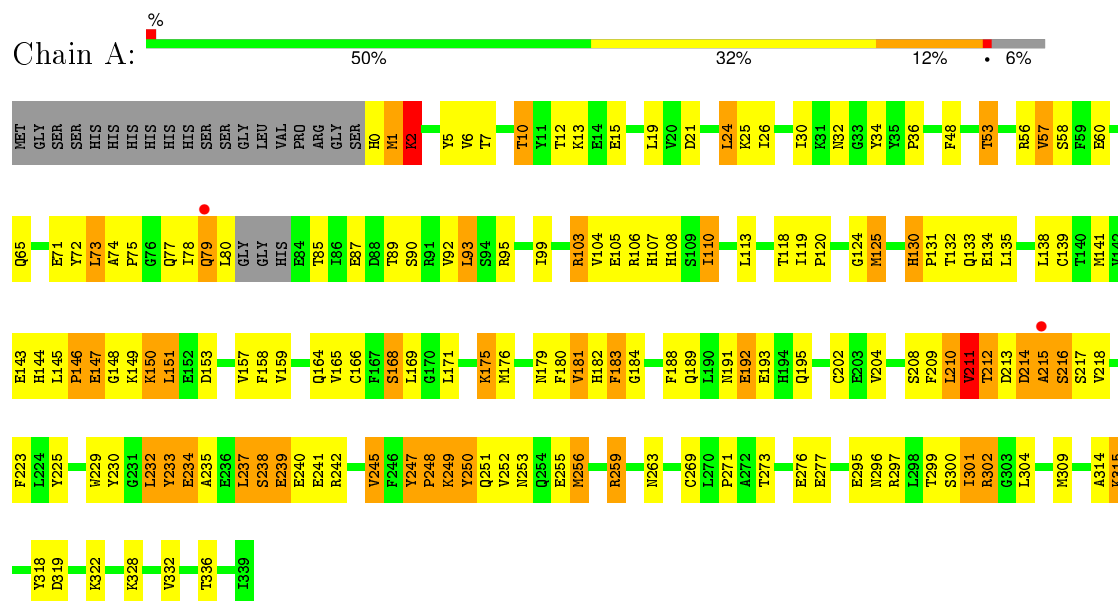
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

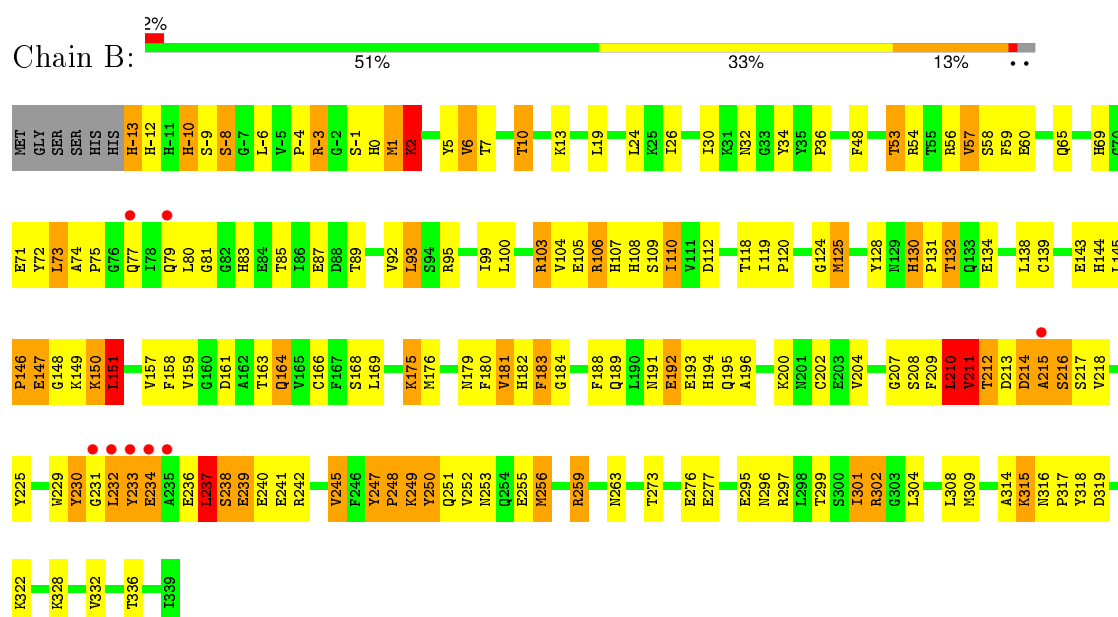
### 3 Residue-property plots

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

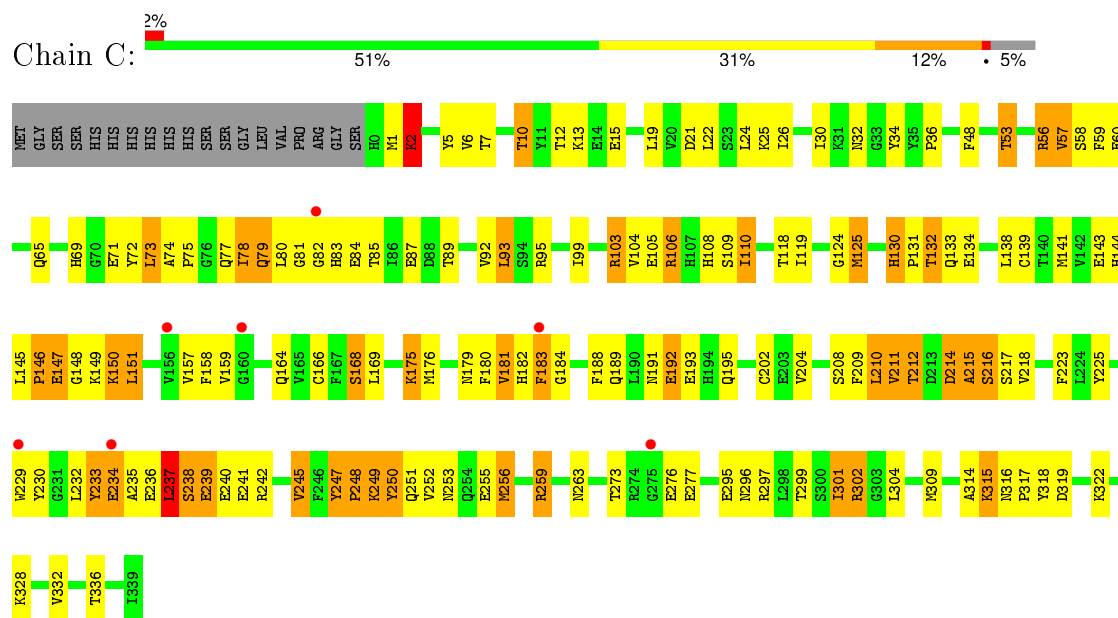
#### • Molecule 1: Putrescine carbamoyltransferase



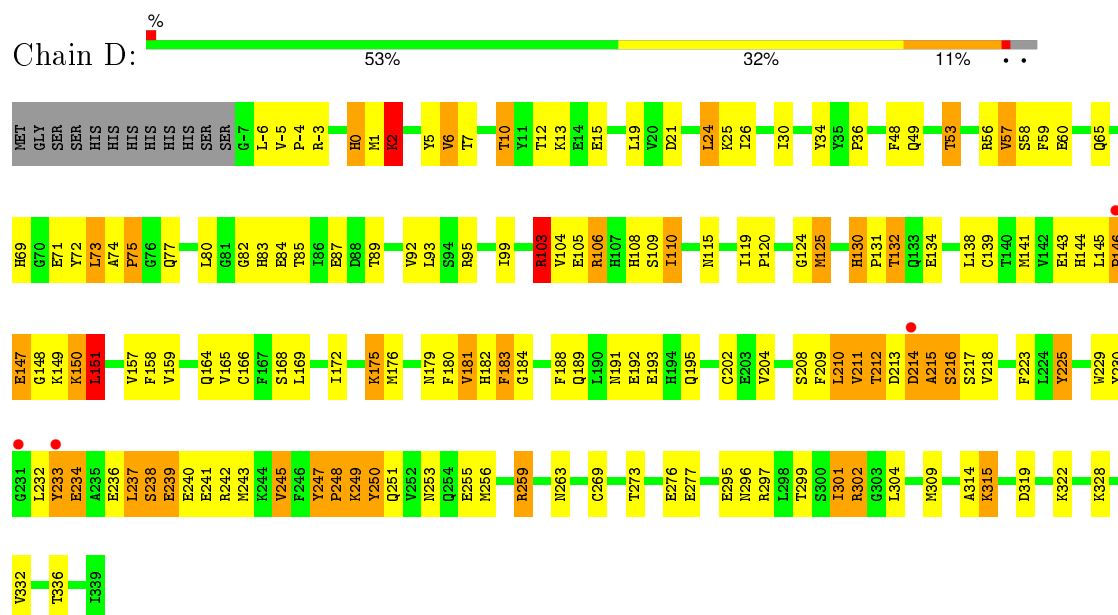
#### • Molecule 1: Putrescine carbamoyltransferase



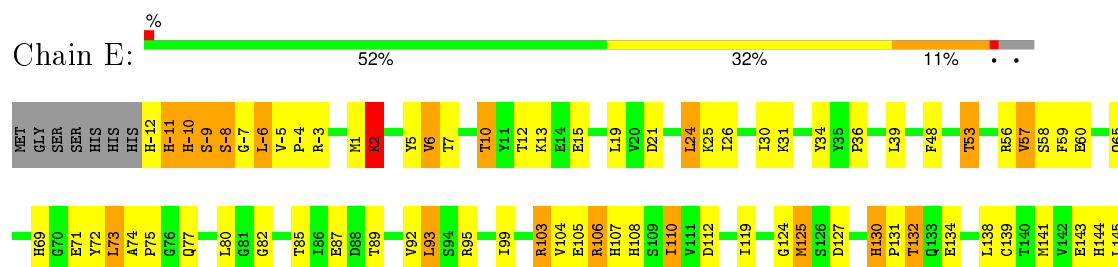
- Molecule 1: Putrescine carbamoyltransferase

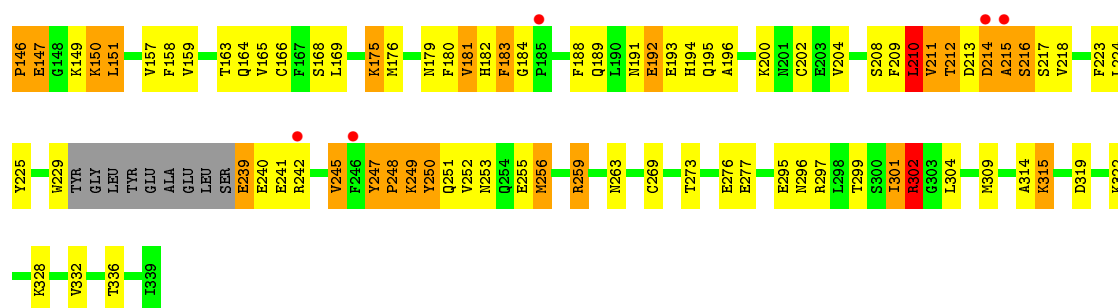


- Molecule 1: Putrescine carbamoyltransferase

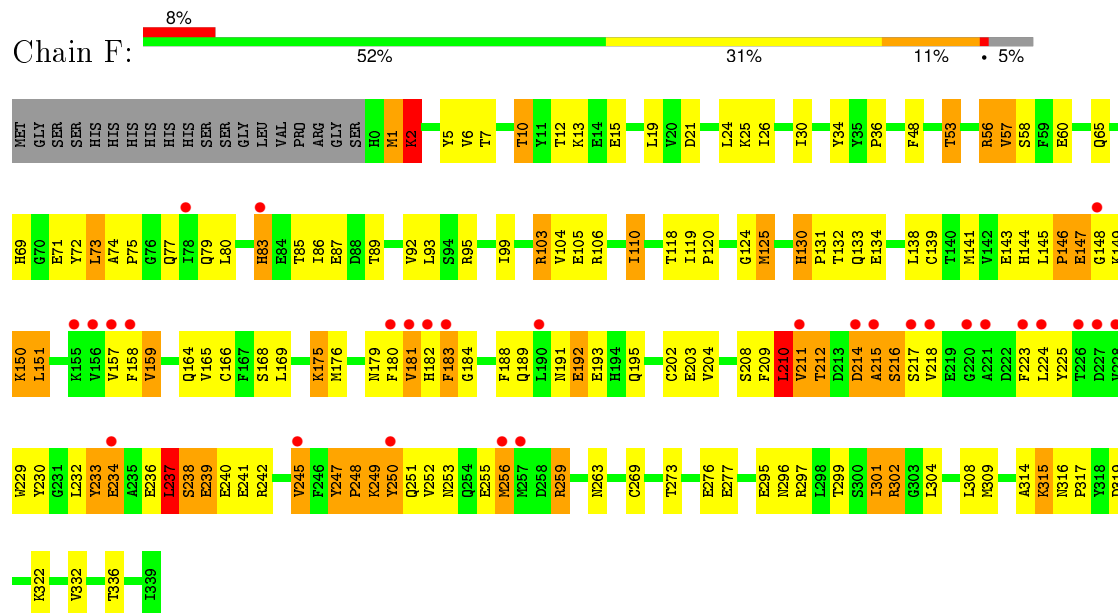


- Molecule 1: Putrescine carbamoyltransferase

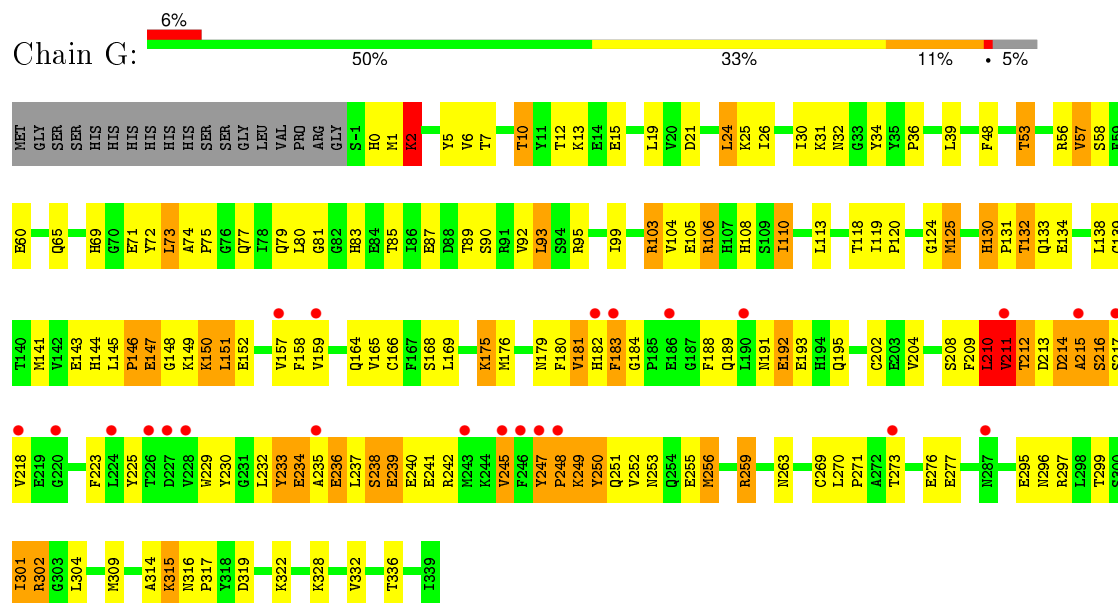




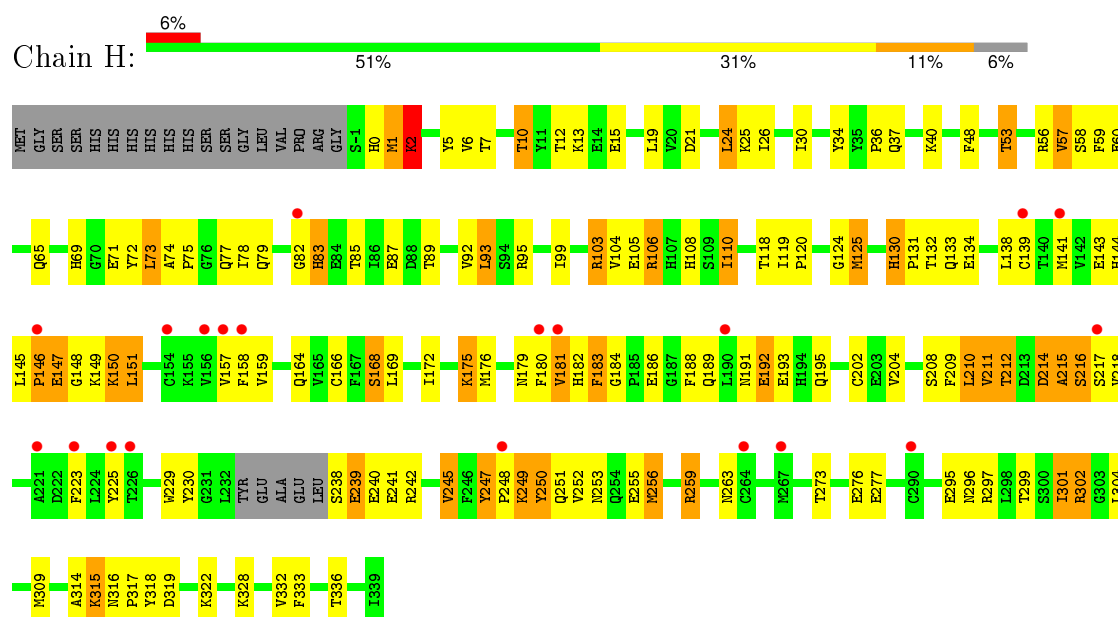
• Molecule 1: Putrescine carbamoyltransferase



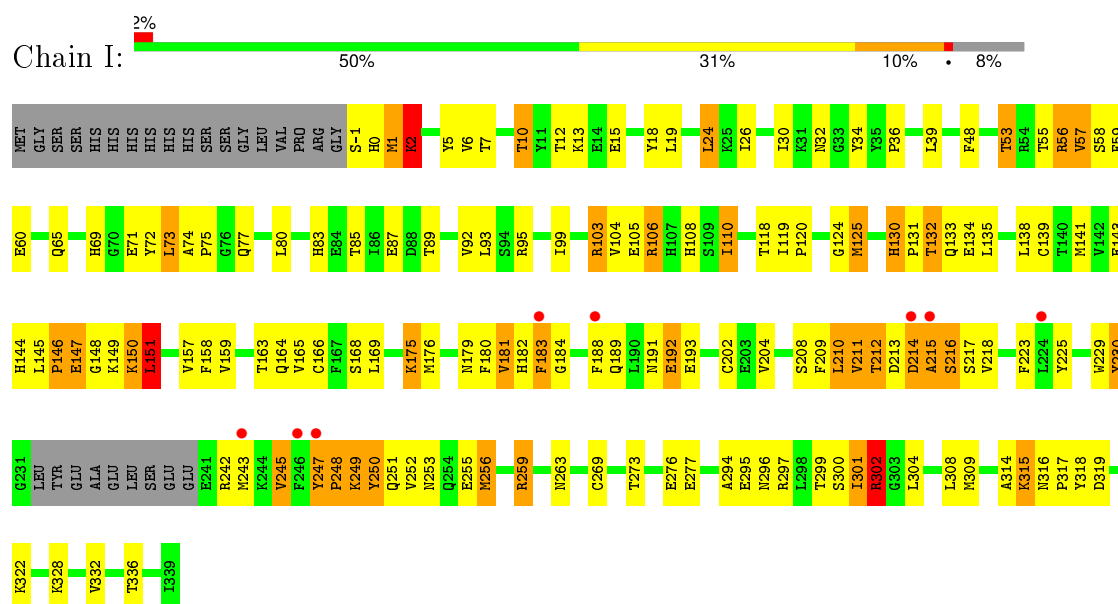
• Molecule 1: Putrescine carbamoyltransferase



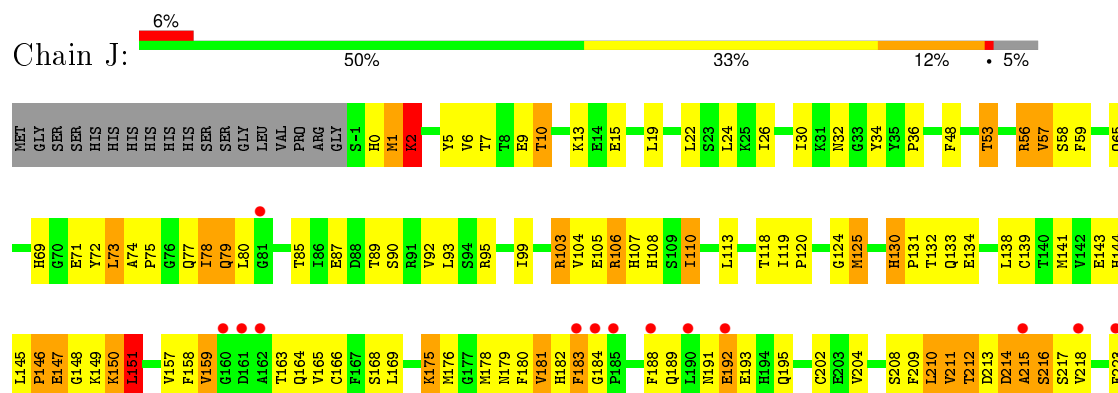
• Molecule 1: Putrescine carbamoyltransferase



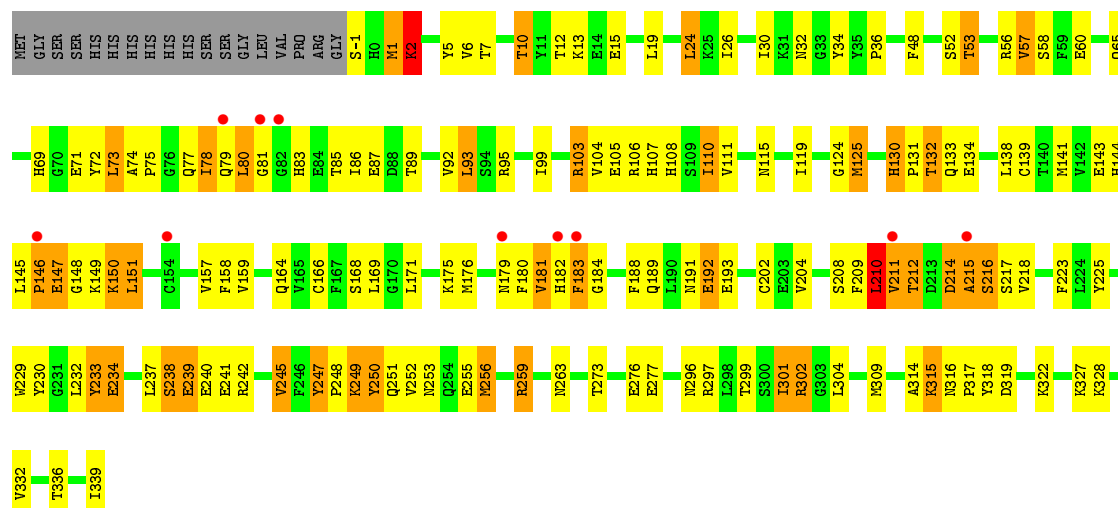
• Molecule 1: Putrescine carbamoyltransferase



• Molecule 1: Putrescine carbamoyltransferase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	273.86 Å   87.79 Å   241.30 Å 90.00°   114.08°   90.00°	Depositor
Resolution (Å)	48.17 – 3.20 49.02 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.17-3.20) 91.4 (49.02-3.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.32 (at 3.19 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.190   ,   0.234 0.174   ,   0.223	Depositor DCC
$R_{free}$ test set	1860 reflections (2.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 76.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 85430 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32142	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.46	0/2687	0.66	0/3626
1	B	0.50	0/2818	0.68	2/3803 (0.1%)
1	C	0.43	0/2705	0.64	0/3650
1	D	0.48	0/2755	0.67	2/3718 (0.1%)
1	E	0.53	0/2743	0.67	2/3699 (0.1%)
1	F	0.44	0/2710	0.64	1/3656 (0.0%)
1	G	0.42	0/2706	0.63	1/3651 (0.0%)
1	H	0.42	0/2676	0.62	0/3608
1	I	0.43	0/2651	0.64	1/3574 (0.0%)
1	J	0.44	0/2697	0.63	0/3640
1	K	0.44	0/2702	0.63	1/3646 (0.0%)
1	L	0.44	0/2718	0.65	1/3667 (0.0%)
All	All	0.45	0/32568	0.65	11/43938 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	1
All	All	0	7

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	302	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	D	237	LEU	N-CA-C	5.64	126.23	111.00
1	E	210	LEU	CA-CB-CG	5.46	127.87	115.30
1	D	103	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	210	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	237	LEU	CA-CB-CG	5.27	127.42	115.30
1	L	210	LEU	CA-CB-CG	5.14	127.11	115.30
1	K	210	LEU	CA-CB-CG	5.13	127.11	115.30
1	G	210	LEU	CA-CB-CG	5.07	126.97	115.30
1	F	210	LEU	CA-CB-CG	5.03	126.87	115.30
1	E	302	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	LEU	Peptide
1	B	237	LEU	Peptide
1	C	237	LEU	Peptide
1	D	236	GLU	Peptide
1	D	237	LEU	Peptide
1	E	-9	SER	Peptide
1	F	237	LEU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2642	0	2564	168	0
1	B	2766	0	2678	209	0
1	C	2659	0	2575	157	0
1	D	2707	0	2625	161	0
1	E	2694	0	2614	206	0
1	F	2664	0	2586	146	2
1	G	2660	0	2569	146	0
1	H	2631	0	2549	138	0
1	I	2606	0	2536	140	0
1	J	2651	0	2564	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2656	0	2563	150	2
1	L	2671	0	2592	156	0
2	A	10	0	0	1	0
2	B	15	0	0	2	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	15	0	0	0	0
2	F	10	0	0	1	0
2	G	15	0	0	0	0
2	H	10	0	0	0	0
2	I	10	0	0	1	0
2	J	10	0	0	0	0
2	K	5	0	0	0	0
2	L	15	0	0	2	0
All	All	32142	0	31015	1806	2

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 29.

All (1806) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:TYR:H	1:E:-11:HIS:CD2	1.55	1.23
1:F:238:SER:HB3	1:F:241:GLU:HB3	1.18	1.17
1:J:238:SER:HB3	1:J:241:GLU:HB3	1.19	1.16
1:H:238:SER:HB3	1:H:241:GLU:HB3	1.17	1.15
1:B:233:TYR:H	1:E:-11:HIS:CG	1.64	1.14
1:B:196:ALA:HB1	1:E:200:LYS:HE2	1.20	1.13
1:L:238:SER:HB3	1:L:241:GLU:HB3	1.16	1.12
1:B:232:LEU:HA	1:E:-11:HIS:HB3	1.32	1.11
1:B:238:SER:HB3	1:B:241:GLU:HB3	1.13	1.10
1:A:238:SER:HB3	1:A:241:GLU:HB3	1.28	1.10
1:G:53:THR:HG23	1:I:77:GLN:HG3	1.24	1.10
1:G:238:SER:HB3	1:G:241:GLU:HB3	1.12	1.09
1:K:238:SER:HB3	1:K:241:GLU:HB3	1.18	1.09
1:D:238:SER:HB3	1:D:241:GLU:HB3	1.31	1.09
1:H:77:GLN:HG3	1:I:53:THR:HG23	1.34	1.09
1:D:77:GLN:HG3	1:E:53:THR:HG23	1.36	1.08
1:E:-4:PRO:HG2	1:E:6:VAL:HG21	1.20	1.07
1:A:53:THR:HG23	1:C:77:GLN:HG3	1.36	1.07
1:B:-3:ARG:HA	1:B:-3:ARG:HE	1.18	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:SER:HB3	1:C:241:GLU:HB3	1.29	1.06
1:F:238:SER:CB	1:F:241:GLU:HB3	1.86	1.05
1:K:103:ARG:HH11	1:K:103:ARG:HG2	1.18	1.05
1:B:103:ARG:HG2	1:B:103:ARG:HH11	1.20	1.05
1:H:103:ARG:HH11	1:H:103:ARG:HG2	1.22	1.04
1:A:238:SER:CB	1:A:241:GLU:HB3	1.88	1.04
1:C:103:ARG:HG2	1:C:103:ARG:HH11	1.17	1.03
1:B:106:ARG:NH2	1:E:112:ASP:OD2	1.89	1.03
1:I:103:ARG:HG2	1:I:103:ARG:HH11	1.18	1.03
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.19	1.03
1:G:103:ARG:HH11	1:G:103:ARG:HG2	1.17	1.03
1:E:103:ARG:HH11	1:E:103:ARG:HG2	1.19	1.03
1:F:103:ARG:HG2	1:F:103:ARG:HH11	1.19	1.03
1:H:238:SER:CB	1:H:241:GLU:HB3	1.89	1.03
1:L:238:SER:CB	1:L:241:GLU:HB3	1.89	1.01
1:C:238:SER:CB	1:C:241:GLU:HB3	1.90	1.01
1:A:210:LEU:HD13	1:A:211:VAL:N	1.74	1.01
1:D:103:ARG:HG2	1:D:103:ARG:HH11	1.23	1.00
1:L:103:ARG:HH11	1:L:103:ARG:HG2	1.22	1.00
1:D:238:SER:CB	1:D:241:GLU:HB3	1.91	0.99
1:J:103:ARG:HG2	1:J:103:ARG:HH11	1.22	0.99
1:K:238:SER:CB	1:K:241:GLU:HB3	1.91	0.99
1:B:238:SER:CB	1:B:241:GLU:HB3	1.93	0.99
1:J:238:SER:CB	1:J:241:GLU:HB3	1.92	0.98
1:G:238:SER:CB	1:G:241:GLU:HB3	1.92	0.98
1:A:77:GLN:HG3	1:B:53:THR:HG23	1.43	0.98
1:E:210:LEU:HD13	1:E:211:VAL:N	1.80	0.95
1:A:215:ALA:HB1	1:A:259:ARG:HE	1.33	0.93
1:D:53:THR:HG23	1:F:77:GLN:HG3	1.49	0.93
1:B:77:GLN:HG3	1:C:53:THR:HG23	1.51	0.92
1:B:233:TYR:N	1:E:-11:HIS:CD2	2.36	0.92
1:D:215:ALA:HB1	1:D:259:ARG:HE	1.33	0.92
1:J:210:LEU:HD13	1:J:211:VAL:N	1.86	0.91
1:D:210:LEU:HD13	1:D:211:VAL:N	1.86	0.90
1:B:231:GLY:O	1:E:-11:HIS:HA	1.70	0.90
1:G:210:LEU:HD13	1:G:211:VAL:N	1.87	0.89
1:J:53:THR:HG23	1:L:77:GLN:HG3	1.53	0.89
1:B:215:ALA:HB1	1:B:259:ARG:HE	1.37	0.89
1:D:-4:PRO:HG2	1:D:6:VAL:HG21	1.54	0.89
1:D:251:GLN:HG3	1:D:276:GLU:O	1.73	0.88
1:E:183:PHE:HD2	1:E:183:PHE:C	1.77	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LEU:HD13	1:C:211:VAL:N	1.87	0.88
1:H:215:ALA:HB1	1:H:259:ARG:HE	1.38	0.88
1:E:215:ALA:HB1	1:E:259:ARG:HE	1.39	0.88
1:E:-4:PRO:CG	1:E:6:VAL:HG21	2.02	0.88
1:G:77:GLN:HG3	1:H:53:THR:HG23	1.54	0.88
1:B:210:LEU:HD13	1:B:211:VAL:N	1.88	0.88
1:B:196:ALA:CB	1:E:200:LYS:HE2	2.05	0.87
1:B:183:PHE:HD2	1:B:183:PHE:O	1.58	0.87
1:B:233:TYR:N	1:E:-11:HIS:CG	2.43	0.87
1:B:-4:PRO:HG2	1:B:6:VAL:HG21	1.55	0.87
1:C:215:ALA:HB1	1:C:259:ARG:HE	1.39	0.86
1:K:215:ALA:HB1	1:K:259:ARG:HE	1.40	0.86
1:G:251:GLN:HG3	1:G:276:GLU:O	1.75	0.86
1:G:215:ALA:HB1	1:G:259:ARG:HE	1.40	0.86
1:K:210:LEU:HD13	1:K:211:VAL:N	1.89	0.86
1:E:259:ARG:HH11	1:E:259:ARG:CG	1.88	0.86
1:G:238:SER:HB3	1:G:241:GLU:CB	2.04	0.86
1:H:210:LEU:HD13	1:H:211:VAL:N	1.91	0.86
1:D:53:THR:OG1	1:F:79:GLN:HG3	1.76	0.85
1:F:210:LEU:HD13	1:F:211:VAL:N	1.89	0.85
1:B:251:GLN:HG3	1:B:276:GLU:O	1.76	0.85
1:B:-4:PRO:CG	1:B:6:VAL:HG21	2.06	0.85
1:F:183:PHE:C	1:F:183:PHE:HD2	1.80	0.85
1:F:238:SER:HB3	1:F:241:GLU:CB	2.03	0.85
1:B:183:PHE:HD2	1:B:183:PHE:C	1.78	0.85
1:B:232:LEU:CA	1:E:-11:HIS:HB3	2.06	0.85
1:H:259:ARG:HH11	1:H:259:ARG:CG	1.89	0.85
1:I:215:ALA:HB1	1:I:259:ARG:HE	1.38	0.85
1:D:183:PHE:C	1:D:183:PHE:HD2	1.80	0.85
1:L:251:GLN:HG3	1:L:276:GLU:O	1.76	0.85
1:G:183:PHE:HD2	1:G:183:PHE:C	1.80	0.85
1:I:103:ARG:HH11	1:I:103:ARG:CG	1.90	0.84
1:E:103:ARG:HH11	1:E:103:ARG:CG	1.88	0.84
1:J:238:SER:HB3	1:J:241:GLU:CB	2.06	0.84
1:C:183:PHE:HD2	1:C:183:PHE:C	1.80	0.84
1:J:183:PHE:HD2	1:J:183:PHE:C	1.81	0.84
1:J:251:GLN:HG3	1:J:276:GLU:O	1.77	0.84
1:B:103:ARG:HH11	1:B:103:ARG:CG	1.91	0.84
1:F:259:ARG:CG	1:F:259:ARG:HH11	1.91	0.84
1:L:215:ALA:HB1	1:L:259:ARG:HE	1.42	0.84
1:I:210:LEU:HD13	1:I:211:VAL:N	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:GLN:HG3	1:F:53:THR:HG23	1.58	0.84
1:B:259:ARG:HH11	1:B:259:ARG:CG	1.91	0.84
1:B:-3:ARG:HA	1:B:-3:ARG:NE	1.90	0.84
1:A:214:ASP:O	1:A:216:SER:N	2.10	0.84
1:I:251:GLN:HG3	1:I:276:GLU:O	1.76	0.84
1:L:79:GLN:C	1:L:81:GLY:H	1.77	0.84
1:K:103:ARG:CG	1:K:103:ARG:HH11	1.91	0.84
1:E:183:PHE:HD2	1:E:183:PHE:O	1.61	0.84
1:J:259:ARG:CG	1:J:259:ARG:HH11	1.91	0.84
1:A:104:VAL:HG11	1:A:110:ILE:HB	1.60	0.84
1:K:238:SER:HB3	1:K:241:GLU:CB	2.07	0.83
1:K:183:PHE:C	1:K:183:PHE:HD2	1.80	0.83
1:I:259:ARG:CG	1:I:259:ARG:HH11	1.91	0.83
1:H:238:SER:HB3	1:H:241:GLU:CB	2.07	0.83
1:F:103:ARG:CG	1:F:103:ARG:HH11	1.91	0.83
1:A:259:ARG:HH11	1:A:259:ARG:CG	1.92	0.83
1:F:215:ALA:HB1	1:F:259:ARG:HE	1.43	0.83
1:J:215:ALA:HB1	1:J:259:ARG:HE	1.42	0.83
1:A:183:PHE:HD2	1:A:183:PHE:C	1.81	0.83
1:L:238:SER:HB3	1:L:241:GLU:CB	2.05	0.83
1:C:259:ARG:CG	1:C:259:ARG:HH11	1.92	0.83
1:A:95:ARG:NH2	2:A:341:SO4:O3	2.11	0.83
1:G:259:ARG:HH11	1:G:259:ARG:CG	1.92	0.83
1:B:232:LEU:HA	1:E:-11:HIS:CB	2.08	0.82
1:K:79:GLN:O	1:K:81:GLY:N	2.12	0.82
1:B:238:SER:HB3	1:B:241:GLU:CB	2.04	0.82
1:I:183:PHE:HD2	1:I:183:PHE:C	1.82	0.82
1:K:104:VAL:HG11	1:K:110:ILE:HB	1.61	0.82
1:D:191:ASN:HB3	1:H:186:GLU:HG3	1.60	0.82
1:B:232:LEU:H	1:B:232:LEU:HD12	1.42	0.82
1:C:251:GLN:HG3	1:C:276:GLU:O	1.79	0.82
1:K:259:ARG:CG	1:K:259:ARG:HH11	1.92	0.82
1:D:191:ASN:CB	1:H:186:GLU:HG3	2.08	0.82
1:L:210:LEU:HD13	1:L:211:VAL:N	1.93	0.82
1:A:251:GLN:HG3	1:A:276:GLU:O	1.80	0.82
1:E:251:GLN:HG3	1:E:276:GLU:O	1.80	0.82
1:F:159:VAL:HB	1:F:183:PHE:CE2	2.15	0.82
1:G:103:ARG:CG	1:G:103:ARG:HH11	1.91	0.82
1:H:183:PHE:C	1:H:183:PHE:HD2	1.81	0.82
1:L:183:PHE:C	1:L:183:PHE:HD2	1.82	0.82
1:C:103:ARG:CG	1:C:103:ARG:HH11	1.92	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:251:GLN:HG3	1:H:276:GLU:O	1.78	0.81
1:B:-9:SER:HB3	1:E:194:HIS:HE1	1.42	0.81
1:C:183:PHE:HD2	1:C:183:PHE:O	1.64	0.81
1:F:251:GLN:HG3	1:F:276:GLU:O	1.79	0.81
1:B:214:ASP:O	1:B:216:SER:N	2.14	0.81
1:K:251:GLN:HG3	1:K:276:GLU:O	1.79	0.81
1:A:297:ARG:HG3	1:A:297:ARG:HH11	1.45	0.81
1:E:-8:SER:OG	1:E:-7:GLY:N	2.11	0.81
1:L:159:VAL:HB	1:L:183:PHE:CE2	2.15	0.81
1:L:259:ARG:CG	1:L:259:ARG:HH11	1.93	0.81
1:J:78:ILE:HG12	1:J:79:GLN:H	1.43	0.81
1:B:200:LYS:HE2	1:E:196:ALA:HB1	1.63	0.81
1:B:159:VAL:HB	1:B:183:PHE:CE2	2.16	0.81
1:E:159:VAL:HB	1:E:183:PHE:CE2	2.15	0.81
1:A:183:PHE:HD2	1:A:183:PHE:O	1.62	0.81
1:D:183:PHE:O	1:D:183:PHE:HD2	1.62	0.81
1:B:231:GLY:O	1:E:-11:HIS:CD2	2.34	0.80
1:A:103:ARG:HH11	1:A:103:ARG:CG	1.92	0.80
1:D:214:ASP:O	1:D:216:SER:N	2.14	0.80
1:D:95:ARG:HB3	1:E:295:GLU:HB2	1.64	0.80
1:H:103:ARG:HH11	1:H:103:ARG:CG	1.95	0.80
1:D:259:ARG:CG	1:D:259:ARG:HH11	1.95	0.80
1:H:214:ASP:O	1:H:216:SER:N	2.15	0.80
1:B:183:PHE:CD2	1:B:183:PHE:O	2.36	0.79
1:I:297:ARG:O	1:I:301:ILE:HG23	1.82	0.79
1:C:214:ASP:O	1:C:216:SER:N	2.15	0.79
1:E:183:PHE:CD2	1:E:183:PHE:C	2.51	0.79
1:D:215:ALA:O	1:D:259:ARG:NH2	2.16	0.79
1:B:-13:HIS:HE1	1:E:106:ARG:NE	1.80	0.79
1:I:104:VAL:HG11	1:I:110:ILE:HB	1.65	0.79
1:C:79:GLN:O	1:C:81:GLY:N	2.16	0.79
1:E:297:ARG:HH11	1:E:297:ARG:HG3	1.47	0.79
1:L:297:ARG:O	1:L:301:ILE:HG23	1.83	0.79
1:F:103:ARG:HG2	1:F:103:ARG:NH1	1.98	0.79
1:B:314:ALA:O	1:B:315:LYS:HB2	1.83	0.78
1:D:183:PHE:CD2	1:D:183:PHE:C	2.55	0.78
1:A:232:LEU:H	1:A:232:LEU:HD12	1.47	0.78
1:C:159:VAL:HB	1:C:183:PHE:CE2	2.18	0.78
1:J:103:ARG:HH11	1:J:103:ARG:CG	1.95	0.78
1:A:215:ALA:HB3	1:L:115:ASN:HB3	1.64	0.78
1:I:214:ASP:O	1:I:216:SER:N	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:183:PHE:CD2	1:J:183:PHE:C	2.55	0.78
1:I:297:ARG:HH11	1:I:297:ARG:HG3	1.49	0.78
1:K:159:VAL:HB	1:K:183:PHE:CE2	2.18	0.78
1:G:214:ASP:O	1:G:216:SER:N	2.17	0.78
1:H:183:PHE:CD2	1:H:183:PHE:C	2.56	0.78
1:J:297:ARG:O	1:J:301:ILE:HG23	1.82	0.78
1:L:103:ARG:HH11	1:L:103:ARG:CG	1.96	0.78
1:E:215:ALA:O	1:E:259:ARG:NH2	2.16	0.78
1:C:215:ALA:O	1:C:259:ARG:NH2	2.17	0.78
1:J:104:VAL:HG11	1:J:110:ILE:HB	1.64	0.78
1:G:297:ARG:O	1:G:301:ILE:HG23	1.84	0.78
1:D:159:VAL:HB	1:D:183:PHE:CE2	2.18	0.78
1:L:214:ASP:O	1:L:216:SER:N	2.16	0.78
1:L:104:VAL:HG11	1:L:110:ILE:HB	1.65	0.78
1:G:104:VAL:HG11	1:G:110:ILE:HB	1.65	0.77
1:A:159:VAL:HB	1:A:183:PHE:CE2	2.18	0.77
1:G:183:PHE:CD2	1:G:183:PHE:C	2.55	0.77
1:F:183:PHE:HD2	1:F:183:PHE:O	1.67	0.77
1:K:183:PHE:HD2	1:K:183:PHE:O	1.66	0.77
1:A:238:SER:HB3	1:A:241:GLU:CB	2.12	0.77
1:D:238:SER:HB3	1:D:241:GLU:CB	2.13	0.77
1:C:297:ARG:O	1:C:301:ILE:HG23	1.85	0.77
1:E:183:PHE:CD2	1:E:183:PHE:O	2.38	0.77
1:E:214:ASP:O	1:E:216:SER:N	2.17	0.77
1:D:104:VAL:HG11	1:D:110:ILE:HB	1.66	0.77
1:K:183:PHE:CD2	1:K:183:PHE:C	2.55	0.77
1:D:-4:PRO:CG	1:D:6:VAL:HG21	2.14	0.77
1:I:183:PHE:HD2	1:I:183:PHE:O	1.68	0.77
1:J:159:VAL:HB	1:J:183:PHE:CE2	2.20	0.77
1:G:183:PHE:HD2	1:G:183:PHE:O	1.67	0.76
1:J:214:ASP:O	1:J:216:SER:N	2.18	0.76
1:G:159:VAL:HB	1:G:183:PHE:CE2	2.20	0.76
1:F:297:ARG:O	1:F:301:ILE:HG23	1.86	0.76
1:C:183:PHE:CD2	1:C:183:PHE:C	2.54	0.76
1:A:144:HIS:O	1:A:146:PRO:HD2	1.86	0.76
1:C:237:LEU:CD1	1:C:238:SER:HB2	2.15	0.76
1:H:159:VAL:HB	1:H:183:PHE:CE2	2.20	0.76
1:B:215:ALA:O	1:B:259:ARG:NH2	2.19	0.76
1:H:95:ARG:HB3	1:I:295:GLU:HB2	1.68	0.76
1:D:183:PHE:O	1:D:183:PHE:CD2	2.40	0.76
1:I:159:VAL:HB	1:I:183:PHE:CE2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:183:PHE:O	1:J:183:PHE:HD2	1.69	0.76
1:C:180:PHE:O	1:C:209:PHE:HA	1.84	0.76
1:K:297:ARG:O	1:K:301:ILE:HG23	1.86	0.76
1:H:104:VAL:HG11	1:H:110:ILE:HB	1.66	0.75
1:B:297:ARG:O	1:B:301:ILE:HG23	1.87	0.75
1:D:297:ARG:O	1:D:301:ILE:HG23	1.86	0.75
1:H:215:ALA:O	1:H:259:ARG:NH2	2.20	0.75
1:K:214:ASP:O	1:K:216:SER:N	2.20	0.75
1:L:183:PHE:O	1:L:183:PHE:HD2	1.67	0.75
1:H:183:PHE:O	1:H:183:PHE:HD2	1.69	0.75
1:H:77:GLN:HG3	1:I:53:THR:CG2	2.16	0.75
1:A:180:PHE:O	1:A:209:PHE:HA	1.87	0.75
1:C:238:SER:HB3	1:C:241:GLU:CB	2.14	0.75
1:A:183:PHE:CD2	1:A:183:PHE:O	2.39	0.75
1:F:297:ARG:HG3	1:F:297:ARG:HH11	1.50	0.75
1:E:104:VAL:HG11	1:E:110:ILE:HB	1.68	0.74
1:A:144:HIS:C	1:A:146:PRO:HD2	2.08	0.74
1:C:104:VAL:HG11	1:C:110:ILE:HB	1.69	0.74
1:C:103:ARG:NH1	1:C:103:ARG:HG2	1.96	0.74
1:K:215:ALA:O	1:K:259:ARG:NH2	2.20	0.74
1:F:104:VAL:HG11	1:F:110:ILE:HB	1.70	0.74
1:G:1:MET:O	1:G:2:LYS:HB3	1.85	0.74
1:G:215:ALA:O	1:G:259:ARG:NH2	2.21	0.74
1:K:180:PHE:O	1:K:209:PHE:HA	1.88	0.74
1:B:103:ARG:HG2	1:B:103:ARG:NH1	1.97	0.74
1:A:183:PHE:CD2	1:A:183:PHE:C	2.55	0.74
1:B:297:ARG:HG3	1:B:297:ARG:HH11	1.53	0.74
1:C:183:PHE:CD2	1:C:183:PHE:O	2.40	0.74
1:J:180:PHE:O	1:J:209:PHE:HA	1.88	0.74
1:E:103:ARG:HG2	1:E:103:ARG:NH1	1.97	0.74
1:I:215:ALA:O	1:I:259:ARG:NH2	2.20	0.74
1:F:180:PHE:O	1:F:209:PHE:HA	1.87	0.74
1:F:83:HIS:N	1:F:83:HIS:ND1	2.33	0.74
1:F:214:ASP:O	1:F:216:SER:N	2.21	0.73
1:G:180:PHE:O	1:G:209:PHE:HA	1.88	0.73
1:C:237:LEU:HD13	1:C:238:SER:HB2	1.70	0.73
1:B:104:VAL:HG11	1:B:110:ILE:HB	1.71	0.73
1:A:210:LEU:CD1	1:A:211:VAL:N	2.52	0.73
1:H:297:ARG:HG3	1:H:297:ARG:HH11	1.54	0.73
1:D:180:PHE:O	1:D:209:PHE:HA	1.89	0.73
1:E:144:HIS:O	1:E:146:PRO:HD2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:259:ARG:HG2	1:H:259:ARG:HH11	1.52	0.73
1:G:297:ARG:HG3	1:G:297:ARG:HH11	1.53	0.73
1:H:103:ARG:NH1	1:H:103:ARG:HG2	2.00	0.73
1:L:134:GLU:HG2	1:L:168:SER:HB3	1.70	0.72
1:B:183:PHE:CD2	1:B:183:PHE:C	2.54	0.72
1:I:183:PHE:CD2	1:I:183:PHE:C	2.57	0.72
1:F:134:GLU:HG2	1:F:168:SER:HB3	1.71	0.72
1:B:-9:SER:O	1:B:-8:SER:O	2.07	0.72
1:K:297:ARG:HG3	1:K:297:ARG:HH11	1.55	0.72
1:J:1:MET:O	1:J:2:LYS:HB3	1.89	0.72
1:C:144:HIS:C	1:C:146:PRO:HD2	2.10	0.72
1:L:180:PHE:O	1:L:209:PHE:HA	1.90	0.72
1:D:103:ARG:CG	1:D:103:ARG:HH11	2.01	0.72
1:H:297:ARG:O	1:H:301:ILE:HG23	1.88	0.72
1:F:215:ALA:O	1:F:259:ARG:NH2	2.23	0.72
1:D:134:GLU:HG2	1:D:168:SER:HB3	1.72	0.72
1:L:1:MET:O	1:L:2:LYS:HB3	1.89	0.72
1:G:103:ARG:NH1	1:G:103:ARG:HG2	1.96	0.71
1:E:210:LEU:CD1	1:E:211:VAL:N	2.53	0.71
1:B:-4:PRO:CD	1:B:6:VAL:HG21	2.19	0.71
1:K:77:GLN:HG3	1:L:53:THR:HG23	1.70	0.71
1:H:249:LYS:O	1:H:251:GLN:N	2.22	0.71
1:A:297:ARG:O	1:A:301:ILE:HG23	1.88	0.71
1:I:144:HIS:C	1:I:146:PRO:HD2	2.10	0.71
1:I:180:PHE:O	1:I:209:PHE:HA	1.90	0.71
1:E:144:HIS:C	1:E:146:PRO:HD2	2.10	0.71
1:H:134:GLU:HG2	1:H:168:SER:HB3	1.73	0.71
1:G:295:GLU:HB2	1:I:95:ARG:HB3	1.73	0.71
1:G:314:ALA:O	1:G:315:LYS:HB2	1.90	0.71
1:F:249:LYS:O	1:F:251:GLN:N	2.23	0.71
1:F:144:HIS:C	1:F:146:PRO:HD2	2.10	0.71
1:E:181:VAL:HA	1:E:210:LEU:H	1.54	0.71
1:D:297:ARG:HH11	1:D:297:ARG:HG3	1.55	0.71
1:A:211:VAL:HG22	1:A:212:THR:H	1.55	0.71
1:E:211:VAL:HG22	1:E:212:THR:H	1.55	0.71
1:B:144:HIS:C	1:B:146:PRO:HD2	2.11	0.71
1:F:211:VAL:HG22	1:F:212:THR:H	1.55	0.71
1:J:215:ALA:O	1:J:259:ARG:NH2	2.24	0.71
1:L:211:VAL:HG22	1:L:212:THR:H	1.56	0.71
1:J:249:LYS:O	1:J:251:GLN:N	2.23	0.70
1:D:144:HIS:C	1:D:146:PRO:HD2	2.11	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:HG2	1:A:103:ARG:NH1	1.98	0.70
1:F:183:PHE:CD2	1:F:183:PHE:O	2.44	0.70
1:C:144:HIS:O	1:C:146:PRO:HD2	1.91	0.70
1:E:314:ALA:O	1:E:315:LYS:HB2	1.89	0.70
1:G:183:PHE:CD2	1:G:183:PHE:O	2.43	0.70
1:L:215:ALA:O	1:L:259:ARG:NH2	2.24	0.70
1:A:249:LYS:O	1:A:251:GLN:N	2.23	0.70
1:K:183:PHE:CD2	1:K:183:PHE:O	2.43	0.70
1:L:79:GLN:O	1:L:81:GLY:N	2.25	0.70
1:H:144:HIS:C	1:H:146:PRO:HD2	2.11	0.70
1:I:314:ALA:O	1:I:315:LYS:HB2	1.90	0.70
1:D:181:VAL:HA	1:D:210:LEU:H	1.56	0.70
1:L:144:HIS:C	1:L:146:PRO:HD2	2.11	0.70
1:G:5:TYR:CD1	1:G:304:LEU:HD21	2.27	0.70
1:H:180:PHE:O	1:H:209:PHE:HA	1.91	0.70
1:G:134:GLU:HG2	1:G:168:SER:HB3	1.73	0.70
1:D:103:ARG:HG2	1:D:103:ARG:NH1	2.02	0.70
1:L:183:PHE:CD2	1:L:183:PHE:C	2.57	0.70
1:K:144:HIS:C	1:K:146:PRO:HD2	2.11	0.70
1:K:144:HIS:O	1:K:146:PRO:HD2	1.92	0.70
1:B:180:PHE:O	1:B:209:PHE:HA	1.92	0.70
1:J:134:GLU:HG2	1:J:168:SER:HB3	1.73	0.70
1:E:180:PHE:O	1:E:209:PHE:HA	1.91	0.70
1:A:215:ALA:HB1	1:A:259:ARG:NE	2.04	0.70
1:I:144:HIS:O	1:I:146:PRO:HD2	1.90	0.70
1:H:314:ALA:O	1:H:315:LYS:HB2	1.91	0.70
1:I:53:THR:O	1:I:57:VAL:HG13	1.91	0.69
1:I:249:LYS:O	1:I:251:GLN:N	2.25	0.69
1:E:134:GLU:HG2	1:E:168:SER:HB3	1.74	0.69
1:E:259:ARG:HH11	1:E:259:ARG:HG2	1.56	0.69
1:H:183:PHE:CD2	1:H:183:PHE:O	2.45	0.69
1:B:95:ARG:HB3	1:C:295:GLU:HB2	1.73	0.69
1:B:-13:HIS:HE1	1:E:106:ARG:HE	1.40	0.69
1:L:103:ARG:NH2	2:L:341:SO4:O2	2.21	0.69
1:C:211:VAL:HG22	1:C:212:THR:H	1.56	0.69
1:J:144:HIS:C	1:J:146:PRO:HD2	2.12	0.69
1:C:249:LYS:O	1:C:251:GLN:N	2.24	0.69
1:G:249:LYS:O	1:G:251:GLN:N	2.24	0.69
1:D:1:MET:O	1:D:2:LYS:HB3	1.91	0.69
1:C:181:VAL:HA	1:C:210:LEU:H	1.57	0.69
1:L:183:PHE:CD2	1:L:183:PHE:O	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLU:HG2	1:B:168:SER:HB3	1.74	0.69
1:K:134:GLU:HG2	1:K:168:SER:HB3	1.74	0.69
1:H:181:VAL:HA	1:H:210:LEU:H	1.58	0.69
1:G:144:HIS:O	1:G:146:PRO:HD2	1.92	0.69
1:B:5:TYR:CD1	1:B:304:LEU:HD21	2.28	0.69
1:A:215:ALA:HB3	1:L:115:ASN:CB	2.22	0.69
1:B:181:VAL:HA	1:B:210:LEU:H	1.56	0.69
1:F:183:PHE:C	1:F:183:PHE:CD2	2.55	0.69
1:F:259:ARG:HG2	1:F:259:ARG:HH11	1.57	0.69
1:G:144:HIS:C	1:G:146:PRO:HD2	2.12	0.69
1:D:230:TYR:HH	1:F:83:HIS:HE2	1.41	0.69
1:E:1:MET:O	1:E:2:LYS:HB3	1.92	0.69
1:J:211:VAL:HG22	1:J:212:THR:H	1.58	0.69
1:C:78:ILE:O	1:C:79:GLN:HG3	1.92	0.69
1:A:259:ARG:HH11	1:A:259:ARG:HG2	1.57	0.68
1:L:79:GLN:C	1:L:81:GLY:N	2.47	0.68
1:C:134:GLU:HG2	1:C:168:SER:HB3	1.75	0.68
1:J:181:VAL:HA	1:J:210:LEU:H	1.59	0.68
1:E:249:LYS:O	1:E:251:GLN:N	2.26	0.68
1:B:211:VAL:HG22	1:B:212:THR:H	1.57	0.68
1:G:181:VAL:HA	1:G:210:LEU:H	1.57	0.68
1:D:5:TYR:CD1	1:D:304:LEU:HD21	2.28	0.68
1:E:319:ASP:HB3	1:E:322:LYS:HB2	1.75	0.68
1:J:183:PHE:O	1:J:183:PHE:CD2	2.46	0.68
1:C:297:ARG:HG3	1:C:297:ARG:HH11	1.59	0.68
1:J:77:GLN:HG3	1:K:53:THR:HG23	1.74	0.68
1:B:259:ARG:HH11	1:B:259:ARG:HG2	1.58	0.68
1:L:2:LYS:HE2	1:L:119:ILE:O	1.93	0.68
1:J:314:ALA:O	1:J:315:LYS:HB2	1.93	0.68
1:B:1:MET:O	1:B:2:LYS:HB3	1.92	0.68
1:A:314:ALA:O	1:A:315:LYS:HB2	1.92	0.68
1:L:78:ILE:HD13	1:L:80:LEU:HB2	1.76	0.68
1:F:144:HIS:O	1:F:146:PRO:HD2	1.94	0.68
1:H:239:GLU:HA	1:H:242:ARG:HH21	1.58	0.68
1:I:259:ARG:HG2	1:I:259:ARG:HH11	1.58	0.68
1:I:181:VAL:HA	1:I:210:LEU:H	1.57	0.67
1:D:211:VAL:HG22	1:D:212:THR:H	1.58	0.67
1:L:297:ARG:HH11	1:L:297:ARG:HG3	1.58	0.67
1:A:5:TYR:CD1	1:A:304:LEU:HD21	2.28	0.67
1:A:215:ALA:O	1:A:259:ARG:NH2	2.28	0.67
1:F:34:TYR:O	1:F:36:PRO:HD3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:TYR:CD1	1:E:304:LEU:HD21	2.30	0.67
1:C:259:ARG:HG2	1:C:259:ARG:HH11	1.59	0.67
1:J:297:ARG:HG3	1:J:297:ARG:HH11	1.59	0.67
1:J:144:HIS:O	1:J:146:PRO:HD2	1.95	0.67
1:I:183:PHE:O	1:I:183:PHE:CD2	2.46	0.67
1:D:53:THR:O	1:D:57:VAL:HG13	1.94	0.67
1:B:196:ALA:HB1	1:E:200:LYS:CE	2.12	0.67
1:D:49:GLN:HE22	1:D:80:LEU:HD22	1.60	0.67
1:G:124:GLY:O	1:G:125:MET:HB2	1.95	0.67
1:H:1:MET:O	1:H:2:LYS:HB3	1.93	0.67
1:K:1:MET:O	1:K:2:LYS:HB3	1.92	0.67
1:K:314:ALA:O	1:K:315:LYS:HB2	1.95	0.67
1:K:249:LYS:O	1:K:251:GLN:N	2.29	0.66
1:D:124:GLY:O	1:D:125:MET:HB2	1.94	0.66
1:F:1:MET:O	1:F:2:LYS:HB3	1.95	0.66
1:K:239:GLU:HA	1:K:242:ARG:HH21	1.60	0.66
1:D:210:LEU:CD1	1:D:211:VAL:N	2.59	0.66
1:E:297:ARG:O	1:E:301:ILE:HG23	1.95	0.66
1:E:48:PHE:O	1:E:75:PRO:HA	1.95	0.66
1:E:124:GLY:O	1:E:125:MET:HB2	1.96	0.66
1:K:103:ARG:NH1	1:K:103:ARG:HG2	1.96	0.66
1:G:7:THR:O	1:G:10:THR:HG23	1.96	0.66
1:A:215:ALA:HB3	1:L:115:ASN:CG	2.14	0.66
1:B:211:VAL:HG13	1:B:212:THR:N	2.10	0.66
1:H:144:HIS:O	1:H:146:PRO:HD2	1.96	0.66
1:L:144:HIS:O	1:L:146:PRO:HD2	1.96	0.66
1:I:302:ARG:HH11	1:I:302:ARG:HG2	1.61	0.66
1:A:237:LEU:O	1:A:238:SER:O	2.13	0.66
1:D:-3:ARG:N	1:D:115:ASN:OD1	2.23	0.66
1:I:211:VAL:HG22	1:I:212:THR:H	1.61	0.66
1:C:5:TYR:CD1	1:C:304:LEU:HD21	2.31	0.66
1:F:239:GLU:HA	1:F:242:ARG:HH21	1.61	0.66
1:D:215:ALA:HB1	1:D:259:ARG:NE	2.09	0.66
1:L:53:THR:O	1:L:57:VAL:HG13	1.96	0.66
1:A:213:ASP:HB2	1:L:111:VAL:HG21	1.78	0.66
1:L:181:VAL:HA	1:L:210:LEU:H	1.61	0.66
1:D:314:ALA:O	1:D:315:LYS:HB2	1.95	0.65
1:A:210:LEU:HD13	1:A:211:VAL:CA	2.25	0.65
1:B:249:LYS:O	1:B:251:GLN:N	2.27	0.65
1:H:211:VAL:HG22	1:H:212:THR:H	1.60	0.65
1:J:259:ARG:HH11	1:J:259:ARG:HG2	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:TYR:CD1	1:H:304:LEU:HD21	2.31	0.65
1:J:302:ARG:HG2	1:J:302:ARG:HH11	1.61	0.65
1:L:239:GLU:HA	1:L:242:ARG:HH21	1.61	0.65
1:C:237:LEU:HG	1:C:242:ARG:HG3	1.77	0.65
1:I:1:MET:O	1:I:2:LYS:HB3	1.96	0.65
1:J:339:ILE:HG21	1:K:15:GLU:HA	1.77	0.65
1:L:80:LEU:HD11	1:L:86:ILE:HD13	1.77	0.65
1:J:78:ILE:HG12	1:J:79:GLN:N	2.11	0.65
1:G:259:ARG:HG2	1:G:259:ARG:HH11	1.60	0.65
1:L:249:LYS:O	1:L:251:GLN:N	2.28	0.65
1:C:314:ALA:O	1:C:315:LYS:HB2	1.95	0.65
1:C:235:ALA:C	1:C:237:LEU:H	1.99	0.65
1:A:210:LEU:HD13	1:A:211:VAL:H	1.57	0.65
1:I:215:ALA:HB1	1:I:259:ARG:NE	2.11	0.65
1:A:295:GLU:HB2	1:C:95:ARG:HB3	1.78	0.65
1:F:124:GLY:O	1:F:125:MET:HB2	1.97	0.65
1:E:53:THR:O	1:E:57:VAL:HG13	1.96	0.65
1:L:5:TYR:CD1	1:L:304:LEU:HD21	2.31	0.65
1:A:1:MET:O	1:A:2:LYS:HB3	1.96	0.65
1:L:314:ALA:O	1:L:315:LYS:HB2	1.96	0.65
1:E:239:GLU:HA	1:E:242:ARG:HH21	1.61	0.65
1:K:181:VAL:HA	1:K:210:LEU:H	1.62	0.65
1:I:249:LYS:HG3	1:I:250:TYR:CD1	2.32	0.65
1:I:134:GLU:HG2	1:I:168:SER:HB3	1.77	0.65
1:J:215:ALA:HB1	1:J:259:ARG:NE	2.12	0.65
1:H:318:TYR:CD1	1:I:32:ASN:C	2.69	0.65
1:A:124:GLY:O	1:A:125:MET:HB2	1.97	0.65
1:D:259:ARG:HG2	1:D:259:ARG:HH11	1.61	0.64
1:D:157:VAL:HG22	1:D:181:VAL:CG1	2.26	0.64
1:B:215:ALA:HB1	1:B:259:ARG:NE	2.09	0.64
1:K:211:VAL:HG22	1:K:212:THR:H	1.61	0.64
1:A:181:VAL:HA	1:A:210:LEU:H	1.61	0.64
1:G:211:VAL:HG22	1:G:212:THR:H	1.62	0.64
1:C:124:GLY:O	1:C:125:MET:HB2	1.95	0.64
1:K:5:TYR:CD1	1:K:304:LEU:HD21	2.33	0.64
1:A:134:GLU:HG2	1:A:168:SER:HB3	1.78	0.64
1:D:249:LYS:HG3	1:D:250:TYR:CD1	2.32	0.64
1:F:181:VAL:HA	1:F:210:LEU:H	1.61	0.64
1:L:302:ARG:HG2	1:L:302:ARG:HH11	1.62	0.64
1:E:210:LEU:HD13	1:E:211:VAL:CA	2.27	0.64
1:B:144:HIS:O	1:B:146:PRO:HD2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:302:ARG:HH11	1:K:302:ARG:HG2	1.61	0.64
1:K:215:ALA:HB1	1:K:259:ARG:NE	2.11	0.64
1:I:34:TYR:O	1:I:36:PRO:HD3	1.97	0.64
1:E:184:GLY:HA2	1:E:250:TYR:CE2	2.33	0.64
1:L:259:ARG:HG2	1:L:259:ARG:HH11	1.61	0.64
1:I:5:TYR:CD1	1:I:304:LEU:HD21	2.33	0.64
1:G:239:GLU:HA	1:G:242:ARG:HH21	1.61	0.64
1:L:103:ARG:NH1	1:L:103:ARG:HG2	2.01	0.64
1:B:210:LEU:CD1	1:B:211:VAL:N	2.60	0.64
1:B:314:ALA:O	1:B:315:LYS:CB	2.44	0.64
1:K:184:GLY:HA2	1:K:250:TYR:CE2	2.33	0.64
1:G:215:ALA:HB1	1:G:259:ARG:NE	2.12	0.64
1:L:249:LYS:HG3	1:L:250:TYR:CD1	2.33	0.64
1:D:295:GLU:HB2	1:F:95:ARG:HB3	1.80	0.64
1:E:-9:SER:O	1:E:-8:SER:HB3	1.98	0.63
1:B:124:GLY:O	1:B:125:MET:HB2	1.98	0.63
1:A:183:PHE:CG	1:A:214:ASP:OD2	2.52	0.63
1:A:249:LYS:HG3	1:A:250:TYR:CD1	2.33	0.63
1:D:215:ALA:CB	1:D:259:ARG:HE	2.08	0.63
1:H:48:PHE:O	1:H:75:PRO:HA	1.98	0.63
1:J:7:THR:O	1:J:10:THR:HG23	1.97	0.63
1:E:7:THR:O	1:E:10:THR:HG23	1.98	0.63
1:A:7:THR:O	1:A:10:THR:HG23	1.98	0.63
1:E:210:LEU:HD13	1:E:211:VAL:H	1.63	0.63
1:A:215:ALA:CB	1:L:115:ASN:HB3	2.27	0.63
1:F:53:THR:O	1:F:57:VAL:HG13	1.99	0.63
1:D:144:HIS:O	1:D:146:PRO:HD2	1.99	0.63
1:L:13:LYS:HA	1:L:176:MET:HE1	1.81	0.63
1:L:124:GLY:O	1:L:125:MET:HB2	1.96	0.63
1:J:5:TYR:CD1	1:J:304:LEU:HD21	2.33	0.63
1:I:302:ARG:HH11	1:I:302:ARG:CG	2.12	0.63
1:E:34:TYR:O	1:E:36:PRO:HD3	1.98	0.63
1:G:79:GLN:O	1:G:81:GLY:N	2.32	0.63
1:J:211:VAL:HG13	1:J:212:THR:N	2.14	0.63
1:I:124:GLY:O	1:I:125:MET:HB2	1.99	0.63
1:K:124:GLY:O	1:K:125:MET:HB2	1.98	0.63
1:C:239:GLU:HA	1:C:242:ARG:HH21	1.63	0.63
1:K:259:ARG:HG2	1:K:259:ARG:HH11	1.62	0.63
1:C:72:TYR:CE2	1:C:74:ALA:HA	2.34	0.63
1:A:53:THR:CG2	1:C:77:GLN:HG3	2.22	0.63
1:L:215:ALA:HB1	1:L:259:ARG:NE	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:124:GLY:O	1:J:125:MET:HB2	1.99	0.63
1:C:319:ASP:HB3	1:C:322:LYS:HB2	1.80	0.63
1:F:5:TYR:CD1	1:F:304:LEU:HD21	2.33	0.63
1:A:302:ARG:HG2	1:A:302:ARG:HH11	1.63	0.63
1:C:2:LYS:HE2	1:C:119:ILE:O	1.99	0.63
1:A:297:ARG:HG3	1:A:297:ARG:NH1	2.14	0.62
1:I:7:THR:O	1:I:10:THR:HG23	1.99	0.62
1:A:53:THR:O	1:A:57:VAL:HG13	1.98	0.62
1:G:319:ASP:HB3	1:G:322:LYS:HB2	1.81	0.62
1:J:239:GLU:HA	1:J:242:ARG:HH21	1.63	0.62
1:H:215:ALA:HB1	1:H:259:ARG:NE	2.11	0.62
1:J:34:TYR:O	1:J:36:PRO:HD3	1.99	0.62
1:H:157:VAL:HG22	1:H:181:VAL:CG1	2.29	0.62
1:E:183:PHE:CG	1:E:214:ASP:OD2	2.53	0.62
1:C:249:LYS:HG3	1:C:250:TYR:CD1	2.35	0.62
1:L:7:THR:O	1:L:10:THR:HG23	1.99	0.62
1:E:95:ARG:HB3	1:F:295:GLU:HB2	1.82	0.62
1:B:34:TYR:O	1:B:36:PRO:HD3	1.99	0.62
1:A:184:GLY:HA2	1:A:250:TYR:CE2	2.35	0.62
1:D:157:VAL:HG22	1:D:181:VAL:HG13	1.82	0.62
1:K:249:LYS:HG3	1:K:250:TYR:CD1	2.35	0.62
1:L:157:VAL:HG22	1:L:181:VAL:CG1	2.30	0.62
1:J:302:ARG:CG	1:J:302:ARG:HH11	2.13	0.62
1:B:48:PHE:O	1:B:75:PRO:HA	2.00	0.62
1:L:78:ILE:HD13	1:L:80:LEU:CB	2.30	0.62
1:I:48:PHE:O	1:I:75:PRO:HA	1.99	0.62
1:I:55:THR:OG1	2:I:341:SO4:O2	2.16	0.62
1:F:211:VAL:HG13	1:F:212:THR:N	2.14	0.62
1:C:210:LEU:CD1	1:C:211:VAL:N	2.62	0.62
1:D:239:GLU:HA	1:D:242:ARG:HH21	1.65	0.62
1:J:191:ASN:ND2	1:J:193:GLU:HB3	2.15	0.62
1:G:236:GLU:C	1:G:238:SER:H	2.03	0.61
1:B:-13:HIS:HE1	1:E:106:ARG:CD	2.13	0.61
1:E:297:ARG:NH1	1:E:297:ARG:HG3	2.15	0.61
1:G:314:ALA:O	1:G:315:LYS:CB	2.48	0.61
1:B:53:THR:O	1:B:57:VAL:HG13	1.99	0.61
1:E:215:ALA:HB1	1:E:259:ARG:NE	2.12	0.61
1:A:239:GLU:HA	1:A:242:ARG:HH21	1.65	0.61
1:D:249:LYS:O	1:D:251:GLN:N	2.32	0.61
1:H:53:THR:O	1:H:57:VAL:HG13	2.00	0.61
1:K:302:ARG:CG	1:K:302:ARG:HH11	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:GLY:O	1:E:-11:HIS:CA	2.48	0.61
1:C:1:MET:O	1:C:2:LYS:HB3	1.99	0.61
1:F:56:ARG:HG3	1:F:72:TYR:CD1	2.35	0.61
1:D:302:ARG:HH11	1:D:302:ARG:HG2	1.64	0.61
1:K:157:VAL:HG22	1:K:181:VAL:HG13	1.82	0.61
1:K:237:LEU:O	1:K:238:SER:O	2.19	0.61
1:C:7:THR:O	1:C:10:THR:HG23	2.01	0.61
1:J:210:LEU:CD1	1:J:211:VAL:N	2.62	0.61
1:B:184:GLY:HA2	1:B:250:TYR:CE2	2.35	0.61
1:I:103:ARG:HG2	1:I:103:ARG:NH1	1.97	0.61
1:G:211:VAL:HG13	1:G:212:THR:N	2.14	0.61
1:H:183:PHE:CG	1:H:214:ASP:OD2	2.54	0.61
1:K:183:PHE:CG	1:K:214:ASP:OD2	2.53	0.61
1:I:259:ARG:NH1	1:I:259:ARG:CG	2.59	0.61
1:H:124:GLY:O	1:H:125:MET:HB2	2.01	0.61
1:J:56:ARG:HG3	1:J:72:TYR:CD1	2.36	0.61
1:K:259:ARG:HG3	1:K:259:ARG:HH11	1.66	0.61
1:G:48:PHE:O	1:G:75:PRO:HA	2.01	0.61
1:J:103:ARG:HG2	1:J:103:ARG:NH1	2.00	0.60
1:E:211:VAL:HG13	1:E:212:THR:N	2.14	0.60
1:A:183:PHE:CD2	1:A:214:ASP:OD2	2.54	0.60
1:G:210:LEU:CD1	1:G:211:VAL:N	2.61	0.60
1:A:211:VAL:HG13	1:A:212:THR:N	2.15	0.60
1:E:249:LYS:HG3	1:E:250:TYR:CD1	2.36	0.60
1:J:184:GLY:HA2	1:J:250:TYR:CE2	2.36	0.60
1:D:191:ASN:ND2	1:D:193:GLU:HB3	2.16	0.60
1:A:2:LYS:HE2	1:A:119:ILE:O	2.01	0.60
1:L:34:TYR:O	1:L:36:PRO:HD3	2.01	0.60
1:F:314:ALA:O	1:F:315:LYS:HB2	2.00	0.60
1:E:314:ALA:O	1:E:315:LYS:CB	2.48	0.60
1:D:2:LYS:HE2	1:D:119:ILE:O	2.01	0.60
1:C:53:THR:O	1:C:57:VAL:HG13	2.01	0.60
1:C:79:GLN:O	1:C:82:GLY:N	2.34	0.60
1:F:249:LYS:HG3	1:F:250:TYR:CD1	2.36	0.60
1:B:-9:SER:HB3	1:E:194:HIS:CE1	2.31	0.60
1:L:48:PHE:O	1:L:75:PRO:HA	2.02	0.60
1:F:302:ARG:HH11	1:F:302:ARG:HG2	1.67	0.60
1:B:200:LYS:NZ	1:E:200:LYS:NZ	2.49	0.60
1:K:53:THR:O	1:K:57:VAL:HG13	2.02	0.60
1:G:53:THR:CG2	1:I:77:GLN:HG3	2.15	0.60
1:E:259:ARG:HH11	1:E:259:ARG:HG3	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:249:LYS:HG3	1:J:250:TYR:CD1	2.37	0.60
1:H:314:ALA:O	1:H:315:LYS:CB	2.49	0.60
1:H:319:ASP:HB3	1:H:322:LYS:HB2	1.82	0.60
1:K:72:TYR:CE2	1:K:74:ALA:HA	2.36	0.60
1:D:332:VAL:O	1:D:336:THR:HG23	2.02	0.60
1:C:215:ALA:HB1	1:C:259:ARG:NE	2.12	0.60
1:K:183:PHE:CD2	1:K:214:ASP:OD2	2.55	0.60
1:F:72:TYR:CE2	1:F:74:ALA:HA	2.37	0.60
1:A:259:ARG:CG	1:A:259:ARG:NH1	2.60	0.60
1:B:249:LYS:HG3	1:B:250:TYR:CD1	2.37	0.60
1:D:7:THR:O	1:D:10:THR:HG23	2.01	0.60
1:B:319:ASP:HB3	1:B:322:LYS:HB2	1.84	0.60
1:L:191:ASN:ND2	1:L:193:GLU:HB3	2.17	0.60
1:F:48:PHE:O	1:F:75:PRO:HA	2.01	0.60
1:K:157:VAL:HG22	1:K:181:VAL:CG1	2.32	0.60
1:A:230:TYR:HA	1:A:242:ARG:HD3	1.84	0.60
1:D:210:LEU:HD13	1:D:211:VAL:CA	2.31	0.59
1:C:211:VAL:HG13	1:C:212:THR:N	2.16	0.59
1:G:259:ARG:HG3	1:G:259:ARG:HH11	1.67	0.59
1:G:191:ASN:ND2	1:G:193:GLU:HB3	2.16	0.59
1:G:72:TYR:CE2	1:G:74:ALA:HA	2.37	0.59
1:B:-13:HIS:CE1	1:E:106:ARG:HD2	2.36	0.59
1:F:215:ALA:HB1	1:F:259:ARG:NE	2.13	0.59
1:E:56:ARG:HG3	1:E:72:TYR:CD1	2.37	0.59
1:C:253:ASN:OD1	1:C:255:GLU:HB3	2.02	0.59
1:H:34:TYR:O	1:H:36:PRO:HD3	2.02	0.59
1:E:13:LYS:HA	1:E:176:MET:HE1	1.84	0.59
1:I:72:TYR:CE2	1:I:74:ALA:HA	2.36	0.59
1:H:183:PHE:CD2	1:H:214:ASP:OD2	2.55	0.59
1:H:210:LEU:CD1	1:H:211:VAL:N	2.64	0.59
1:J:2:LYS:HE2	1:J:119:ILE:O	2.02	0.59
1:H:72:TYR:CE2	1:H:74:ALA:HA	2.37	0.59
1:I:314:ALA:O	1:I:315:LYS:CB	2.49	0.59
1:F:319:ASP:HB3	1:F:322:LYS:HB2	1.84	0.59
1:B:233:TYR:N	1:E:-11:HIS:HB3	2.17	0.59
1:E:2:LYS:HE2	1:E:119:ILE:O	2.01	0.59
1:G:34:TYR:O	1:G:36:PRO:HD3	2.01	0.59
1:H:7:THR:O	1:H:10:THR:HG23	2.02	0.59
1:E:157:VAL:HG22	1:E:181:VAL:CG1	2.33	0.59
1:K:48:PHE:O	1:K:75:PRO:HA	2.02	0.59
1:L:72:TYR:CE2	1:L:74:ALA:HA	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:332:VAL:O	1:K:336:THR:HG23	2.02	0.59
1:A:302:ARG:HH11	1:A:302:ARG:CG	2.15	0.59
1:C:99:ILE:HB	1:C:309:MET:HE3	1.83	0.59
1:G:249:LYS:HG3	1:G:250:TYR:CD1	2.38	0.59
1:K:211:VAL:HG13	1:K:212:THR:N	2.17	0.59
1:C:302:ARG:HH11	1:C:302:ARG:CG	2.16	0.59
1:C:183:PHE:CD2	1:C:214:ASP:OD2	2.56	0.59
1:F:259:ARG:HG3	1:F:259:ARG:HH11	1.67	0.59
1:I:191:ASN:ND2	1:I:193:GLU:HB3	2.17	0.59
1:B:175:LYS:HB3	1:B:176:MET:HE3	1.83	0.59
1:E:183:PHE:CD2	1:E:214:ASP:OD2	2.56	0.59
1:H:211:VAL:HG13	1:H:212:THR:N	2.18	0.59
1:K:314:ALA:O	1:K:315:LYS:CB	2.51	0.59
1:L:302:ARG:CG	1:L:302:ARG:HH11	2.15	0.59
1:B:332:VAL:O	1:B:336:THR:HG23	2.03	0.59
1:J:259:ARG:HH11	1:J:259:ARG:HG3	1.67	0.58
1:F:191:ASN:ND2	1:F:193:GLU:HB3	2.18	0.58
1:A:157:VAL:HG22	1:A:181:VAL:CG1	2.33	0.58
1:H:249:LYS:HG3	1:H:250:TYR:CD1	2.38	0.58
1:C:34:TYR:O	1:C:36:PRO:HD3	2.02	0.58
1:B:7:THR:O	1:B:10:THR:HG23	2.03	0.58
1:B:-13:HIS:CE1	1:E:106:ARG:HE	2.22	0.58
1:J:210:LEU:HD13	1:J:211:VAL:CA	2.34	0.58
1:B:210:LEU:HD13	1:B:211:VAL:CA	2.33	0.58
1:I:259:ARG:HH11	1:I:259:ARG:HG3	1.66	0.58
1:C:314:ALA:O	1:C:315:LYS:CB	2.51	0.58
1:K:191:ASN:ND2	1:K:193:GLU:HB3	2.17	0.58
1:F:175:LYS:HB3	1:F:176:MET:HE3	1.83	0.58
1:I:319:ASP:HB3	1:I:322:LYS:HB2	1.85	0.58
1:K:85:THR:HB	1:K:87:GLU:OE1	2.03	0.58
1:D:158:PHE:CE2	1:D:166:CYS:HB2	2.38	0.58
1:H:302:ARG:HH11	1:H:302:ARG:HG2	1.67	0.58
1:D:48:PHE:O	1:D:75:PRO:HA	2.04	0.58
1:B:239:GLU:HA	1:B:242:ARG:HH21	1.69	0.58
1:C:13:LYS:HA	1:C:176:MET:HE1	1.84	0.58
1:J:253:ASN:OD1	1:J:255:GLU:HB3	2.04	0.58
1:E:332:VAL:O	1:E:336:THR:HG23	2.03	0.58
1:G:157:VAL:HG22	1:G:181:VAL:CG1	2.33	0.58
1:I:157:VAL:HG22	1:I:181:VAL:CG1	2.32	0.58
1:L:157:VAL:HG22	1:L:181:VAL:HG13	1.86	0.58
1:G:2:LYS:HE2	1:G:119:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:314:ALA:O	1:J:315:LYS:CB	2.50	0.58
1:A:191:ASN:ND2	1:A:193:GLU:HB3	2.18	0.58
1:H:191:ASN:ND2	1:H:193:GLU:HB3	2.18	0.58
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.65	0.58
1:B:157:VAL:HG22	1:B:181:VAL:CG1	2.33	0.58
1:J:48:PHE:O	1:J:75:PRO:HA	2.03	0.58
1:E:175:LYS:HB3	1:E:176:MET:HE3	1.84	0.58
1:B:191:ASN:ND2	1:B:193:GLU:HB3	2.19	0.58
1:L:332:VAL:O	1:L:336:THR:HG23	2.04	0.58
1:G:53:THR:O	1:G:57:VAL:HG13	2.03	0.58
1:D:314:ALA:O	1:D:315:LYS:CB	2.51	0.58
1:G:183:PHE:HE1	1:G:218:VAL:CG1	2.16	0.58
1:D:302:ARG:HH11	1:D:302:ARG:CG	2.15	0.58
1:E:72:TYR:CE2	1:E:74:ALA:HA	2.39	0.58
1:B:230:TYR:HA	1:B:242:ARG:HD3	1.85	0.58
1:B:71:GLU:HG2	1:C:60:GLU:HG2	1.85	0.58
1:I:253:ASN:OD1	1:I:255:GLU:HB3	2.03	0.58
1:I:175:LYS:HB3	1:I:176:MET:HE3	1.85	0.58
1:E:-12:HIS:O	1:E:-11:HIS:CG	2.57	0.58
1:B:-3:ARG:CA	1:B:-3:ARG:HE	2.06	0.58
1:A:157:VAL:HG22	1:A:181:VAL:HG13	1.86	0.57
1:D:183:PHE:CD2	1:D:214:ASP:OD2	2.57	0.57
1:B:183:PHE:CD2	1:B:214:ASP:OD2	2.57	0.57
1:H:183:PHE:HE1	1:H:218:VAL:CG1	2.18	0.57
1:G:259:ARG:NH1	1:G:259:ARG:CG	2.60	0.57
1:K:2:LYS:HE2	1:K:119:ILE:O	2.04	0.57
1:J:72:TYR:CE2	1:J:74:ALA:HA	2.39	0.57
1:D:72:TYR:CE2	1:D:74:ALA:HA	2.39	0.57
1:B:232:LEU:C	1:E:-11:HIS:HB3	2.22	0.57
1:I:297:ARG:NH1	1:I:297:ARG:HG3	2.19	0.57
1:D:230:TYR:HA	1:D:242:ARG:HD3	1.86	0.57
1:L:314:ALA:O	1:L:315:LYS:CB	2.51	0.57
1:B:253:ASN:OD1	1:B:255:GLU:HB3	2.05	0.57
1:B:183:PHE:CG	1:B:214:ASP:OD2	2.57	0.57
1:C:183:PHE:CG	1:C:214:ASP:OD2	2.56	0.57
1:C:183:PHE:HE1	1:C:218:VAL:CG1	2.18	0.57
1:C:82:GLY:C	1:C:84:GLU:H	2.07	0.57
1:A:314:ALA:O	1:A:315:LYS:CB	2.49	0.57
1:K:13:LYS:HA	1:K:176:MET:HE1	1.84	0.57
1:B:72:TYR:CE2	1:B:74:ALA:HA	2.40	0.57
1:E:191:ASN:ND2	1:E:193:GLU:HB3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:VAL:HG13	1:D:212:THR:N	2.18	0.57
1:I:183:PHE:HE1	1:I:218:VAL:CG1	2.18	0.57
1:B:-6:LEU:HD13	1:B:128:TYR:CE1	2.40	0.57
1:A:72:TYR:CE2	1:A:74:ALA:HA	2.39	0.57
1:D:183:PHE:HE1	1:D:218:VAL:CG1	2.16	0.57
1:A:48:PHE:O	1:A:75:PRO:HA	2.05	0.57
1:D:-4:PRO:CD	1:D:6:VAL:HG21	2.33	0.57
1:F:157:VAL:HG22	1:F:181:VAL:CG1	2.35	0.57
1:H:253:ASN:OD1	1:H:255:GLU:HB3	2.04	0.57
1:F:85:THR:HB	1:F:87:GLU:OE1	2.04	0.57
1:E:259:ARG:NH1	1:E:259:ARG:CG	2.57	0.57
1:I:211:VAL:HG13	1:I:212:THR:N	2.20	0.57
1:J:78:ILE:CG1	1:J:79:GLN:N	2.67	0.57
1:B:131:PRO:HA	1:B:134:GLU:HG3	1.86	0.57
1:G:13:LYS:HA	1:G:176:MET:HE1	1.86	0.57
1:G:302:ARG:HG2	1:G:302:ARG:HH11	1.69	0.57
1:A:85:THR:HB	1:A:87:GLU:OE1	2.05	0.57
1:C:210:LEU:HD13	1:C:211:VAL:CA	2.34	0.57
1:B:210:LEU:HD13	1:B:211:VAL:H	1.69	0.57
1:C:48:PHE:O	1:C:75:PRO:HA	2.04	0.57
1:J:237:LEU:O	1:J:238:SER:O	2.22	0.57
1:J:13:LYS:HA	1:J:176:MET:HE1	1.87	0.57
1:H:85:THR:HB	1:H:87:GLU:OE1	2.05	0.57
1:H:210:LEU:HD13	1:H:211:VAL:CA	2.35	0.57
1:I:215:ALA:CB	1:I:259:ARG:HE	2.16	0.57
1:E:-7:GLY:O	1:E:-6:LEU:HB2	2.03	0.57
1:F:302:ARG:HH11	1:F:302:ARG:CG	2.17	0.57
1:J:183:PHE:CD2	1:J:214:ASP:OD2	2.58	0.56
1:A:13:LYS:HA	1:A:176:MET:HE1	1.87	0.56
1:E:71:GLU:HG2	1:F:60:GLU:HG2	1.87	0.56
1:D:85:THR:HB	1:D:87:GLU:OE1	2.05	0.56
1:C:259:ARG:HH11	1:C:259:ARG:HG3	1.68	0.56
1:K:249:LYS:HE3	1:K:250:TYR:CZ	2.40	0.56
1:J:183:PHE:HE1	1:J:218:VAL:CG1	2.18	0.56
1:I:157:VAL:HG22	1:I:181:VAL:HG13	1.86	0.56
1:H:2:LYS:HE2	1:H:119:ILE:O	2.06	0.56
1:F:2:LYS:HE2	1:F:119:ILE:O	2.05	0.56
1:H:302:ARG:HH11	1:H:302:ARG:CG	2.17	0.56
1:K:319:ASP:HB3	1:K:322:LYS:HB2	1.86	0.56
1:J:15:GLU:HA	1:L:339:ILE:HG21	1.87	0.56
1:B:302:ARG:HH11	1:B:302:ARG:HG2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:147:GLU:O	1:K:149:LYS:N	2.37	0.56
1:G:157:VAL:HG22	1:G:181:VAL:HG13	1.88	0.56
1:C:184:GLY:HA2	1:C:250:TYR:CE2	2.40	0.56
1:F:210:LEU:HD13	1:F:211:VAL:CA	2.34	0.56
1:F:58:SER:C	1:F:301:ILE:HD11	2.26	0.56
1:D:58:SER:C	1:D:301:ILE:HD11	2.26	0.56
1:D:319:ASP:HB3	1:D:322:LYS:HB2	1.86	0.56
1:D:-4:PRO:HG2	1:D:6:VAL:CG2	2.32	0.56
1:G:184:GLY:HA2	1:G:250:TYR:CE2	2.40	0.56
1:K:210:LEU:CD1	1:K:211:VAL:N	2.65	0.56
1:F:183:PHE:HE1	1:F:218:VAL:CG1	2.18	0.56
1:L:210:LEU:HD13	1:L:211:VAL:CA	2.35	0.56
1:B:56:ARG:HG3	1:B:72:TYR:CD1	2.41	0.56
1:G:175:LYS:HB3	1:G:176:MET:HE3	1.88	0.56
1:C:85:THR:HB	1:C:87:GLU:OE1	2.06	0.56
1:A:215:ALA:CB	1:A:259:ARG:HE	2.15	0.56
1:I:2:LYS:HE2	1:I:119:ILE:O	2.05	0.56
1:G:253:ASN:OD1	1:G:255:GLU:HB3	2.06	0.56
1:F:7:THR:O	1:F:10:THR:HG23	2.06	0.56
1:B:183:PHE:HE1	1:B:218:VAL:CG1	2.19	0.56
1:A:253:ASN:OD1	1:A:255:GLU:HB3	2.05	0.56
1:C:328:LYS:O	1:C:332:VAL:HG23	2.06	0.56
1:J:53:THR:O	1:J:57:VAL:HG13	2.05	0.56
1:G:183:PHE:CD2	1:G:214:ASP:OD2	2.58	0.56
1:L:183:PHE:HE1	1:L:218:VAL:CG1	2.18	0.56
1:I:85:THR:HB	1:I:87:GLU:OE1	2.06	0.56
1:C:103:ARG:NH1	1:C:103:ARG:CG	2.62	0.55
1:H:157:VAL:HG22	1:H:181:VAL:HG13	1.87	0.55
1:I:249:LYS:HE3	1:I:250:TYR:CZ	2.41	0.55
1:D:13:LYS:HA	1:D:176:MET:HE1	1.88	0.55
1:K:253:ASN:OD1	1:K:255:GLU:HB3	2.07	0.55
1:G:71:GLU:HG2	1:H:60:GLU:HG2	1.88	0.55
1:D:259:ARG:HG3	1:D:259:ARG:HH11	1.71	0.55
1:B:249:LYS:HE3	1:B:250:TYR:CZ	2.41	0.55
1:I:184:GLY:HA2	1:I:250:TYR:CE2	2.41	0.55
1:G:297:ARG:NH1	1:G:297:ARG:HG3	2.21	0.55
1:G:131:PRO:HA	1:G:134:GLU:HG3	1.88	0.55
1:G:125:MET:HG3	1:G:130:HIS:CG	2.41	0.55
1:C:302:ARG:HH11	1:C:302:ARG:HG2	1.71	0.55
1:L:26:ILE:O	1:L:30:ILE:HG13	2.06	0.55
1:J:157:VAL:HG22	1:J:181:VAL:CG1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:184:GLY:HA2	1:L:250:TYR:CE2	2.41	0.55
1:D:34:TYR:O	1:D:36:PRO:HD3	2.06	0.55
1:E:4:PRO:HG2	1:E:6:VAL:CG2	2.14	0.55
1:C:237:LEU:HG	1:C:242:ARG:CG	2.36	0.55
1:D:-4:PRO:HA	1:D:115:ASN:OD1	2.05	0.55
1:D:-5:VAL:HG13	1:D:-4:PRO:HD2	1.88	0.55
1:C:157:VAL:HG22	1:C:181:VAL:HG13	1.87	0.55
1:I:210:LEU:CD1	1:I:211:VAL:N	2.67	0.55
1:B:108:HIS:CD2	1:E:108:HIS:CD2	2.95	0.55
1:J:183:PHE:CG	1:J:214:ASP:OD2	2.59	0.55
1:A:175:LYS:HB3	1:A:176:MET:HE3	1.88	0.55
1:G:332:VAL:O	1:G:336:THR:HG23	2.06	0.55
1:E:253:ASN:OD1	1:E:255:GLU:HB3	2.06	0.55
1:C:230:TYR:HA	1:C:242:ARG:HD3	1.88	0.55
1:E:249:LYS:HE3	1:E:250:TYR:CZ	2.41	0.55
1:J:259:ARG:CG	1:J:259:ARG:NH1	2.60	0.55
1:A:319:ASP:HB3	1:A:322:LYS:HB2	1.89	0.55
1:G:85:THR:HB	1:G:87:GLU:OE1	2.06	0.55
1:B:112:ASP:OD2	1:E:106:ARG:NH2	2.40	0.55
1:B:85:THR:HB	1:B:87:GLU:OE1	2.06	0.55
1:C:191:ASN:ND2	1:C:193:GLU:HB3	2.22	0.55
1:C:215:ALA:CB	1:C:259:ARG:HE	2.16	0.55
1:F:183:PHE:CG	1:F:214:ASP:OD2	2.60	0.55
1:F:159:VAL:HB	1:F:183:PHE:CZ	2.42	0.55
1:L:159:VAL:HB	1:L:183:PHE:CZ	2.42	0.55
1:D:131:PRO:HA	1:D:134:GLU:HG3	1.89	0.55
1:K:175:LYS:HB3	1:K:176:MET:HE3	1.88	0.55
1:G:302:ARG:CG	1:G:302:ARG:HH11	2.19	0.55
1:C:237:LEU:HD12	1:C:238:SER:HB2	1.85	0.55
1:D:249:LYS:HG3	1:D:250:TYR:CE1	2.42	0.55
1:I:56:ARG:HG3	1:I:72:TYR:CD1	2.42	0.55
1:I:230:TYR:HA	1:I:242:ARG:HD3	1.89	0.55
1:G:210:LEU:HD13	1:G:211:VAL:CA	2.36	0.55
1:E:183:PHE:HE1	1:E:218:VAL:CG1	2.20	0.55
1:K:7:THR:O	1:K:10:THR:HG23	2.07	0.55
1:D:159:VAL:HB	1:D:183:PHE:CZ	2.43	0.54
1:K:183:PHE:HE1	1:K:218:VAL:CG1	2.20	0.54
1:J:157:VAL:HG22	1:J:181:VAL:HG13	1.90	0.54
1:B:214:ASP:O	1:B:215:ALA:C	2.45	0.54
1:H:259:ARG:NH1	1:H:259:ARG:CG	2.57	0.54
1:H:215:ALA:CB	1:H:259:ARG:HE	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:210:LEU:HD13	1:K:211:VAL:CA	2.37	0.54
1:C:157:VAL:HG22	1:C:181:VAL:CG1	2.37	0.54
1:F:183:PHE:CD2	1:F:214:ASP:OD2	2.60	0.54
1:F:259:ARG:NH1	1:F:259:ARG:CG	2.59	0.54
1:L:56:ARG:HG3	1:L:72:TYR:CD1	2.42	0.54
1:D:56:ARG:HG3	1:D:72:TYR:CD1	2.43	0.54
1:B:302:ARG:HH11	1:B:302:ARG:CG	2.20	0.54
1:A:183:PHE:CD1	1:A:214:ASP:OD2	2.61	0.54
1:J:210:LEU:HD13	1:J:211:VAL:H	1.70	0.54
1:H:184:GLY:HA2	1:H:250:TYR:CE2	2.43	0.54
1:L:253:ASN:OD1	1:L:255:GLU:HB3	2.08	0.54
1:F:253:ASN:OD1	1:F:255:GLU:HB3	2.07	0.54
1:A:237:LEU:HD12	1:A:238:SER:HB2	1.89	0.54
1:G:235:ALA:O	1:G:236:GLU:CB	2.54	0.54
1:B:157:VAL:HG22	1:B:181:VAL:HG13	1.89	0.54
1:C:214:ASP:O	1:C:215:ALA:C	2.45	0.54
1:F:249:LYS:HE3	1:F:250:TYR:CZ	2.43	0.54
1:L:211:VAL:HG13	1:L:212:THR:N	2.22	0.54
1:B:2:LYS:HE2	1:B:119:ILE:O	2.07	0.54
1:L:158:PHE:CE2	1:L:166:CYS:HB2	2.43	0.54
1:E:157:VAL:HG22	1:E:181:VAL:HG13	1.89	0.54
1:I:210:LEU:HD13	1:I:211:VAL:CA	2.38	0.54
1:D:5:TYR:CE1	1:D:304:LEU:HD21	2.43	0.54
1:G:56:ARG:HG3	1:G:72:TYR:CD1	2.43	0.54
1:C:332:VAL:O	1:C:336:THR:HG23	2.08	0.54
1:K:34:TYR:O	1:K:36:PRO:HD3	2.07	0.54
1:L:99:ILE:HB	1:L:309:MET:HE3	1.90	0.54
1:H:247:TYR:CD1	1:H:247:TYR:O	2.61	0.54
1:F:332:VAL:O	1:F:336:THR:HG23	2.08	0.54
1:B:233:TYR:N	1:E:-11:HIS:CB	2.71	0.54
1:I:214:ASP:O	1:I:215:ALA:C	2.46	0.54
1:F:297:ARG:HG3	1:F:297:ARG:NH1	2.20	0.54
1:A:56:ARG:HG3	1:A:72:TYR:CD1	2.43	0.54
1:L:85:THR:HB	1:L:87:GLU:OE1	2.07	0.54
1:L:319:ASP:HB3	1:L:322:LYS:HB2	1.90	0.54
1:G:236:GLU:C	1:G:238:SER:N	2.61	0.54
1:D:183:PHE:CG	1:D:214:ASP:OD2	2.60	0.54
1:H:259:ARG:HG3	1:H:259:ARG:HH11	1.70	0.54
1:F:210:LEU:CD1	1:F:211:VAL:N	2.65	0.54
1:I:183:PHE:CG	1:I:214:ASP:OD2	2.61	0.54
1:D:60:GLU:HG2	1:F:71:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:SER:C	1:B:301:ILE:HD11	2.27	0.54
1:B:328:LYS:O	1:B:332:VAL:HG23	2.08	0.54
1:K:159:VAL:HB	1:K:183:PHE:CZ	2.43	0.53
1:I:183:PHE:CD2	1:I:214:ASP:OD2	2.61	0.53
1:D:58:SER:HB3	1:D:301:ILE:HD13	1.90	0.53
1:F:56:ARG:HG3	1:F:72:TYR:CE1	2.43	0.53
1:K:339:ILE:HG21	1:L:15:GLU:HA	1.89	0.53
1:C:159:VAL:HB	1:C:183:PHE:CZ	2.43	0.53
1:G:183:PHE:CG	1:G:214:ASP:OD2	2.61	0.53
1:L:183:PHE:CG	1:L:214:ASP:OD2	2.61	0.53
1:C:82:GLY:O	1:C:84:GLU:N	2.40	0.53
1:A:159:VAL:HB	1:A:183:PHE:CZ	2.43	0.53
1:G:215:ALA:CB	1:G:259:ARG:HE	2.19	0.53
1:L:78:ILE:HG12	1:L:79:GLN:H	1.73	0.53
1:C:58:SER:C	1:C:301:ILE:HD11	2.28	0.53
1:K:56:ARG:HG3	1:K:72:TYR:CD1	2.43	0.53
1:A:12:THR:OG1	1:A:15:GLU:HG3	2.08	0.53
1:E:159:VAL:HB	1:E:183:PHE:CZ	2.43	0.53
1:J:147:GLU:O	1:J:149:LYS:N	2.41	0.53
1:L:73:LEU:N	1:L:73:LEU:HD13	2.23	0.53
1:L:259:ARG:CG	1:L:259:ARG:NH1	2.62	0.53
1:C:158:PHE:CE2	1:C:166:CYS:HB2	2.44	0.53
1:A:214:ASP:O	1:A:215:ALA:C	2.46	0.53
1:A:183:PHE:HE1	1:A:218:VAL:CG1	2.22	0.53
1:A:249:LYS:HG3	1:A:250:TYR:CE1	2.44	0.53
1:H:297:ARG:HG3	1:H:297:ARG:NH1	2.23	0.53
1:C:131:PRO:HA	1:C:134:GLU:HG3	1.91	0.53
1:H:5:TYR:CE1	1:H:304:LEU:HD21	2.43	0.53
1:I:-1:SER:HB3	1:I:2:LYS:HG3	1.90	0.53
1:D:328:LYS:O	1:D:332:VAL:HG23	2.09	0.53
1:F:13:LYS:HA	1:F:176:MET:HE1	1.90	0.53
1:C:147:GLU:O	1:C:149:LYS:N	2.41	0.53
1:E:214:ASP:HB2	1:E:249:LYS:HD2	1.90	0.53
1:L:259:ARG:HG3	1:L:259:ARG:HH11	1.69	0.53
1:J:230:TYR:HA	1:J:242:ARG:HD3	1.91	0.53
1:J:236:GLU:O	1:J:237:LEU:O	2.25	0.53
1:K:236:GLU:O	1:K:237:LEU:C	2.47	0.53
1:C:210:LEU:HD13	1:C:211:VAL:H	1.71	0.53
1:G:58:SER:C	1:G:301:ILE:HD11	2.29	0.53
1:I:125:MET:HG3	1:I:130:HIS:CG	2.43	0.53
1:C:56:ARG:HG3	1:C:72:TYR:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:LYS:O	1:E:332:VAL:HG23	2.09	0.53
1:I:12:THR:OG1	1:I:15:GLU:HG3	2.09	0.53
1:F:184:GLY:HA2	1:F:250:TYR:CE2	2.44	0.53
1:L:2:LYS:HE2	1:L:119:ILE:C	2.29	0.53
1:J:295:GLU:HB2	1:L:95:ARG:HB3	1.91	0.53
1:E:183:PHE:CD1	1:E:214:ASP:OD2	2.62	0.53
1:K:297:ARG:HG3	1:K:297:ARG:NH1	2.23	0.53
1:H:131:PRO:HA	1:H:134:GLU:HG3	1.89	0.53
1:H:175:LYS:HB3	1:H:176:MET:HE3	1.90	0.53
1:E:85:THR:HB	1:E:87:GLU:OE1	2.08	0.53
1:E:302:ARG:HG2	1:E:302:ARG:HH11	1.73	0.53
1:E:-11:HIS:O	1:E:-10:HIS:O	2.27	0.52
1:A:259:ARG:HH11	1:A:259:ARG:HG3	1.70	0.52
1:L:210:LEU:CD1	1:L:211:VAL:N	2.68	0.52
1:L:131:PRO:HA	1:L:134:GLU:HG3	1.91	0.52
1:F:131:PRO:HA	1:F:134:GLU:HG3	1.90	0.52
1:E:214:ASP:O	1:E:215:ALA:C	2.47	0.52
1:K:214:ASP:HB2	1:K:249:LYS:HD2	1.91	0.52
1:A:95:ARG:HB3	1:B:295:GLU:HB2	1.91	0.52
1:H:56:ARG:HG3	1:H:72:TYR:CD1	2.44	0.52
1:G:147:GLU:O	1:G:149:LYS:N	2.43	0.52
1:D:214:ASP:O	1:D:215:ALA:C	2.48	0.52
1:L:230:TYR:HA	1:L:242:ARG:HD3	1.91	0.52
1:L:5:TYR:CE1	1:L:304:LEU:HD21	2.45	0.52
1:L:125:MET:HG3	1:L:130:HIS:CG	2.44	0.52
1:H:99:ILE:HG13	1:H:120:PRO:HB2	1.91	0.52
1:L:147:GLU:O	1:L:149:LYS:N	2.42	0.52
1:J:188:PHE:CE2	1:J:245:VAL:HG21	2.45	0.52
1:L:183:PHE:CD2	1:L:214:ASP:OD2	2.62	0.52
1:J:214:ASP:O	1:J:215:ALA:C	2.47	0.52
1:H:58:SER:C	1:H:301:ILE:HD11	2.29	0.52
1:D:53:THR:HG1	1:F:79:GLN:HG3	1.72	0.52
1:H:159:VAL:HB	1:H:183:PHE:CZ	2.45	0.52
1:C:249:LYS:C	1:C:251:GLN:H	2.13	0.52
1:I:159:VAL:HB	1:I:183:PHE:CZ	2.45	0.52
1:I:249:LYS:HE3	1:I:250:TYR:CE1	2.44	0.52
1:J:159:VAL:HB	1:J:183:PHE:CZ	2.45	0.52
1:B:5:TYR:CE1	1:B:304:LEU:HD21	2.44	0.52
1:F:314:ALA:O	1:F:315:LYS:CB	2.56	0.52
1:E:192:GLU:H	1:E:192:GLU:CD	2.13	0.52
1:A:238:SER:HB2	1:A:241:GLU:HB3	1.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:SER:HB2	1:C:241:GLU:HB3	1.87	0.52
1:B:106:ARG:HH21	1:E:112:ASP:CG	2.13	0.52
1:E:215:ALA:CB	1:E:259:ARG:HE	2.16	0.52
1:F:157:VAL:HG22	1:F:181:VAL:HG13	1.91	0.52
1:L:214:ASP:O	1:L:215:ALA:C	2.47	0.52
1:C:175:LYS:HB3	1:C:176:MET:HE3	1.91	0.52
1:A:34:TYR:O	1:A:36:PRO:HD3	2.09	0.52
1:G:5:TYR:CE1	1:G:304:LEU:HD21	2.44	0.52
1:K:73:LEU:N	1:K:73:LEU:HD13	2.25	0.52
1:L:150:LYS:O	1:L:151:LEU:CB	2.57	0.52
1:I:103:ARG:NH1	1:I:103:ARG:CG	2.61	0.52
1:J:99:ILE:HB	1:J:309:MET:HE3	1.91	0.52
1:J:73:LEU:HD13	1:J:73:LEU:N	2.25	0.52
1:G:57:VAL:HG12	1:I:73:LEU:HD11	1.91	0.52
1:F:249:LYS:C	1:F:251:GLN:H	2.12	0.52
1:A:58:SER:C	1:A:301:ILE:HD11	2.30	0.52
1:H:230:TYR:HA	1:H:242:ARG:HD3	1.92	0.52
1:I:131:PRO:HA	1:I:134:GLU:HG3	1.91	0.52
1:B:192:GLU:H	1:B:192:GLU:CD	2.13	0.52
1:G:159:VAL:HB	1:G:183:PHE:CZ	2.44	0.51
1:L:249:LYS:HE3	1:L:250:TYR:CZ	2.45	0.51
1:I:58:SER:C	1:I:301:ILE:HD11	2.31	0.51
1:B:104:VAL:HG21	1:B:109:SER:OG	2.10	0.51
1:G:230:TYR:HA	1:G:242:ARG:HD3	1.91	0.51
1:E:302:ARG:HH11	1:E:302:ARG:CG	2.23	0.51
1:H:147:GLU:O	1:H:149:LYS:N	2.43	0.51
1:B:147:GLU:O	1:B:149:LYS:N	2.44	0.51
1:I:26:ILE:O	1:I:30:ILE:HG13	2.10	0.51
1:G:229:TRP:CZ2	1:G:277:GLU:HA	2.45	0.51
1:K:21:ASP:O	1:K:25:LYS:HG2	2.10	0.51
1:B:231:GLY:C	1:E:-11:HIS:HD2	2.14	0.51
1:G:236:GLU:O	1:G:238:SER:N	2.43	0.51
1:L:249:LYS:HG3	1:L:250:TYR:CE1	2.46	0.51
1:J:249:LYS:C	1:J:251:GLN:H	2.12	0.51
1:B:125:MET:HG3	1:B:130:HIS:CG	2.46	0.51
1:D:247:TYR:O	1:D:247:TYR:CD1	2.63	0.51
1:D:249:LYS:HE3	1:D:250:TYR:CZ	2.46	0.51
1:H:249:LYS:C	1:H:251:GLN:H	2.12	0.51
1:H:318:TYR:HD1	1:I:32:ASN:HA	1.74	0.51
1:H:13:LYS:HA	1:H:176:MET:HE1	1.91	0.51
1:A:99:ILE:HG13	1:A:120:PRO:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:328:LYS:O	1:I:332:VAL:HG23	2.10	0.51
1:E:147:GLU:O	1:E:149:LYS:N	2.44	0.51
1:C:249:LYS:HE3	1:C:250:TYR:CZ	2.46	0.51
1:K:249:LYS:HE3	1:K:250:TYR:CE1	2.46	0.51
1:I:259:ARG:NH1	1:I:259:ARG:HG3	2.25	0.51
1:K:133:GLN:NE2	1:K:297:ARG:HD3	2.26	0.51
1:E:-12:HIS:O	1:E:-11:HIS:ND1	2.43	0.51
1:F:230:TYR:HA	1:F:242:ARG:HD3	1.93	0.51
1:J:85:THR:HB	1:J:87:GLU:OE1	2.10	0.51
1:F:147:GLU:O	1:F:149:LYS:N	2.44	0.51
1:H:73:LEU:HD13	1:H:73:LEU:N	2.25	0.51
1:D:184:GLY:HA2	1:D:250:TYR:CE2	2.46	0.51
1:F:259:ARG:HG3	1:F:259:ARG:NH1	2.26	0.51
1:J:249:LYS:HE3	1:J:250:TYR:CZ	2.45	0.51
1:E:58:SER:C	1:E:301:ILE:HD11	2.31	0.51
1:D:297:ARG:NH1	1:D:297:ARG:HG3	2.23	0.51
1:L:52:SER:OG	2:L:342:SO4:O2	2.16	0.51
1:D:147:GLU:O	1:D:149:LYS:N	2.44	0.51
1:L:247:TYR:O	1:L:247:TYR:CD1	2.64	0.51
1:B:249:LYS:C	1:B:251:GLN:H	2.14	0.51
1:C:297:ARG:HG3	1:C:297:ARG:NH1	2.26	0.51
1:A:5:TYR:CE1	1:A:304:LEU:HD21	2.46	0.51
1:B:150:LYS:O	1:B:151:LEU:CB	2.59	0.51
1:A:238:SER:CB	1:A:241:GLU:CB	2.77	0.51
1:D:210:LEU:HD13	1:D:211:VAL:H	1.70	0.51
1:D:210:LEU:HD13	1:D:211:VAL:O	2.11	0.51
1:L:12:THR:OG1	1:L:15:GLU:HG3	2.11	0.51
1:K:229:TRP:CZ2	1:K:277:GLU:HA	2.46	0.51
1:F:238:SER:CB	1:F:241:GLU:CB	2.75	0.51
1:A:249:LYS:HE3	1:A:250:TYR:CZ	2.46	0.51
1:F:247:TYR:CD1	1:F:247:TYR:O	2.64	0.51
1:C:125:MET:HG3	1:C:130:HIS:CG	2.46	0.51
1:K:99:ILE:HB	1:K:309:MET:HE3	1.92	0.51
1:B:188:PHE:CE2	1:B:245:VAL:HG21	2.46	0.51
1:G:214:ASP:HB2	1:G:249:LYS:HD2	1.92	0.50
1:J:259:ARG:NH1	1:J:259:ARG:HG3	2.26	0.50
1:B:-1:SER:HB3	1:B:2:LYS:HG3	1.92	0.50
1:B:99:ILE:HB	1:B:309:MET:HE3	1.93	0.50
1:I:147:GLU:O	1:I:149:LYS:N	2.44	0.50
1:D:150:LYS:O	1:D:151:LEU:CB	2.59	0.50
1:K:214:ASP:O	1:K:215:ALA:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:LYS:HE3	1:G:250:TYR:CZ	2.46	0.50
1:L:215:ALA:CB	1:L:259:ARG:HE	2.20	0.50
1:L:328:LYS:O	1:L:332:VAL:HG23	2.12	0.50
1:L:202:CYS:C	1:L:204:VAL:H	2.14	0.50
1:D:253:ASN:OD1	1:D:255:GLU:HB3	2.10	0.50
1:E:247:TYR:CD1	1:E:247:TYR:O	2.63	0.50
1:B:159:VAL:HB	1:B:183:PHE:CZ	2.45	0.50
1:F:214:ASP:O	1:F:215:ALA:C	2.50	0.50
1:I:249:LYS:HG3	1:I:250:TYR:CE1	2.45	0.50
1:E:5:TYR:CE1	1:E:304:LEU:HD21	2.45	0.50
1:J:191:ASN:HD21	1:J:193:GLU:HB3	1.76	0.50
1:A:147:GLU:O	1:A:149:LYS:N	2.45	0.50
1:L:232:LEU:O	1:L:234:GLU:N	2.44	0.50
1:H:158:PHE:CE2	1:H:166:CYS:HB2	2.46	0.50
1:J:232:LEU:O	1:J:234:GLU:N	2.45	0.50
1:K:103:ARG:CG	1:K:103:ARG:NH1	2.62	0.50
1:G:214:ASP:O	1:G:215:ALA:C	2.50	0.50
1:F:58:SER:HB3	1:F:301:ILE:HD13	1.93	0.50
1:F:125:MET:HG3	1:F:130:HIS:CG	2.47	0.50
1:J:332:VAL:O	1:J:336:THR:HG23	2.11	0.50
1:B:202:CYS:C	1:B:204:VAL:H	2.15	0.50
1:D:238:SER:HB2	1:D:241:GLU:HB3	1.84	0.50
1:B:215:ALA:CB	1:B:259:ARG:HE	2.16	0.50
1:J:247:TYR:CD1	1:J:247:TYR:O	2.65	0.50
1:I:247:TYR:O	1:I:247:TYR:CD1	2.65	0.50
1:F:188:PHE:CE2	1:F:245:VAL:HG21	2.46	0.50
1:D:259:ARG:NH1	1:D:259:ARG:CG	2.62	0.50
1:H:210:LEU:HD13	1:H:211:VAL:O	2.12	0.50
1:L:297:ARG:NH1	1:L:297:ARG:HG3	2.25	0.50
1:B:58:SER:HB3	1:B:301:ILE:HD13	1.94	0.50
1:E:125:MET:HG3	1:E:130:HIS:CG	2.46	0.50
1:B:99:ILE:HG13	1:B:120:PRO:HB2	1.92	0.50
1:C:73:LEU:HD13	1:C:73:LEU:N	2.27	0.50
1:A:249:LYS:C	1:A:251:GLN:H	2.14	0.50
1:I:214:ASP:HB2	1:I:249:LYS:HD2	1.94	0.50
1:J:319:ASP:HB3	1:J:322:LYS:HB2	1.93	0.50
1:D:73:LEU:HD11	1:E:57:VAL:HG12	1.93	0.50
1:J:125:MET:HG3	1:J:130:HIS:CG	2.47	0.50
1:D:150:LYS:O	1:D:151:LEU:HB3	2.12	0.50
1:F:158:PHE:CE2	1:F:166:CYS:HB2	2.47	0.50
1:E:150:LYS:O	1:E:151:LEU:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ASN:HD21	1:B:193:GLU:HB3	1.76	0.50
1:H:150:LYS:O	1:H:151:LEU:CB	2.59	0.50
1:C:150:LYS:O	1:C:151:LEU:CB	2.60	0.50
1:A:71:GLU:HG2	1:B:60:GLU:HG2	1.94	0.50
1:B:54:ARG:NH2	2:B:342:SO4:O3	2.44	0.49
1:B:158:PHE:CE2	1:B:166:CYS:HB2	2.46	0.49
1:H:26:ILE:O	1:H:30:ILE:HG13	2.12	0.49
1:D:0:HIS:N	1:D:0:HIS:ND1	2.60	0.49
1:A:229:TRP:CZ2	1:A:277:GLU:HA	2.48	0.49
1:K:259:ARG:HG3	1:K:259:ARG:NH1	2.26	0.49
1:J:214:ASP:HB2	1:J:249:LYS:HD2	1.95	0.49
1:L:80:LEU:HD13	1:L:86:ILE:HD12	1.94	0.49
1:A:0:HIS:O	1:A:1:MET:C	2.49	0.49
1:G:232:LEU:O	1:G:234:GLU:N	2.45	0.49
1:D:99:ILE:HG13	1:D:120:PRO:HB2	1.94	0.49
1:C:12:THR:OG1	1:C:15:GLU:HG3	2.12	0.49
1:J:26:ILE:O	1:J:30:ILE:HG13	2.13	0.49
1:A:259:ARG:HG3	1:A:259:ARG:NH1	2.27	0.49
1:G:210:LEU:HD13	1:G:211:VAL:H	1.71	0.49
1:E:249:LYS:C	1:E:251:GLN:H	2.15	0.49
1:B:13:LYS:HA	1:B:176:MET:HE1	1.94	0.49
1:G:150:LYS:O	1:G:151:LEU:CB	2.59	0.49
1:C:247:TYR:CD1	1:C:247:TYR:O	2.65	0.49
1:B:231:GLY:O	1:E:-11:HIS:CG	2.65	0.49
1:K:12:THR:OG1	1:K:15:GLU:HG3	2.13	0.49
1:E:191:ASN:O	1:E:195:GLN:HG3	2.11	0.49
1:H:316:ASN:N	1:H:317:PRO:HD3	2.26	0.49
1:F:229:TRP:CZ2	1:F:277:GLU:HA	2.48	0.49
1:A:158:PHE:CE2	1:A:166:CYS:HB2	2.48	0.49
1:I:141:MET:HE3	1:I:223:PHE:CD1	2.47	0.49
1:K:150:LYS:O	1:K:151:LEU:CB	2.60	0.49
1:B:214:ASP:HB2	1:B:249:LYS:HD2	1.93	0.49
1:A:232:LEU:H	1:A:232:LEU:CD1	2.22	0.49
1:A:0:HIS:O	1:A:2:LYS:N	2.46	0.49
1:A:247:TYR:O	1:A:247:TYR:CD1	2.66	0.49
1:H:71:GLU:HG2	1:I:60:GLU:HG2	1.94	0.49
1:C:192:GLU:H	1:C:192:GLU:CD	2.14	0.49
1:L:80:LEU:CD1	1:L:86:ILE:CD1	2.91	0.49
1:G:145:LEU:O	1:G:146:PRO:O	2.30	0.49
1:K:99:ILE:HG13	1:K:120:PRO:HB2	1.94	0.49
1:B:-13:HIS:HE1	1:E:106:ARG:HD2	1.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ARG:NH1	1:D:259:ARG:HG3	2.28	0.49
1:B:247:TYR:O	1:B:248:PRO:O	2.30	0.49
1:K:191:ASN:HD21	1:K:193:GLU:HB3	1.76	0.49
1:L:316:ASN:N	1:L:317:PRO:HD3	2.26	0.49
1:B:233:TYR:H	1:E:-11:HIS:CB	2.21	0.49
1:B:249:LYS:HE3	1:B:250:TYR:CE1	2.48	0.49
1:H:214:ASP:O	1:H:215:ALA:C	2.51	0.49
1:B:-4:PRO:HG2	1:B:6:VAL:CG2	2.37	0.49
1:C:249:LYS:HG3	1:C:250:TYR:CE1	2.48	0.49
1:G:249:LYS:C	1:G:251:GLN:H	2.15	0.49
1:J:58:SER:C	1:J:301:ILE:HD11	2.33	0.49
1:K:230:TYR:HA	1:K:242:ARG:HD3	1.93	0.49
1:A:131:PRO:HA	1:A:134:GLU:HG3	1.94	0.49
1:K:125:MET:HG3	1:K:130:HIS:CG	2.48	0.49
1:E:188:PHE:CE2	1:E:245:VAL:HG21	2.48	0.49
1:A:150:LYS:O	1:A:151:LEU:CB	2.60	0.49
1:J:150:LYS:O	1:J:151:LEU:CB	2.60	0.49
1:C:229:TRP:CZ2	1:C:277:GLU:HA	2.48	0.49
2:B:341:SO4:O2	1:E:-12:HIS:NE2	2.46	0.49
1:K:183:PHE:CD1	1:K:214:ASP:OD2	2.66	0.49
1:A:58:SER:HB3	1:A:301:ILE:HD13	1.94	0.49
1:E:71:GLU:HG2	1:F:60:GLU:CG	2.43	0.49
1:I:202:CYS:C	1:I:204:VAL:H	2.15	0.49
1:K:232:LEU:O	1:K:234:GLU:N	2.46	0.49
1:E:58:SER:HB3	1:E:301:ILE:HD13	1.95	0.49
1:G:58:SER:HB3	1:G:301:ILE:HD13	1.95	0.49
1:G:191:ASN:HD21	1:G:193:GLU:HB3	1.78	0.49
1:A:191:ASN:HD21	1:A:193:GLU:HB3	1.77	0.49
1:G:158:PHE:CE2	1:G:166:CYS:HB2	2.47	0.49
1:I:150:LYS:O	1:I:151:LEU:CB	2.60	0.49
1:I:165:VAL:HG11	1:I:269:CYS:SG	2.53	0.49
1:J:165:VAL:HG11	1:J:269:CYS:SG	2.52	0.49
1:A:192:GLU:H	1:A:192:GLU:CD	2.15	0.49
1:G:316:ASN:N	1:G:317:PRO:HD3	2.28	0.49
1:J:133:GLN:NE2	1:J:297:ARG:HD3	2.28	0.48
1:K:165:VAL:HG11	1:K:269:CYS:SG	2.53	0.48
1:A:332:VAL:O	1:A:336:THR:HG23	2.12	0.48
1:K:58:SER:C	1:K:301:ILE:HD11	2.34	0.48
1:J:131:PRO:HA	1:J:134:GLU:HG3	1.94	0.48
1:B:229:TRP:CZ2	1:B:277:GLU:HA	2.48	0.48
1:B:150:LYS:O	1:B:151:LEU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:TRP:CZ2	1:H:277:GLU:HA	2.48	0.48
1:K:247:TYR:CD1	1:K:247:TYR:O	2.66	0.48
1:B:145:LEU:O	1:B:146:PRO:O	2.30	0.48
1:B:179:ASN:HA	1:B:208:SER:OG	2.14	0.48
1:A:79:GLN:O	1:A:80:LEU:C	2.51	0.48
1:B:252:VAL:HA	1:B:256:MET:HE2	1.95	0.48
1:B:259:ARG:HG3	1:B:259:ARG:NH1	2.25	0.48
1:C:58:SER:HB3	1:C:301:ILE:HD13	1.94	0.48
1:K:131:PRO:HA	1:K:134:GLU:HG3	1.94	0.48
1:K:5:TYR:CE1	1:K:304:LEU:HD21	2.48	0.48
1:H:249:LYS:HE3	1:H:250:TYR:CZ	2.48	0.48
1:E:191:ASN:HD21	1:E:193:GLU:HB3	1.78	0.48
1:H:12:THR:OG1	1:H:15:GLU:HG3	2.13	0.48
1:E:202:CYS:C	1:E:204:VAL:H	2.16	0.48
1:E:259:ARG:NH1	1:E:259:ARG:HG3	2.25	0.48
1:K:249:LYS:C	1:K:251:GLN:H	2.14	0.48
1:J:150:LYS:O	1:J:151:LEU:HB3	2.13	0.48
1:C:238:SER:CB	1:C:241:GLU:CB	2.80	0.48
1:L:249:LYS:HE3	1:L:250:TYR:CE1	2.48	0.48
1:H:125:MET:HG3	1:H:130:HIS:CG	2.48	0.48
1:G:12:THR:OG1	1:G:15:GLU:HG3	2.13	0.48
1:A:165:VAL:HG11	1:A:269:CYS:SG	2.53	0.48
1:F:232:LEU:O	1:F:234:GLU:N	2.46	0.48
1:K:71:GLU:HG2	1:L:60:GLU:HG2	1.95	0.48
1:B:232:LEU:HA	1:E:-11:HIS:CA	2.43	0.48
1:A:150:LYS:O	1:A:151:LEU:HB3	2.14	0.48
1:A:328:LYS:O	1:A:332:VAL:HG23	2.14	0.48
1:D:229:TRP:CZ2	1:D:277:GLU:HA	2.49	0.48
1:B:213:ASP:CG	1:B:213:ASP:O	2.52	0.48
1:A:103:ARG:NH1	1:A:103:ARG:CG	2.63	0.48
1:J:249:LYS:HG3	1:J:250:TYR:CE1	2.49	0.48
1:E:131:PRO:HA	1:E:134:GLU:HG3	1.95	0.48
1:A:247:TYR:O	1:A:247:TYR:CG	2.67	0.48
1:D:202:CYS:C	1:D:204:VAL:H	2.16	0.48
1:K:202:CYS:C	1:K:204:VAL:H	2.17	0.48
1:E:229:TRP:CZ2	1:E:277:GLU:HA	2.49	0.48
1:B:247:TYR:O	1:B:247:TYR:CD1	2.67	0.48
1:C:214:ASP:HB2	1:C:249:LYS:HD2	1.95	0.48
1:J:191:ASN:O	1:J:195:GLN:HG3	2.14	0.48
1:B:202:CYS:HB3	1:B:207:GLY:H	1.79	0.48
1:H:150:LYS:O	1:H:151:LEU:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:VAL:HA	1:E:256:MET:HE2	1.96	0.48
1:I:229:TRP:CZ2	1:I:277:GLU:HA	2.49	0.48
1:F:249:LYS:HE3	1:F:250:TYR:CE1	2.48	0.47
1:J:78:ILE:O	1:J:80:LEU:N	2.47	0.47
1:J:56:ARG:HG3	1:J:72:TYR:CE1	2.48	0.47
1:F:191:ASN:HD21	1:F:193:GLU:HB3	1.79	0.47
1:H:191:ASN:HD21	1:H:193:GLU:HB3	1.78	0.47
1:I:13:LYS:HA	1:I:176:MET:HE1	1.96	0.47
1:J:175:LYS:HB3	1:J:176:MET:HE3	1.96	0.47
1:E:12:THR:OG1	1:E:15:GLU:HG3	2.14	0.47
1:A:214:ASP:HB2	1:A:249:LYS:HD2	1.96	0.47
1:J:53:THR:CG2	1:L:77:GLN:HG3	2.34	0.47
1:K:210:LEU:HD13	1:K:211:VAL:H	1.76	0.47
1:L:249:LYS:C	1:L:251:GLN:H	2.16	0.47
1:E:59:PHE:CD2	1:E:301:ILE:HD12	2.49	0.47
1:C:1:MET:O	1:C:1:MET:HG3	2.14	0.47
1:A:247:TYR:O	1:A:248:PRO:O	2.31	0.47
1:C:202:CYS:C	1:C:204:VAL:H	2.17	0.47
1:G:247:TYR:O	1:G:247:TYR:CD1	2.67	0.47
1:K:318:TYR:CD1	1:L:32:ASN:C	2.87	0.47
1:F:182:HIS:CE1	1:F:189:GLN:HA	2.49	0.47
1:J:229:TRP:CZ2	1:J:277:GLU:HA	2.49	0.47
1:H:214:ASP:HB2	1:H:249:LYS:HD2	1.96	0.47
1:E:56:ARG:HG3	1:E:72:TYR:CE1	2.49	0.47
1:D:232:LEU:O	1:D:234:GLU:N	2.47	0.47
1:C:214:ASP:HB3	1:C:215:ALA:H	1.45	0.47
1:I:5:TYR:CE1	1:I:304:LEU:HD21	2.50	0.47
1:H:139:CYS:O	1:H:143:GLU:HG3	2.15	0.47
1:G:21:ASP:O	1:G:25:LYS:HG2	2.13	0.47
1:K:158:PHE:CE2	1:K:166:CYS:HB2	2.48	0.47
1:A:249:LYS:HB2	1:A:250:TYR:H	1.45	0.47
1:B:297:ARG:HG3	1:B:297:ARG:NH1	2.21	0.47
1:H:69:HIS:CD2	1:H:71:GLU:HG3	2.50	0.47
1:H:21:ASP:O	1:H:25:LYS:HG2	2.14	0.47
1:G:192:GLU:H	1:G:192:GLU:CD	2.18	0.47
1:F:150:LYS:O	1:F:151:LEU:CB	2.62	0.47
1:A:26:ILE:O	1:A:30:ILE:HG13	2.14	0.47
1:K:192:GLU:H	1:K:192:GLU:CD	2.17	0.47
1:B:232:LEU:HA	1:E:-11:HIS:C	2.35	0.47
1:B:232:LEU:N	1:B:232:LEU:HD12	2.21	0.47
1:E:210:LEU:CD1	1:E:211:VAL:CA	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:PHE:CD1	1:B:214:ASP:OD2	2.68	0.47
1:B:259:ARG:NH1	1:B:259:ARG:CG	2.59	0.47
1:K:249:LYS:HG3	1:K:250:TYR:CE1	2.49	0.47
1:K:247:TYR:O	1:K:248:PRO:O	2.32	0.47
1:I:249:LYS:C	1:I:251:GLN:H	2.15	0.47
1:D:95:ARG:CB	1:E:295:GLU:HB2	2.41	0.47
1:E:2:LYS:HE2	1:E:119:ILE:C	2.36	0.47
1:C:2:LYS:HE2	1:C:119:ILE:C	2.34	0.47
1:I:191:ASN:HD21	1:I:193:GLU:HB3	1.79	0.47
1:A:248:PRO:HB3	1:L:87:GLU:OE2	2.15	0.47
1:J:328:LYS:O	1:J:332:VAL:HG23	2.14	0.47
1:C:150:LYS:O	1:C:151:LEU:HB3	2.15	0.47
1:K:69:HIS:CD2	1:K:71:GLU:HG3	2.49	0.47
1:F:150:LYS:O	1:F:151:LEU:HB3	2.14	0.47
1:G:73:LEU:HD13	1:G:73:LEU:N	2.30	0.47
1:K:188:PHE:CE2	1:K:245:VAL:HG21	2.49	0.47
1:C:232:LEU:O	1:C:234:GLU:N	2.48	0.47
1:H:202:CYS:C	1:H:204:VAL:H	2.17	0.47
1:F:214:ASP:HB3	1:F:215:ALA:H	1.44	0.47
1:A:232:LEU:O	1:A:234:GLU:N	2.48	0.47
1:C:5:TYR:CE1	1:C:304:LEU:HD21	2.50	0.47
1:K:150:LYS:O	1:K:151:LEU:HB3	2.14	0.47
1:G:202:CYS:C	1:G:204:VAL:H	2.15	0.47
1:F:249:LYS:HG3	1:F:250:TYR:CE1	2.48	0.47
1:L:259:ARG:NH1	1:L:259:ARG:HG3	2.28	0.47
1:L:58:SER:C	1:L:301:ILE:HD11	2.34	0.47
1:I:192:GLU:H	1:I:192:GLU:CD	2.18	0.47
1:C:259:ARG:NH1	1:C:259:ARG:HG3	2.28	0.47
1:I:58:SER:HB3	1:I:301:ILE:HD13	1.97	0.47
1:G:182:HIS:CE1	1:G:189:GLN:HA	2.50	0.47
1:B:73:LEU:N	1:B:73:LEU:HD13	2.30	0.47
1:H:93:LEU:HD12	1:H:93:LEU:HA	1.82	0.47
1:A:249:LYS:HE3	1:A:250:TYR:CE1	2.50	0.46
1:D:124:GLY:O	1:D:125:MET:CB	2.62	0.46
1:C:191:ASN:O	1:C:195:GLN:HG3	2.15	0.46
1:J:71:GLU:HG2	1:K:60:GLU:HG2	1.98	0.46
1:B:232:LEU:HD23	1:E:-10:HIS:HB3	1.98	0.46
1:D:179:ASN:HA	1:D:208:SER:OG	2.15	0.46
1:D:26:ILE:O	1:D:30:ILE:HG13	2.16	0.46
1:L:150:LYS:O	1:L:151:LEU:HB3	2.14	0.46
1:C:247:TYR:O	1:C:248:PRO:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:252:VAL:HA	1:F:256:MET:HE2	1.97	0.46
1:F:99:ILE:HG13	1:F:120:PRO:HB2	1.96	0.46
1:E:26:ILE:O	1:E:30:ILE:HG13	2.15	0.46
1:B:139:CYS:O	1:B:143:GLU:HG3	2.16	0.46
1:H:182:HIS:CE1	1:H:189:GLN:HA	2.49	0.46
1:C:188:PHE:CE2	1:C:245:VAL:HG21	2.50	0.46
1:L:93:LEU:HD12	1:L:93:LEU:HA	1.76	0.46
1:G:141:MET:HE3	1:G:223:PHE:CD1	2.51	0.46
1:B:249:LYS:HG3	1:B:250:TYR:CE1	2.51	0.46
1:J:297:ARG:HG3	1:J:297:ARG:NH1	2.26	0.46
1:G:296:ASN:HA	1:G:299:THR:HB	1.97	0.46
1:J:182:HIS:CE1	1:J:189:GLN:HA	2.49	0.46
1:B:236:GLU:O	1:B:238:SER:N	2.46	0.46
1:H:259:ARG:NH1	1:H:259:ARG:HG3	2.28	0.46
1:B:210:LEU:HD13	1:B:211:VAL:O	2.15	0.46
1:I:210:LEU:HD13	1:I:211:VAL:O	2.16	0.46
1:G:150:LYS:O	1:G:151:LEU:HB3	2.16	0.46
1:I:150:LYS:O	1:I:151:LEU:HB3	2.16	0.46
1:D:12:THR:OG1	1:D:15:GLU:HG3	2.15	0.46
1:C:237:LEU:CG	1:C:242:ARG:HG3	2.45	0.46
1:C:133:GLN:NE2	1:C:297:ARG:HD3	2.30	0.46
1:I:69:HIS:CD2	1:I:71:GLU:HG3	2.51	0.46
1:A:179:ASN:HA	1:A:208:SER:OG	2.16	0.46
1:L:229:TRP:CZ2	1:L:277:GLU:HA	2.50	0.46
1:A:210:LEU:CD1	1:A:211:VAL:CA	2.91	0.46
1:D:214:ASP:HB3	1:D:215:ALA:H	1.44	0.46
1:J:215:ALA:CB	1:J:259:ARG:HE	2.21	0.46
1:J:297:ARG:HA	1:J:297:ARG:HD2	1.79	0.46
1:G:2:LYS:HE2	1:G:119:ILE:C	2.36	0.46
1:D:141:MET:HE3	1:D:223:PHE:CD1	2.51	0.46
1:I:182:HIS:CE1	1:I:189:GLN:HA	2.51	0.46
1:I:99:ILE:HB	1:I:309:MET:HE3	1.95	0.46
1:A:202:CYS:C	1:A:204:VAL:H	2.18	0.46
1:L:188:PHE:CE2	1:L:245:VAL:HG21	2.51	0.46
1:A:232:LEU:CD1	1:A:235:ALA:HB3	2.46	0.46
1:H:82:GLY:O	1:H:83:HIS:CB	2.63	0.46
1:G:188:PHE:CE2	1:G:245:VAL:HG21	2.51	0.46
1:I:139:CYS:O	1:I:143:GLU:HG3	2.16	0.46
1:D:71:GLU:HG2	1:E:60:GLU:HG2	1.97	0.46
1:H:192:GLU:H	1:H:192:GLU:CD	2.19	0.46
1:B:106:ARG:HB3	1:B:108:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:183:PHE:CD1	1:H:214:ASP:OD2	2.69	0.46
1:I:214:ASP:HB3	1:I:215:ALA:H	1.45	0.46
1:L:80:LEU:CD1	1:L:86:ILE:HD13	2.44	0.46
1:J:327:LYS:HG3	1:K:34:TYR:CE2	2.51	0.46
1:L:296:ASN:HA	1:L:299:THR:HB	1.98	0.46
1:B:26:ILE:O	1:B:30:ILE:HG13	2.16	0.46
1:I:188:PHE:CE2	1:I:245:VAL:HG21	2.51	0.46
1:F:316:ASN:N	1:F:317:PRO:HD3	2.30	0.46
1:F:192:GLU:CD	1:F:192:GLU:H	2.18	0.46
1:A:73:LEU:HD11	1:B:57:VAL:HG12	1.98	0.46
1:H:249:LYS:HG3	1:H:250:TYR:CE1	2.50	0.46
1:K:247:TYR:CG	1:K:247:TYR:O	2.68	0.46
1:G:259:ARG:HG3	1:G:259:ARG:NH1	2.26	0.46
1:B:131:PRO:HD2	1:B:132:THR:HG22	1.98	0.46
1:H:332:VAL:O	1:H:336:THR:HG23	2.16	0.46
1:A:21:ASP:O	1:A:25:LYS:HG2	2.17	0.46
1:C:182:HIS:CE1	1:C:189:GLN:HA	2.51	0.46
1:B:161:ASP:OD1	1:E:-10:HIS:HD2	1.99	0.45
1:D:214:ASP:HB2	1:D:249:LYS:HD2	1.97	0.45
1:G:210:LEU:HD13	1:G:211:VAL:O	2.16	0.45
1:F:215:ALA:CB	1:F:259:ARG:HE	2.21	0.45
1:A:2:LYS:HE2	1:A:119:ILE:C	2.35	0.45
1:K:26:ILE:O	1:K:30:ILE:HG13	2.15	0.45
1:G:139:CYS:O	1:G:143:GLU:HG3	2.16	0.45
1:C:235:ALA:C	1:C:237:LEU:N	2.66	0.45
1:B:59:PHE:CD2	1:B:301:ILE:HD12	2.51	0.45
1:B:208:SER:C	1:B:209:PHE:HD1	2.18	0.45
1:G:328:LYS:O	1:G:332:VAL:HG23	2.16	0.45
1:B:318:TYR:CD1	1:C:32:ASN:C	2.90	0.45
1:C:21:ASP:O	1:C:25:LYS:HG2	2.17	0.45
1:C:296:ASN:HA	1:C:299:THR:HB	1.97	0.45
1:B:200:LYS:NZ	1:E:200:LYS:HZ1	2.13	0.45
1:G:297:ARG:HD2	1:G:297:ARG:HA	1.77	0.45
1:G:179:ASN:HA	1:G:208:SER:OG	2.15	0.45
1:D:99:ILE:HB	1:D:309:MET:HE1	1.97	0.45
1:G:249:LYS:HB2	1:G:250:TYR:H	1.55	0.45
1:F:133:GLN:NE2	1:F:297:ARG:HD3	2.32	0.45
1:J:5:TYR:CE1	1:J:304:LEU:HD21	2.52	0.45
1:H:191:ASN:O	1:H:195:GLN:HG3	2.17	0.45
1:B:191:ASN:O	1:B:195:GLN:HG3	2.15	0.45
1:A:56:ARG:HG3	1:A:72:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:VAL:HG11	1:D:269:CYS:SG	2.57	0.45
1:H:333:PHE:CZ	1:I:18:TYR:CE1	3.05	0.45
1:A:125:MET:HG3	1:A:130:HIS:CG	2.52	0.45
1:G:247:TYR:O	1:G:248:PRO:O	2.35	0.45
1:C:316:ASN:N	1:C:317:PRO:HD3	2.30	0.45
1:J:316:ASN:N	1:J:317:PRO:HD3	2.32	0.45
1:F:202:CYS:C	1:F:204:VAL:H	2.19	0.45
1:E:141:MET:HE3	1:E:223:PHE:CD1	2.52	0.45
1:J:247:TYR:CG	1:J:247:TYR:O	2.69	0.45
1:D:191:ASN:HD21	1:D:193:GLU:HB3	1.81	0.45
1:E:150:LYS:O	1:E:151:LEU:HB3	2.15	0.45
1:F:26:ILE:O	1:F:30:ILE:HG13	2.17	0.45
1:K:213:ASP:O	1:K:213:ASP:CG	2.55	0.45
1:F:308:LEU:HD23	1:F:308:LEU:HA	1.76	0.45
1:D:249:LYS:C	1:D:251:GLN:H	2.19	0.45
1:H:133:GLN:NE2	1:H:297:ARG:HD3	2.31	0.45
1:L:131:PRO:HD2	1:L:132:THR:HG22	1.97	0.45
1:L:179:ASN:HA	1:L:208:SER:OG	2.17	0.45
1:K:328:LYS:O	1:K:332:VAL:HG23	2.17	0.45
1:K:191:ASN:O	1:K:195:GLN:HG3	2.17	0.45
1:H:252:VAL:HA	1:H:256:MET:HE2	1.99	0.45
1:A:182:HIS:CE1	1:A:189:GLN:HA	2.52	0.45
1:J:192:GLU:H	1:J:192:GLU:CD	2.20	0.45
1:A:93:LEU:HA	1:A:93:LEU:HD12	1.74	0.45
1:H:249:LYS:HE3	1:H:250:TYR:CE1	2.51	0.45
1:F:210:LEU:HD13	1:F:211:VAL:O	2.17	0.45
1:B:194:HIS:NE2	1:E:-8:SER:CB	2.80	0.45
1:J:2:LYS:HE2	1:J:119:ILE:C	2.36	0.45
1:G:131:PRO:HD2	1:G:132:THR:HG22	1.99	0.45
1:I:332:VAL:O	1:I:336:THR:HG23	2.15	0.45
1:F:296:ASN:HA	1:F:299:THR:HB	1.99	0.45
1:F:237:LEU:O	1:F:238:SER:HB2	2.16	0.45
1:F:247:TYR:O	1:F:248:PRO:O	2.35	0.45
1:G:56:ARG:HG3	1:G:72:TYR:CE1	2.52	0.45
1:I:179:ASN:HA	1:I:208:SER:OG	2.16	0.45
1:J:296:ASN:HA	1:J:299:THR:HB	1.99	0.45
1:A:32:ASN:C	1:C:318:TYR:CD1	2.90	0.45
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.86	0.45
1:E:249:LYS:HG3	1:E:250:TYR:CE1	2.51	0.45
1:G:249:LYS:HE3	1:G:250:TYR:CE1	2.52	0.45
1:G:249:LYS:HG3	1:G:250:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:210:LEU:HD13	1:L:211:VAL:O	2.17	0.45
1:A:13:LYS:HA	1:A:176:MET:CE	2.47	0.45
1:D:175:LYS:HB3	1:D:176:MET:HE3	1.98	0.45
1:J:99:ILE:HG13	1:J:120:PRO:HB2	1.98	0.45
1:A:139:CYS:O	1:A:143:GLU:HG3	2.17	0.45
1:K:182:HIS:CE1	1:K:189:GLN:HA	2.52	0.45
1:D:82:GLY:O	1:D:84:GLU:N	2.50	0.45
1:I:158:PHE:CE2	1:I:166:CYS:HB2	2.52	0.45
1:C:22:LEU:O	1:C:26:ILE:HG13	2.17	0.45
1:C:26:ILE:O	1:C:30:ILE:HG13	2.17	0.45
1:J:308:LEU:HD23	1:J:308:LEU:HA	1.76	0.45
1:F:247:TYR:CG	1:F:247:TYR:O	2.70	0.44
1:E:21:ASP:O	1:E:25:LYS:HG2	2.16	0.44
1:G:252:VAL:HA	1:G:256:MET:HE2	1.99	0.44
1:D:182:HIS:CE1	1:D:189:GLN:HA	2.52	0.44
1:F:103:ARG:CG	1:F:103:ARG:NH1	2.62	0.44
1:B:247:TYR:O	1:B:247:TYR:CG	2.70	0.44
1:E:184:GLY:HA2	1:E:250:TYR:HE2	1.81	0.44
1:J:249:LYS:HE3	1:J:250:TYR:CE1	2.52	0.44
1:K:145:LEU:O	1:K:146:PRO:O	2.34	0.44
1:H:2:LYS:HE2	1:H:119:ILE:C	2.37	0.44
1:F:191:ASN:O	1:F:195:GLN:HG3	2.17	0.44
1:C:247:TYR:O	1:C:247:TYR:CG	2.70	0.44
1:I:73:LEU:N	1:I:73:LEU:HD13	2.32	0.44
1:E:-4:PRO:CD	1:E:6:VAL:HG21	2.47	0.44
1:E:106:ARG:HB3	1:E:108:HIS:CD2	2.53	0.44
1:E:210:LEU:HD13	1:E:211:VAL:O	2.17	0.44
1:F:214:ASP:HB2	1:F:249:LYS:HD2	1.99	0.44
1:D:191:ASN:O	1:D:195:GLN:HG3	2.17	0.44
1:K:297:ARG:HA	1:K:297:ARG:HD2	1.83	0.44
1:E:110:ILE:O	1:E:110:ILE:HD13	2.17	0.44
1:F:5:TYR:CE1	1:F:304:LEU:HD21	2.52	0.44
1:B:71:GLU:HG2	1:C:60:GLU:CG	2.47	0.44
1:E:69:HIS:CD2	1:E:71:GLU:HG3	2.52	0.44
1:E:247:TYR:CG	1:E:247:TYR:O	2.70	0.44
1:G:60:GLU:HG2	1:I:71:GLU:HG2	2.00	0.44
1:L:252:VAL:HA	1:L:256:MET:HE2	1.99	0.44
1:K:270:LEU:HB3	1:K:271:PRO:HA	2.00	0.44
1:F:12:THR:HG23	1:F:15:GLU:OE1	2.17	0.44
1:B:79:GLN:O	1:B:81:GLY:N	2.50	0.44
1:F:21:ASP:O	1:F:25:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:VAL:HA	1:C:256:MET:HE2	1.99	0.44
1:K:139:CYS:O	1:K:143:GLU:HG3	2.17	0.44
1:E:213:ASP:O	1:E:213:ASP:CG	2.55	0.44
1:D:243:MET:HE1	1:D:247:TYR:CD2	2.52	0.44
1:E:73:LEU:HG	1:F:53:THR:HG22	1.99	0.44
1:D:2:LYS:HE2	1:D:119:ILE:C	2.37	0.44
1:I:2:LYS:HE2	1:I:119:ILE:C	2.38	0.44
1:J:22:LEU:O	1:J:26:ILE:HG13	2.17	0.44
1:C:69:HIS:CD2	1:C:71:GLU:HG3	2.53	0.44
1:F:141:MET:HE3	1:F:223:PHE:CD1	2.53	0.44
1:E:139:CYS:O	1:E:143:GLU:HG3	2.18	0.44
1:K:308:LEU:HA	1:K:308:LEU:HD23	1.76	0.44
1:B:232:LEU:CD1	1:B:232:LEU:H	2.19	0.44
1:E:249:LYS:HE3	1:E:250:TYR:CE1	2.52	0.44
1:K:58:SER:HB3	1:K:301:ILE:HD13	1.97	0.44
1:H:179:ASN:HA	1:H:208:SER:OG	2.17	0.44
1:B:202:CYS:C	1:B:204:VAL:N	2.70	0.44
1:G:93:LEU:HD12	1:G:93:LEU:HA	1.75	0.44
1:G:24:LEU:HA	1:G:24:LEU:HD12	1.83	0.44
1:J:210:LEU:HD13	1:J:211:VAL:O	2.17	0.44
1:G:32:ASN:C	1:I:318:TYR:CD1	2.91	0.44
1:B:296:ASN:HA	1:B:299:THR:HB	1.98	0.44
1:E:107:HIS:O	1:E:108:HIS:C	2.56	0.44
1:D:103:ARG:NH1	1:D:103:ARG:CG	2.69	0.44
1:A:215:ALA:O	1:L:115:ASN:OD1	2.35	0.44
1:K:214:ASP:HB3	1:K:215:ALA:H	1.45	0.44
1:L:249:LYS:HB2	1:L:250:TYR:H	1.51	0.44
1:C:179:ASN:HA	1:C:208:SER:OG	2.18	0.44
1:L:202:CYS:C	1:L:204:VAL:N	2.71	0.44
1:L:182:HIS:CE1	1:L:189:GLN:HA	2.53	0.44
1:J:158:PHE:CE2	1:J:166:CYS:HB2	2.52	0.44
1:C:210:LEU:HD13	1:C:211:VAL:O	2.18	0.44
1:L:78:ILE:CD1	1:L:80:LEU:HB2	2.47	0.44
1:L:210:LEU:HD13	1:L:211:VAL:H	1.79	0.44
1:L:133:GLN:NE2	1:L:297:ARG:HD3	2.33	0.44
1:G:133:GLN:NE2	1:G:297:ARG:HD3	2.32	0.44
1:A:144:HIS:C	1:A:146:PRO:CD	2.83	0.44
1:D:125:MET:HG3	1:D:130:HIS:CG	2.53	0.44
1:L:247:TYR:O	1:L:247:TYR:CG	2.70	0.44
1:B:182:HIS:CE1	1:B:189:GLN:HA	2.53	0.44
1:B:93:LEU:HD12	1:B:93:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:PHE:CE2	1:A:214:ASP:OD2	2.70	0.44
1:E:73:LEU:HD13	1:E:73:LEU:N	2.33	0.44
1:K:59:PHE:CD2	1:K:301:ILE:HD12	2.52	0.44
1:D:59:PHE:CD2	1:D:301:ILE:HD12	2.53	0.44
1:H:145:LEU:O	1:H:146:PRO:O	2.36	0.44
1:D:1:MET:HE3	1:D:1:MET:HB3	1.65	0.44
1:K:2:LYS:HE2	1:K:119:ILE:C	2.37	0.44
1:H:99:ILE:HB	1:H:309:MET:HE3	1.99	0.44
1:D:139:CYS:O	1:D:143:GLU:HG3	2.17	0.44
1:H:296:ASN:HA	1:H:299:THR:HB	1.99	0.44
1:A:135:LEU:HG	1:A:300:SER:HB2	2.00	0.44
1:B:-9:SER:CB	1:E:194:HIS:HE1	2.22	0.43
1:I:145:LEU:O	1:I:146:PRO:O	2.36	0.43
1:F:239:GLU:HA	1:F:242:ARG:NH2	2.31	0.43
1:L:139:CYS:O	1:L:143:GLU:HG3	2.18	0.43
1:L:24:LEU:HA	1:L:24:LEU:HD12	1.87	0.43
1:L:192:GLU:H	1:L:192:GLU:CD	2.22	0.43
1:B:232:LEU:O	1:B:234:GLU:N	2.50	0.43
1:A:215:ALA:CB	1:A:259:ARG:NE	2.77	0.43
1:B:248:PRO:HB2	1:B:249:LYS:H	1.59	0.43
1:C:183:PHE:CD1	1:C:214:ASP:OD2	2.71	0.43
1:J:247:TYR:O	1:J:248:PRO:O	2.36	0.43
1:C:59:PHE:CD2	1:C:301:ILE:HD12	2.53	0.43
1:K:179:ASN:HA	1:K:208:SER:OG	2.19	0.43
1:J:179:ASN:HA	1:J:208:SER:OG	2.18	0.43
1:D:249:LYS:HE3	1:D:250:TYR:CE1	2.53	0.43
1:B:214:ASP:HB3	1:B:215:ALA:H	1.43	0.43
1:B:215:ALA:CB	1:B:259:ARG:NE	2.79	0.43
1:F:145:LEU:O	1:F:146:PRO:O	2.37	0.43
1:E:131:PRO:HD2	1:E:132:THR:HG22	1.99	0.43
1:D:238:SER:CB	1:D:241:GLU:CB	2.79	0.43
1:D:73:LEU:HG	1:E:53:THR:HG22	2.01	0.43
1:B:194:HIS:CE1	1:E:-8:SER:HB3	2.53	0.43
1:E:124:GLY:O	1:E:125:MET:CB	2.65	0.43
1:D:158:PHE:CZ	1:D:166:CYS:HB2	2.53	0.43
1:J:202:CYS:C	1:J:204:VAL:H	2.21	0.43
1:A:188:PHE:CE2	1:A:245:VAL:HG21	2.53	0.43
1:A:318:TYR:CD1	1:B:32:ASN:C	2.92	0.43
1:D:210:LEU:CD1	1:D:211:VAL:CA	2.96	0.43
1:K:208:SER:O	1:K:209:PHE:HB3	2.18	0.43
1:E:145:LEU:O	1:E:146:PRO:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:HIS:O	1:A:2:LYS:HG3	2.18	0.43
1:C:302:ARG:HH11	1:C:302:ARG:CB	2.31	0.43
1:J:213:ASP:CG	1:J:213:ASP:O	2.56	0.43
1:I:24:LEU:HD12	1:I:24:LEU:HA	1.86	0.43
1:D:-5:VAL:HA	1:D:-4:PRO:HD3	1.86	0.43
1:L:297:ARG:HD2	1:L:297:ARG:HA	1.80	0.43
1:B:297:ARG:HD2	1:B:297:ARG:HA	1.71	0.43
1:C:124:GLY:O	1:C:125:MET:CB	2.66	0.43
1:H:56:ARG:HG3	1:H:72:TYR:CE1	2.54	0.43
1:E:247:TYR:O	1:E:248:PRO:O	2.37	0.43
1:I:99:ILE:HG13	1:I:120:PRO:HB2	2.01	0.43
1:F:165:VAL:HG11	1:F:269:CYS:SG	2.59	0.43
1:C:141:MET:HE3	1:C:223:PHE:CD1	2.53	0.43
1:F:80:LEU:HD21	1:F:86:ILE:HD12	2.00	0.43
1:K:248:PRO:HB2	1:K:249:LYS:H	1.60	0.43
1:B:-9:SER:HA	1:E:127:ASP:O	2.18	0.43
1:B:194:HIS:CE1	1:E:-8:SER:CB	3.02	0.43
1:I:59:PHE:CD2	1:I:301:ILE:HD12	2.54	0.43
1:A:213:ASP:O	1:A:213:ASP:CG	2.57	0.43
1:K:151:LEU:O	1:K:178:MET:HE3	2.19	0.43
1:K:141:MET:HE3	1:K:223:PHE:CD1	2.53	0.43
1:F:237:LEU:HD13	1:F:238:SER:OG	2.19	0.43
1:C:249:LYS:HE3	1:C:250:TYR:CE1	2.54	0.43
1:D:131:PRO:HD2	1:D:132:THR:HG22	2.00	0.43
1:J:5:TYR:CE1	1:J:131:PRO:HB2	2.53	0.43
1:I:247:TYR:CG	1:I:247:TYR:O	2.72	0.43
1:G:202:CYS:C	1:G:204:VAL:N	2.71	0.43
1:I:106:ARG:HB3	1:I:108:HIS:CD2	2.54	0.43
1:H:141:MET:HE3	1:H:223:PHE:CD1	2.53	0.43
1:E:39:LEU:CD2	1:E:309:MET:HG3	2.49	0.43
1:D:24:LEU:HA	1:D:24:LEU:HD12	1.84	0.43
1:L:237:LEU:O	1:L:238:SER:C	2.57	0.43
1:L:214:ASP:HB2	1:L:249:LYS:HD2	2.01	0.43
1:A:124:GLY:O	1:A:125:MET:CB	2.66	0.43
1:I:56:ARG:HG3	1:I:72:TYR:CE1	2.53	0.43
1:A:141:MET:HE3	1:A:223:PHE:CD1	2.54	0.43
1:J:141:MET:HE3	1:J:223:PHE:CD1	2.53	0.43
1:C:93:LEU:HA	1:C:93:LEU:HD12	1.72	0.43
1:F:73:LEU:N	1:F:73:LEU:HD13	2.33	0.43
1:A:184:GLY:HA2	1:A:250:TYR:HE2	1.80	0.43
1:G:69:HIS:CD2	1:G:71:GLU:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:THR:OG1	1:F:15:GLU:HG3	2.18	0.43
1:K:106:ARG:HB3	1:K:108:HIS:CD2	2.54	0.43
1:E:-5:VAL:HG12	1:E:-5:VAL:O	2.18	0.42
1:J:59:PHE:CD2	1:J:301:ILE:HD12	2.54	0.42
1:B:209:PHE:CD1	1:B:209:PHE:N	2.87	0.42
1:E:239:GLU:HA	1:E:242:ARG:NH2	2.32	0.42
1:A:71:GLU:HG2	1:B:60:GLU:CG	2.48	0.42
1:G:99:ILE:HG13	1:G:120:PRO:HB2	2.01	0.42
1:K:296:ASN:HA	1:K:299:THR:HB	2.01	0.42
1:H:24:LEU:HD12	1:H:24:LEU:HA	1.81	0.42
1:D:248:PRO:HB2	1:D:249:LYS:H	1.57	0.42
1:B:2:LYS:HE2	1:B:119:ILE:C	2.40	0.42
1:I:247:TYR:O	1:I:248:PRO:O	2.37	0.42
1:G:232:LEU:O	1:G:233:TYR:C	2.58	0.42
1:L:141:MET:HE3	1:L:223:PHE:CD1	2.53	0.42
1:I:316:ASN:N	1:I:317:PRO:HD3	2.34	0.42
1:A:296:ASN:HA	1:A:299:THR:HB	2.01	0.42
1:F:224:LEU:HA	1:F:224:LEU:HD12	1.91	0.42
1:F:210:LEU:HD13	1:F:211:VAL:H	1.77	0.42
1:B:-10:HIS:HB3	1:B:-9:SER:H	1.53	0.42
1:B:-6:LEU:HD13	1:B:128:TYR:CZ	2.54	0.42
1:H:328:LYS:O	1:H:332:VAL:HG23	2.18	0.42
1:J:90:SER:OG	1:J:113:LEU:HD12	2.18	0.42
1:G:26:ILE:O	1:G:30:ILE:HG13	2.19	0.42
1:F:297:ARG:HD2	1:F:297:ARG:HA	1.76	0.42
1:F:179:ASN:HA	1:F:208:SER:OG	2.19	0.42
1:A:191:ASN:O	1:A:195:GLN:HG3	2.19	0.42
1:L:69:HIS:CD2	1:L:71:GLU:HG3	2.53	0.42
1:C:211:VAL:HG22	1:C:212:THR:N	2.31	0.42
1:J:249:LYS:HB2	1:J:250:TYR:H	1.53	0.42
1:I:297:ARG:HD2	1:I:297:ARG:HA	1.72	0.42
1:H:247:TYR:O	1:H:247:TYR:CG	2.72	0.42
1:I:163:THR:O	1:I:166:CYS:HB3	2.20	0.42
1:G:95:ARG:HB3	1:H:295:GLU:HB2	2.01	0.42
1:I:252:VAL:HA	1:I:256:MET:HE2	2.01	0.42
1:G:90:SER:OG	1:G:113:LEU:HD12	2.18	0.42
1:E:-7:GLY:O	1:E:-6:LEU:CB	2.66	0.42
1:C:145:LEU:O	1:C:146:PRO:O	2.37	0.42
1:J:145:LEU:O	1:J:146:PRO:O	2.37	0.42
1:J:232:LEU:O	1:J:233:TYR:C	2.58	0.42
1:G:247:TYR:O	1:G:247:TYR:CG	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:69:HIS:CD2	1:J:71:GLU:HG3	2.55	0.42
1:E:99:ILE:HB	1:E:309:MET:HE1	2.01	0.42
1:I:135:LEU:HG	1:I:300:SER:HB2	2.00	0.42
1:K:252:VAL:HA	1:K:256:MET:HE2	2.01	0.42
1:J:252:VAL:HG13	1:J:256:MET:HG2	2.01	0.42
1:H:58:SER:HB3	1:H:301:ILE:HD13	2.01	0.42
1:E:144:HIS:C	1:E:146:PRO:CD	2.85	0.42
1:L:145:LEU:O	1:L:146:PRO:O	2.36	0.42
1:G:191:ASN:O	1:G:195:GLN:HG3	2.19	0.42
1:L:158:PHE:CZ	1:L:166:CYS:HB2	2.54	0.42
1:I:202:CYS:C	1:I:204:VAL:N	2.73	0.42
1:I:39:LEU:CD2	1:I:309:MET:HG3	2.50	0.42
1:C:139:CYS:O	1:C:143:GLU:HG3	2.19	0.42
1:J:139:CYS:O	1:J:143:GLU:HG3	2.19	0.42
1:B:100:LEU:HA	1:B:100:LEU:HD23	1.90	0.42
1:I:296:ASN:HA	1:I:299:THR:HB	2.01	0.42
1:J:238:SER:CB	1:J:241:GLU:CB	2.80	0.42
1:A:214:ASP:HB3	1:A:215:ALA:H	1.42	0.42
1:B:184:GLY:HA2	1:B:250:TYR:HE2	1.83	0.42
1:E:249:LYS:HB2	1:E:250:TYR:H	1.50	0.42
1:I:210:LEU:HD13	1:I:211:VAL:H	1.76	0.42
1:D:104:VAL:HG21	1:D:109:SER:OG	2.19	0.42
1:L:208:SER:O	1:L:209:PHE:HB3	2.19	0.42
1:D:145:LEU:O	1:D:146:PRO:O	2.38	0.42
1:L:56:ARG:HG3	1:L:72:TYR:CE1	2.54	0.42
1:J:252:VAL:HA	1:J:256:MET:HE2	2.02	0.42
1:E:165:VAL:HG11	1:E:269:CYS:SG	2.59	0.42
1:A:252:VAL:HA	1:A:256:MET:HE2	2.01	0.42
1:G:270:LEU:HB3	1:G:271:PRO:HA	2.02	0.42
1:B:163:THR:HA	1:E:-10:HIS:HA	2.01	0.42
1:H:103:ARG:NH1	1:H:103:ARG:CG	2.65	0.42
1:A:104:VAL:CG1	1:A:110:ILE:HB	2.41	0.42
1:B:208:SER:C	1:B:209:PHE:CD1	2.93	0.42
1:C:191:ASN:HD21	1:C:193:GLU:HB3	1.84	0.42
1:A:60:GLU:HG2	1:C:71:GLU:HG2	2.00	0.42
1:G:165:VAL:HG11	1:G:269:CYS:SG	2.59	0.42
1:B:-13:HIS:CE1	1:E:106:ARG:NE	2.72	0.42
1:D:215:ALA:CB	1:D:259:ARG:NE	2.77	0.42
1:A:271:PRO:HB3	1:C:84:GLU:OE2	2.19	0.42
1:K:239:GLU:HA	1:K:242:ARG:NH2	2.30	0.42
1:B:69:HIS:CD2	1:B:71:GLU:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:CYS:C	1:C:204:VAL:N	2.73	0.42
1:D:296:ASN:HA	1:D:299:THR:HB	2.02	0.42
1:E:-5:VAL:HA	1:E:-4:PRO:HD3	1.62	0.41
1:A:77:GLN:HG3	1:B:53:THR:CG2	2.31	0.41
1:G:215:ALA:CB	1:G:259:ARG:NE	2.81	0.41
1:A:145:LEU:N	1:A:146:PRO:CD	2.83	0.41
1:H:104:VAL:CG1	1:H:110:ILE:HB	2.45	0.41
1:L:191:ASN:HD21	1:L:193:GLU:HB3	1.80	0.41
1:A:151:LEU:C	1:A:153:ASP:N	2.73	0.41
1:J:151:LEU:O	1:J:178:MET:HE2	2.20	0.41
1:D:21:ASP:O	1:D:25:LYS:HG2	2.20	0.41
1:L:107:HIS:O	1:L:108:HIS:C	2.58	0.41
1:G:213:ASP:CG	1:G:213:ASP:O	2.58	0.41
1:L:232:LEU:O	1:L:233:TYR:C	2.58	0.41
1:J:106:ARG:HB3	1:J:108:HIS:CD2	2.55	0.41
1:E:296:ASN:HA	1:E:299:THR:HB	2.02	0.41
1:E:163:THR:O	1:E:166:CYS:HB3	2.20	0.41
1:E:158:PHE:CE2	1:E:166:CYS:HB2	2.55	0.41
1:J:104:VAL:CG1	1:J:110:ILE:HB	2.43	0.41
1:I:243:MET:HE1	1:I:247:TYR:CD2	2.55	0.41
1:D:247:TYR:CG	1:D:247:TYR:O	2.73	0.41
1:C:144:HIS:C	1:C:146:PRO:CD	2.86	0.41
1:G:239:GLU:HA	1:G:242:ARG:NH2	2.31	0.41
1:D:60:GLU:CG	1:F:71:GLU:HG2	2.51	0.41
1:D:241:GLU:O	1:D:245:VAL:HG12	2.21	0.41
1:B:106:ARG:NH2	1:E:112:ASP:CG	2.63	0.41
1:G:103:ARG:CG	1:G:103:ARG:NH1	2.62	0.41
1:D:249:LYS:HB2	1:D:250:TYR:H	1.56	0.41
1:B:183:PHE:CE2	1:B:214:ASP:OD2	2.74	0.41
1:E:183:PHE:CE2	1:E:214:ASP:OD2	2.73	0.41
1:K:183:PHE:CE2	1:K:214:ASP:OD2	2.73	0.41
1:H:210:LEU:HD13	1:H:211:VAL:H	1.78	0.41
1:J:215:ALA:CB	1:J:259:ARG:NE	2.82	0.41
1:E:297:ARG:HD2	1:E:297:ARG:HA	1.72	0.41
1:I:131:PRO:HD2	1:I:132:THR:HG22	2.03	0.41
1:K:232:LEU:O	1:K:233:TYR:C	2.58	0.41
1:K:163:THR:O	1:K:166:CYS:HB3	2.21	0.41
1:D:106:ARG:HB3	1:D:108:HIS:CD2	2.55	0.41
1:H:106:ARG:HB3	1:H:108:HIS:CD2	2.55	0.41
1:H:214:ASP:HB3	1:H:215:ALA:H	1.45	0.41
1:G:208:SER:C	1:G:209:PHE:HD1	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:32:ASN:C	1:L:318:TYR:CD1	2.94	0.41
1:B:308:LEU:HD23	1:B:308:LEU:HA	1.80	0.41
1:D:188:PHE:CE2	1:D:245:VAL:HG21	2.56	0.41
1:I:215:ALA:CB	1:I:259:ARG:NE	2.80	0.41
1:J:214:ASP:HB3	1:J:215:ALA:H	1.44	0.41
1:J:58:SER:HB3	1:J:301:ILE:HD13	2.03	0.41
1:A:145:LEU:O	1:A:146:PRO:O	2.39	0.41
1:C:208:SER:O	1:C:209:PHE:HB3	2.19	0.41
1:C:104:VAL:HG21	1:C:109:SER:OG	2.21	0.41
1:B:56:ARG:HG3	1:B:72:TYR:CE1	2.55	0.41
1:K:40:LYS:O	1:K:41:ASN:HB2	2.21	0.41
1:B:164:GLN:H	1:B:164:GLN:CD	2.24	0.41
1:F:237:LEU:HD22	1:F:237:LEU:HA	1.80	0.41
1:B:107:HIS:O	1:B:108:HIS:C	2.58	0.41
1:H:208:SER:O	1:H:209:PHE:HB3	2.20	0.41
1:D:202:CYS:C	1:D:204:VAL:N	2.73	0.41
1:J:107:HIS:O	1:J:108:HIS:C	2.58	0.41
1:E:182:HIS:CE1	1:E:189:GLN:HA	2.56	0.41
1:I:213:ASP:CG	1:I:213:ASP:O	2.58	0.41
1:F:236:GLU:O	1:F:237:LEU:C	2.59	0.41
1:H:241:GLU:O	1:H:245:VAL:HG12	2.20	0.41
1:H:188:PHE:CE2	1:H:245:VAL:HG21	2.55	0.41
1:L:103:ARG:NH1	1:L:103:ARG:CG	2.65	0.41
1:D:210:LEU:HD13	1:D:211:VAL:C	2.41	0.41
1:C:215:ALA:CB	1:C:259:ARG:NE	2.80	0.41
1:F:248:PRO:HB2	1:F:249:LYS:H	1.60	0.41
1:J:248:PRO:HB2	1:J:249:LYS:H	1.60	0.41
1:A:133:GLN:NE2	1:A:297:ARG:HD3	2.36	0.41
1:I:294:ALA:O	1:I:297:ARG:HB2	2.21	0.41
1:L:58:SER:HB3	1:L:301:ILE:HD13	2.02	0.41
1:A:232:LEU:O	1:A:233:TYR:C	2.58	0.41
1:F:297:ARG:NH1	2:F:341:SO4:O3	2.54	0.41
1:F:208:SER:O	1:F:209:PHE:HB3	2.21	0.41
1:H:134:GLU:HB3	1:H:172:ILE:HB	2.03	0.41
1:C:131:PRO:HD2	1:C:132:THR:HG22	2.02	0.41
1:F:2:LYS:HE2	1:F:119:ILE:C	2.41	0.41
1:J:34:TYR:CE2	1:L:327:LYS:HG3	2.56	0.41
1:D:158:PHE:HA	1:D:225:TYR:O	2.21	0.41
1:A:99:ILE:HB	1:A:309:MET:HE3	2.02	0.41
1:E:202:CYS:C	1:E:204:VAL:N	2.73	0.41
1:D:232:LEU:O	1:D:233:TYR:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:CYS:C	1:H:204:VAL:N	2.74	0.41
1:D:69:HIS:CD2	1:D:71:GLU:HG3	2.56	0.41
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.92	0.41
1:C:106:ARG:HB3	1:C:108:HIS:CD2	2.56	0.41
1:G:106:ARG:HB3	1:G:108:HIS:CD2	2.56	0.41
1:I:308:LEU:HD23	1:I:308:LEU:HA	1.73	0.41
1:D:247:TYR:O	1:D:248:PRO:O	2.39	0.41
1:J:183:PHE:CD1	1:J:214:ASP:OD2	2.74	0.41
1:K:144:HIS:C	1:K:146:PRO:CD	2.87	0.41
1:K:131:PRO:HD2	1:K:132:THR:HG22	2.03	0.41
1:F:69:HIS:CD2	1:F:71:GLU:HG3	2.56	0.41
1:C:158:PHE:CZ	1:C:166:CYS:HB2	2.56	0.41
1:A:151:LEU:C	1:A:153:ASP:H	2.25	0.41
1:K:259:ARG:NH1	1:K:259:ARG:CG	2.61	0.40
1:I:133:GLN:NE2	1:I:297:ARG:HD3	2.35	0.40
1:H:59:PHE:CD2	1:H:301:ILE:HD12	2.56	0.40
1:D:134:GLU:HB3	1:D:172:ILE:HB	2.03	0.40
1:E:208:SER:C	1:E:209:PHE:HD1	2.24	0.40
1:E:13:LYS:HA	1:E:176:MET:CE	2.50	0.40
1:D:82:GLY:C	1:D:84:GLU:H	2.24	0.40
1:B:316:ASN:N	1:B:317:PRO:HD3	2.35	0.40
1:J:289:ILE:HD13	1:J:289:ILE:HG21	1.87	0.40
1:E:24:LEU:HA	1:E:24:LEU:HD12	1.82	0.40
1:E:31:LYS:HG2	1:E:31:LYS:O	2.20	0.40
1:K:184:GLY:HA2	1:K:250:TYR:HE2	1.81	0.40
1:G:214:ASP:HB3	1:G:215:ALA:H	1.44	0.40
1:A:232:LEU:HD13	1:A:235:ALA:HB3	2.02	0.40
1:E:132:THR:HG22	1:E:132:THR:H	1.54	0.40
1:A:213:ASP:HB2	1:L:111:VAL:CG2	2.50	0.40
1:I:5:TYR:CE1	1:I:131:PRO:HB2	2.55	0.40
1:L:124:GLY:O	1:L:125:MET:CB	2.67	0.40
1:K:56:ARG:HG3	1:K:72:TYR:CE1	2.56	0.40
1:D:56:ARG:HG3	1:D:72:TYR:CE1	2.57	0.40
1:L:296:ASN:HA	1:L:299:THR:CB	2.52	0.40
1:G:39:LEU:CD2	1:G:309:MET:HG3	2.51	0.40
1:H:37:GLN:HB3	1:H:40:LYS:HG3	2.02	0.40
1:D:213:ASP:CG	1:D:213:ASP:O	2.60	0.40
1:C:259:ARG:CG	1:C:259:ARG:NH1	2.61	0.40
1:F:58:SER:O	1:F:301:ILE:HD11	2.21	0.40
1:F:124:GLY:O	1:F:125:MET:CB	2.67	0.40
1:E:241:GLU:O	1:E:245:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:ILE:HB	1:F:309:MET:HE1	2.02	0.40
1:J:163:THR:O	1:J:166:CYS:HB3	2.21	0.40
1:A:90:SER:OG	1:A:113:LEU:HD12	2.21	0.40
1:K:52:SER:OG	1:K:55:THR:HB	2.22	0.40
1:E:93:LEU:HD12	1:E:93:LEU:HA	1.71	0.40
1:K:215:ALA:CB	1:K:259:ARG:HE	2.19	0.40
1:E:179:ASN:HA	1:E:208:SER:OG	2.21	0.40
1:K:134:GLU:HB3	1:K:172:ILE:HB	2.03	0.40
1:J:7:THR:HG23	1:J:9:GLU:H	1.87	0.40
1:B:229:TRP:O	1:B:230:TYR:C	2.60	0.40
1:K:13:LYS:HA	1:K:176:MET:CE	2.51	0.40
1:F:232:LEU:O	1:F:233:TYR:C	2.59	0.40
1:C:232:LEU:O	1:C:233:TYR:C	2.59	0.40
1:J:323:GLN:HG3	1:K:32:ASN:O	2.20	0.40
1:F:139:CYS:O	1:F:143:GLU:HG3	2.21	0.40
1:G:31:LYS:O	1:G:31:LYS:HG2	2.21	0.40
1:E:103:ARG:NH1	1:E:103:ARG:CG	2.60	0.40
1:E:215:ALA:CB	1:E:259:ARG:NE	2.81	0.40
1:L:132:THR:H	1:L:132:THR:HG22	1.53	0.40
1:K:202:CYS:C	1:K:204:VAL:N	2.74	0.40
1:J:95:ARG:HB3	1:K:295:GLU:HB2	2.02	0.40
1:A:107:HIS:O	1:A:108:HIS:C	2.58	0.40
1:L:171:LEU:HA	1:L:171:LEU:HD12	1.97	0.40
1:E:224:LEU:HA	1:E:224:LEU:HD12	1.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:GLU:OE1	1:K:106:ARG:NH2[2_556]	1.88	0.32
1:F:203:GLU:O	1:K:106:ARG:NH1[2_556]	2.15	0.05

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/359 (93%)	288 (86%)	25 (8%)	20 (6%)	2	16
1	B	351/359 (98%)	303 (86%)	26 (7%)	22 (6%)	2	13
1	C	338/359 (94%)	288 (85%)	27 (8%)	23 (7%)	1	11
1	D	345/359 (96%)	295 (86%)	32 (9%)	18 (5%)	2	19
1	E	339/359 (94%)	294 (87%)	26 (8%)	19 (6%)	2	18
1	F	338/359 (94%)	291 (86%)	29 (9%)	18 (5%)	2	19
1	G	339/359 (94%)	291 (86%)	27 (8%)	21 (6%)	2	14
1	H	332/359 (92%)	283 (85%)	32 (10%)	17 (5%)	2	20
1	I	328/359 (91%)	286 (87%)	25 (8%)	17 (5%)	2	19
1	J	339/359 (94%)	290 (86%)	29 (9%)	20 (6%)	2	16
1	K	339/359 (94%)	293 (86%)	26 (8%)	20 (6%)	2	16
1	L	339/359 (94%)	289 (85%)	32 (9%)	18 (5%)	2	19
All	All	4060/4308 (94%)	3491 (86%)	336 (8%)	233 (6%)	2	17

All (233) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	125	MET
1	A	146	PRO
1	A	214	ASP
1	A	215	ALA
1	A	233	TYR
1	A	238	SER
1	A	248	PRO
1	A	249	LYS
1	A	250	TYR
1	B	-8	SER
1	B	83	HIS
1	B	125	MET
1	B	146	PRO
1	B	151	LEU
1	B	214	ASP
1	B	215	ALA
1	B	233	TYR
1	B	237	LEU

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Mol	Chain	Res	Type
1	B	248	PRO
1	B	249	LYS
1	B	250	TYR
1	C	80	LEU
1	C	125	MET
1	C	146	PRO
1	C	151	LEU
1	C	214	ASP
1	C	215	ALA
1	C	233	TYR
1	C	238	SER
1	C	248	PRO
1	C	249	LYS
1	C	250	TYR
1	D	83	HIS
1	D	125	MET
1	D	146	PRO
1	D	151	LEU
1	D	214	ASP
1	D	215	ALA
1	D	233	TYR
1	D	238	SER
1	D	248	PRO
1	D	249	LYS
1	D	250	TYR
1	E	-10	HIS
1	E	-8	SER
1	E	80	LEU
1	E	125	MET
1	E	146	PRO
1	E	214	ASP
1	E	215	ALA
1	E	248	PRO
1	E	250	TYR
1	F	125	MET
1	F	146	PRO
1	F	214	ASP
1	F	215	ALA
1	F	233	TYR
1	F	237	LEU
1	F	238	SER
1	F	248	PRO

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Mol	Chain	Res	Type
1	F	249	LYS
1	F	250	TYR
1	G	80	LEU
1	G	83	HIS
1	G	125	MET
1	G	146	PRO
1	G	151	LEU
1	G	214	ASP
1	G	215	ALA
1	G	233	TYR
1	G	237	LEU
1	G	248	PRO
1	G	249	LYS
1	G	250	TYR
1	H	79	GLN
1	H	83	HIS
1	H	125	MET
1	H	146	PRO
1	H	151	LEU
1	H	214	ASP
1	H	215	ALA
1	H	248	PRO
1	H	249	LYS
1	H	250	TYR
1	I	80	LEU
1	I	125	MET
1	I	146	PRO
1	I	151	LEU
1	I	214	ASP
1	I	215	ALA
1	I	248	PRO
1	I	250	TYR
1	J	2	LYS
1	J	79	GLN
1	J	125	MET
1	J	146	PRO
1	J	214	ASP
1	J	215	ALA
1	J	233	TYR
1	J	237	LEU
1	J	238	SER
1	J	248	PRO

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Mol	Chain	Res	Type
1	J	250	TYR
1	K	80	LEU
1	K	125	MET
1	K	146	PRO
1	K	151	LEU
1	K	214	ASP
1	K	215	ALA
1	K	233	TYR
1	K	238	SER
1	K	248	PRO
1	K	249	LYS
1	K	250	TYR
1	L	80	LEU
1	L	125	MET
1	L	146	PRO
1	L	151	LEU
1	L	214	ASP
1	L	215	ALA
1	L	233	TYR
1	L	248	PRO
1	L	249	LYS
1	L	250	TYR
1	A	1	MET
1	A	151	LEU
1	A	211	VAL
1	A	216	SER
1	A	234	GLU
1	B	2	LYS
1	B	211	VAL
1	B	216	SER
1	C	2	LYS
1	C	83	HIS
1	C	211	VAL
1	C	216	SER
1	C	234	GLU
1	C	237	LEU
1	D	2	LYS
1	D	211	VAL
1	D	216	SER
1	D	234	GLU
1	E	-11	HIS
1	E	-6	LEU

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Mol	Chain	Res	Type
1	E	2	LYS
1	E	151	LEU
1	E	211	VAL
1	E	216	SER
1	E	249	LYS
1	F	2	LYS
1	F	151	LEU
1	F	211	VAL
1	F	216	SER
1	G	2	LYS
1	G	211	VAL
1	G	216	SER
1	G	234	GLU
1	G	236	GLU
1	H	2	LYS
1	H	211	VAL
1	H	216	SER
1	I	2	LYS
1	I	83	HIS
1	I	211	VAL
1	I	216	SER
1	I	249	LYS
1	J	151	LEU
1	J	211	VAL
1	J	216	SER
1	J	234	GLU
1	J	249	LYS
1	K	2	LYS
1	K	216	SER
1	K	234	GLU
1	K	237	LEU
1	L	2	LYS
1	L	211	VAL
1	L	216	SER
1	L	238	SER
1	B	80	LEU
1	B	234	GLU
1	D	315	LYS
1	E	82	GLY
1	F	148	GLY
1	F	234	GLU
1	G	315	LYS

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Mol	Chain	Res	Type
1	I	315	LYS
1	K	211	VAL
1	L	234	GLU
1	A	315	LYS
1	B	-10	HIS
1	B	230	TYR
1	B	315	LYS
1	C	79	GLN
1	C	148	GLY
1	C	315	LYS
1	E	315	LYS
1	F	315	LYS
1	H	315	LYS
1	J	230	TYR
1	J	315	LYS
1	K	148	GLY
1	K	315	LYS
1	L	315	LYS
1	A	78	ILE
1	C	236	GLU
1	H	78	ILE
1	H	247	TYR
1	I	148	GLY
1	L	247	TYR
1	A	79	GLN
1	C	78	ILE
1	D	247	TYR
1	E	247	TYR
1	G	152	GLU
1	H	148	GLY
1	I	230	TYR
1	J	148	GLY
1	A	247	TYR
1	G	148	GLY
1	G	247	TYR
1	L	148	GLY
1	A	148	GLY
1	B	247	TYR
1	C	247	TYR
1	F	247	TYR
1	I	247	TYR
1	J	247	TYR

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Mol	Chain	Res	Type
1	K	78	ILE
1	D	148	GLY
1	K	247	TYR
1	B	148	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/313 (92%)	244 (85%)	44 (15%)	3	17
1	B	302/313 (96%)	252 (83%)	50 (17%)	3	13
1	C	289/313 (92%)	245 (85%)	44 (15%)	3	17
1	D	294/313 (94%)	250 (85%)	44 (15%)	3	17
1	E	296/313 (95%)	255 (86%)	41 (14%)	4	20
1	F	291/313 (93%)	245 (84%)	46 (16%)	3	15
1	G	289/313 (92%)	245 (85%)	44 (15%)	3	17
1	H	288/313 (92%)	244 (85%)	44 (15%)	3	17
1	I	286/313 (91%)	243 (85%)	43 (15%)	3	17
1	J	287/313 (92%)	242 (84%)	45 (16%)	3	15
1	K	288/313 (92%)	243 (84%)	45 (16%)	3	15
1	L	292/313 (93%)	248 (85%)	44 (15%)	3	17
All	All	3490/3756 (93%)	2956 (85%)	534 (15%)	3	17

All (534) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	6	VAL
1	A	10	THR
1	A	19	LEU
1	A	24	LEU
1	A	53	THR

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Mol	Chain	Res	Type
1	A	57	VAL
1	A	65	GLN
1	A	73	LEU
1	A	89	THR
1	A	92	VAL
1	A	93	LEU
1	A	103	ARG
1	A	105	GLU
1	A	106	ARG
1	A	110	ILE
1	A	118	THR
1	A	130	HIS
1	A	132	THR
1	A	138	LEU
1	A	147	GLU
1	A	150	LYS
1	A	164	GLN
1	A	168	SER
1	A	169	LEU
1	A	175	LYS
1	A	181	VAL
1	A	183	PHE
1	A	192	GLU
1	A	210	LEU
1	A	211	VAL
1	A	212	THR
1	A	217	SER
1	A	225	TYR
1	A	232	LEU
1	A	239	GLU
1	A	240	GLU
1	A	245	VAL
1	A	256	MET
1	A	259	ARG
1	A	263	ASN
1	A	273	THR
1	A	301	ILE
1	A	302	ARG
1	B	-13	HIS
1	B	-12	HIS
1	B	-3	ARG
1	B	0	HIS

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Mol	Chain	Res	Type
1	B	1	MET
1	B	2	LYS
1	B	6	VAL
1	B	10	THR
1	B	19	LEU
1	B	24	LEU
1	B	53	THR
1	B	57	VAL
1	B	65	GLN
1	B	73	LEU
1	B	89	THR
1	B	92	VAL
1	B	93	LEU
1	B	103	ARG
1	B	105	GLU
1	B	106	ARG
1	B	110	ILE
1	B	118	THR
1	B	130	HIS
1	B	132	THR
1	B	138	LEU
1	B	147	GLU
1	B	150	LYS
1	B	151	LEU
1	B	164	GLN
1	B	169	LEU
1	B	175	LYS
1	B	181	VAL
1	B	183	PHE
1	B	192	GLU
1	B	210	LEU
1	B	211	VAL
1	B	212	THR
1	B	217	SER
1	B	225	TYR
1	B	232	LEU
1	B	238	SER
1	B	239	GLU
1	B	240	GLU
1	B	245	VAL
1	B	256	MET
1	B	259	ARG

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Mol	Chain	Res	Type
1	B	263	ASN
1	B	273	THR
1	B	301	ILE
1	B	302	ARG
1	C	2	LYS
1	C	6	VAL
1	C	10	THR
1	C	19	LEU
1	C	24	LEU
1	C	53	THR
1	C	56	ARG
1	C	57	VAL
1	C	65	GLN
1	C	73	LEU
1	C	89	THR
1	C	92	VAL
1	C	93	LEU
1	C	103	ARG
1	C	105	GLU
1	C	106	ARG
1	C	110	ILE
1	C	118	THR
1	C	130	HIS
1	C	132	THR
1	C	138	LEU
1	C	147	GLU
1	C	150	LYS
1	C	164	GLN
1	C	168	SER
1	C	169	LEU
1	C	175	LYS
1	C	181	VAL
1	C	183	PHE
1	C	192	GLU
1	C	210	LEU
1	C	212	THR
1	C	217	SER
1	C	225	TYR
1	C	237	LEU
1	C	239	GLU
1	C	240	GLU
1	C	245	VAL

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Mol	Chain	Res	Type
1	C	256	MET
1	C	259	ARG
1	C	263	ASN
1	C	273	THR
1	C	301	ILE
1	C	302	ARG
1	D	-6	LEU
1	D	0	HIS
1	D	2	LYS
1	D	6	VAL
1	D	10	THR
1	D	19	LEU
1	D	24	LEU
1	D	53	THR
1	D	57	VAL
1	D	65	GLN
1	D	73	LEU
1	D	75	PRO
1	D	89	THR
1	D	92	VAL
1	D	93	LEU
1	D	103	ARG
1	D	105	GLU
1	D	106	ARG
1	D	110	ILE
1	D	130	HIS
1	D	132	THR
1	D	138	LEU
1	D	147	GLU
1	D	150	LYS
1	D	151	LEU
1	D	164	GLN
1	D	169	LEU
1	D	175	LYS
1	D	181	VAL
1	D	183	PHE
1	D	192	GLU
1	D	210	LEU
1	D	212	THR
1	D	217	SER
1	D	225	TYR
1	D	239	GLU

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Mol	Chain	Res	Type
1	D	240	GLU
1	D	245	VAL
1	D	256	MET
1	D	259	ARG
1	D	263	ASN
1	D	273	THR
1	D	301	ILE
1	D	302	ARG
1	E	-3	ARG
1	E	2	LYS
1	E	6	VAL
1	E	10	THR
1	E	19	LEU
1	E	24	LEU
1	E	53	THR
1	E	57	VAL
1	E	65	GLN
1	E	73	LEU
1	E	89	THR
1	E	92	VAL
1	E	93	LEU
1	E	103	ARG
1	E	105	GLU
1	E	106	ARG
1	E	110	ILE
1	E	130	HIS
1	E	132	THR
1	E	138	LEU
1	E	147	GLU
1	E	150	LYS
1	E	164	GLN
1	E	169	LEU
1	E	175	LYS
1	E	181	VAL
1	E	183	PHE
1	E	192	GLU
1	E	210	LEU
1	E	212	THR
1	E	217	SER
1	E	225	TYR
1	E	239	GLU
1	E	240	GLU

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Mol	Chain	Res	Type
1	E	245	VAL
1	E	256	MET
1	E	259	ARG
1	E	263	ASN
1	E	273	THR
1	E	301	ILE
1	E	302	ARG
1	F	1	MET
1	F	2	LYS
1	F	6	VAL
1	F	10	THR
1	F	19	LEU
1	F	24	LEU
1	F	53	THR
1	F	56	ARG
1	F	57	VAL
1	F	65	GLN
1	F	73	LEU
1	F	83	HIS
1	F	89	THR
1	F	92	VAL
1	F	93	LEU
1	F	103	ARG
1	F	105	GLU
1	F	106	ARG
1	F	110	ILE
1	F	118	THR
1	F	130	HIS
1	F	132	THR
1	F	138	LEU
1	F	147	GLU
1	F	150	LYS
1	F	159	VAL
1	F	164	GLN
1	F	169	LEU
1	F	175	LYS
1	F	181	VAL
1	F	183	PHE
1	F	192	GLU
1	F	210	LEU
1	F	212	THR
1	F	217	SER

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Mol	Chain	Res	Type
1	F	225	TYR
1	F	237	LEU
1	F	239	GLU
1	F	240	GLU
1	F	245	VAL
1	F	256	MET
1	F	259	ARG
1	F	263	ASN
1	F	273	THR
1	F	301	ILE
1	F	302	ARG
1	G	0	HIS
1	G	2	LYS
1	G	6	VAL
1	G	10	THR
1	G	19	LEU
1	G	24	LEU
1	G	53	THR
1	G	57	VAL
1	G	65	GLN
1	G	73	LEU
1	G	89	THR
1	G	92	VAL
1	G	93	LEU
1	G	103	ARG
1	G	105	GLU
1	G	106	ARG
1	G	110	ILE
1	G	118	THR
1	G	130	HIS
1	G	132	THR
1	G	138	LEU
1	G	147	GLU
1	G	150	LYS
1	G	164	GLN
1	G	169	LEU
1	G	175	LYS
1	G	181	VAL
1	G	183	PHE
1	G	192	GLU
1	G	210	LEU
1	G	211	VAL

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Mol	Chain	Res	Type
1	G	212	THR
1	G	217	SER
1	G	225	TYR
1	G	238	SER
1	G	239	GLU
1	G	240	GLU
1	G	245	VAL
1	G	256	MET
1	G	259	ARG
1	G	263	ASN
1	G	273	THR
1	G	301	ILE
1	G	302	ARG
1	H	0	HIS
1	H	1	MET
1	H	2	LYS
1	H	6	VAL
1	H	10	THR
1	H	19	LEU
1	H	24	LEU
1	H	53	THR
1	H	57	VAL
1	H	65	GLN
1	H	73	LEU
1	H	89	THR
1	H	92	VAL
1	H	93	LEU
1	H	103	ARG
1	H	105	GLU
1	H	106	ARG
1	H	110	ILE
1	H	118	THR
1	H	130	HIS
1	H	132	THR
1	H	138	LEU
1	H	147	GLU
1	H	150	LYS
1	H	164	GLN
1	H	168	SER
1	H	169	LEU
1	H	175	LYS
1	H	181	VAL

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Mol	Chain	Res	Type
1	H	183	PHE
1	H	192	GLU
1	H	210	LEU
1	H	212	THR
1	H	217	SER
1	H	225	TYR
1	H	239	GLU
1	H	240	GLU
1	H	245	VAL
1	H	256	MET
1	H	259	ARG
1	H	263	ASN
1	H	273	THR
1	H	301	ILE
1	H	302	ARG
1	I	0	HIS
1	I	1	MET
1	I	2	LYS
1	I	6	VAL
1	I	10	THR
1	I	19	LEU
1	I	24	LEU
1	I	53	THR
1	I	56	ARG
1	I	57	VAL
1	I	65	GLN
1	I	73	LEU
1	I	89	THR
1	I	92	VAL
1	I	93	LEU
1	I	103	ARG
1	I	105	GLU
1	I	106	ARG
1	I	110	ILE
1	I	118	THR
1	I	130	HIS
1	I	132	THR
1	I	138	LEU
1	I	147	GLU
1	I	150	LYS
1	I	151	LEU
1	I	164	GLN

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Mol	Chain	Res	Type
1	I	169	LEU
1	I	175	LYS
1	I	181	VAL
1	I	183	PHE
1	I	192	GLU
1	I	210	LEU
1	I	212	THR
1	I	217	SER
1	I	225	TYR
1	I	245	VAL
1	I	256	MET
1	I	259	ARG
1	I	263	ASN
1	I	273	THR
1	I	301	ILE
1	I	302	ARG
1	J	0	HIS
1	J	1	MET
1	J	2	LYS
1	J	6	VAL
1	J	10	THR
1	J	19	LEU
1	J	24	LEU
1	J	53	THR
1	J	56	ARG
1	J	57	VAL
1	J	65	GLN
1	J	73	LEU
1	J	78	ILE
1	J	89	THR
1	J	92	VAL
1	J	93	LEU
1	J	103	ARG
1	J	105	GLU
1	J	106	ARG
1	J	110	ILE
1	J	118	THR
1	J	130	HIS
1	J	132	THR
1	J	138	LEU
1	J	147	GLU
1	J	150	LYS

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Mol	Chain	Res	Type
1	J	151	LEU
1	J	159	VAL
1	J	164	GLN
1	J	169	LEU
1	J	175	LYS
1	J	181	VAL
1	J	183	PHE
1	J	192	GLU
1	J	210	LEU
1	J	212	THR
1	J	217	SER
1	J	225	TYR
1	J	245	VAL
1	J	256	MET
1	J	259	ARG
1	J	263	ASN
1	J	273	THR
1	J	301	ILE
1	J	302	ARG
1	K	0	HIS
1	K	1	MET
1	K	2	LYS
1	K	6	VAL
1	K	10	THR
1	K	19	LEU
1	K	24	LEU
1	K	53	THR
1	K	56	ARG
1	K	57	VAL
1	K	65	GLN
1	K	73	LEU
1	K	89	THR
1	K	92	VAL
1	K	93	LEU
1	K	103	ARG
1	K	105	GLU
1	K	106	ARG
1	K	110	ILE
1	K	118	THR
1	K	130	HIS
1	K	132	THR
1	K	138	LEU

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Mol	Chain	Res	Type
1	K	147	GLU
1	K	150	LYS
1	K	164	GLN
1	K	168	SER
1	K	169	LEU
1	K	175	LYS
1	K	181	VAL
1	K	183	PHE
1	K	192	GLU
1	K	210	LEU
1	K	212	THR
1	K	217	SER
1	K	225	TYR
1	K	239	GLU
1	K	240	GLU
1	K	245	VAL
1	K	256	MET
1	K	259	ARG
1	K	263	ASN
1	K	273	THR
1	K	301	ILE
1	K	302	ARG
1	L	-1	SER
1	L	1	MET
1	L	2	LYS
1	L	6	VAL
1	L	10	THR
1	L	19	LEU
1	L	24	LEU
1	L	53	THR
1	L	57	VAL
1	L	65	GLN
1	L	73	LEU
1	L	78	ILE
1	L	83	HIS
1	L	89	THR
1	L	92	VAL
1	L	93	LEU
1	L	103	ARG
1	L	105	GLU
1	L	106	ARG
1	L	110	ILE

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Mol	Chain	Res	Type
1	L	130	HIS
1	L	132	THR
1	L	138	LEU
1	L	147	GLU
1	L	150	LYS
1	L	164	GLN
1	L	169	LEU
1	L	175	LYS
1	L	181	VAL
1	L	183	PHE
1	L	192	GLU
1	L	210	LEU
1	L	212	THR
1	L	217	SER
1	L	225	TYR
1	L	239	GLU
1	L	240	GLU
1	L	245	VAL
1	L	256	MET
1	L	259	ARG
1	L	263	ASN
1	L	273	THR
1	L	301	ILE
1	L	302	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	B	-13	HIS
1	B	108	HIS
1	D	49	GLN
1	E	-11	HIS
1	E	50	GLN
1	E	108	HIS
1	E	194	HIS
1	F	50	GLN
1	H	50	GLN
1	I	50	GLN
1	J	115	ASN
1	K	69	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	340	-	4,4,4	0.17	0	6,6,6	0.29	0
2	SO4	A	341	-	4,4,4	0.13	0	6,6,6	0.36	0
2	SO4	B	340	-	4,4,4	0.23	0	6,6,6	0.43	0
2	SO4	B	341	-	4,4,4	0.26	0	6,6,6	0.43	0
2	SO4	B	342	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	C	340	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	C	341	-	4,4,4	0.19	0	6,6,6	0.18	0
2	SO4	D	340	-	4,4,4	0.30	0	6,6,6	0.49	0
2	SO4	D	341	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	E	340	-	4,4,4	0.07	0	6,6,6	0.22	0
2	SO4	E	341	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	E	342	-	4,4,4	0.14	0	6,6,6	0.30	0
2	SO4	F	340	-	4,4,4	0.20	0	6,6,6	0.16	0
2	SO4	F	341	-	4,4,4	0.11	0	6,6,6	0.25	0
2	SO4	G	340	-	4,4,4	0.28	0	6,6,6	0.29	0
2	SO4	G	341	-	4,4,4	0.18	0	6,6,6	0.23	0
2	SO4	G	342	-	4,4,4	0.21	0	6,6,6	0.15	0
2	SO4	H	340	-	4,4,4	0.20	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	H	341	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	I	340	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	I	341	-	4,4,4	0.19	0	6,6,6	0.20	0
2	SO4	J	340	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	J	341	-	4,4,4	0.18	0	6,6,6	0.19	0
2	SO4	K	340	-	4,4,4	0.23	0	6,6,6	0.64	0
2	SO4	L	340	-	4,4,4	0.23	0	6,6,6	0.27	0
2	SO4	L	341	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	L	342	-	4,4,4	0.17	0	6,6,6	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	340	-	-	0/0/0/0	0/0/0/0
2	SO4	A	341	-	-	0/0/0/0	0/0/0/0
2	SO4	B	340	-	-	0/0/0/0	0/0/0/0
2	SO4	B	341	-	-	0/0/0/0	0/0/0/0
2	SO4	B	342	-	-	0/0/0/0	0/0/0/0
2	SO4	C	340	-	-	0/0/0/0	0/0/0/0
2	SO4	C	341	-	-	0/0/0/0	0/0/0/0
2	SO4	D	340	-	-	0/0/0/0	0/0/0/0
2	SO4	D	341	-	-	0/0/0/0	0/0/0/0
2	SO4	E	340	-	-	0/0/0/0	0/0/0/0
2	SO4	E	341	-	-	0/0/0/0	0/0/0/0
2	SO4	E	342	-	-	0/0/0/0	0/0/0/0
2	SO4	F	340	-	-	0/0/0/0	0/0/0/0
2	SO4	F	341	-	-	0/0/0/0	0/0/0/0
2	SO4	G	340	-	-	0/0/0/0	0/0/0/0
2	SO4	G	341	-	-	0/0/0/0	0/0/0/0
2	SO4	G	342	-	-	0/0/0/0	0/0/0/0
2	SO4	H	340	-	-	0/0/0/0	0/0/0/0
2	SO4	H	341	-	-	0/0/0/0	0/0/0/0
2	SO4	I	340	-	-	0/0/0/0	0/0/0/0
2	SO4	I	341	-	-	0/0/0/0	0/0/0/0
2	SO4	J	340	-	-	0/0/0/0	0/0/0/0
2	SO4	J	341	-	-	0/0/0/0	0/0/0/0
2	SO4	K	340	-	-	0/0/0/0	0/0/0/0
2	SO4	L	340	-	-	0/0/0/0	0/0/0/0
2	SO4	L	341	-	-	0/0/0/0	0/0/0/0
2	SO4	L	342	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	341	SO4	1	0
2	B	341	SO4	1	0
2	B	342	SO4	1	0
2	F	341	SO4	1	0
2	I	341	SO4	1	0
2	L	341	SO4	1	0
2	L	342	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	337/359 (93%)	-0.08	2 (0%) 90 84	41, 74, 137, 219	0
1	B	353/359 (98%)	0.01	8 (2%) 64 49	39, 69, 144, 211	0
1	C	340/359 (94%)	-0.01	7 (2%) 67 52	43, 75, 141, 207	0
1	D	347/359 (96%)	-0.06	4 (1%) 81 69	40, 74, 137, 208	0
1	E	343/359 (95%)	-0.07	5 (1%) 76 63	34, 67, 127, 209	0
1	F	340/359 (94%)	0.25	29 (8%) 13 7	38, 82, 147, 224	0
1	G	341/359 (94%)	0.18	23 (6%) 21 12	46, 76, 144, 209	0
1	H	336/359 (93%)	0.25	20 (5%) 25 14	44, 80, 141, 208	0
1	I	332/359 (92%)	0.01	8 (2%) 62 47	44, 76, 136, 208	0
1	J	341/359 (94%)	0.14	21 (6%) 24 13	46, 81, 147, 224	0
1	K	341/359 (94%)	0.07	10 (2%) 55 41	46, 80, 148, 210	0
1	L	341/359 (94%)	0.02	10 (2%) 55 41	38, 79, 149, 238	0
All	All	4092/4308 (94%)	0.06	147 (3%) 46 31	34, 76, 144, 238	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	GLU	5.4
1	B	231	GLY	4.8
1	B	233	TYR	4.6
1	J	81	GLY	4.6
1	G	218	VAL	4.5
1	L	82	GLY	4.5
1	H	225	TYR	4.3
1	G	246	PHE	4.3
1	J	234	GLU	4.3
1	K	81	GLY	4.3
1	G	183	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	215	ALA	4.3
1	L	211	VAL	4.1
1	J	161	ASP	4.0
1	B	79	GLN	4.0
1	F	180	PHE	3.8
1	F	217	SER	3.7
1	F	226	THR	3.7
1	H	154	CYS	3.7
1	F	221	ALA	3.7
1	F	148	GLY	3.7
1	F	181	VAL	3.7
1	L	81	GLY	3.7
1	G	248	PRO	3.6
1	F	183	PHE	3.5
1	K	159	VAL	3.4
1	L	79	GLN	3.4
1	F	182	HIS	3.4
1	D	146	PRO	3.4
1	B	232	LEU	3.3
1	J	162	ALA	3.2
1	G	226	THR	3.2
1	F	220	GLY	3.2
1	F	156	VAL	3.1
1	F	157	VAL	3.1
1	J	339	ILE	3.1
1	F	190	LEU	3.0
1	I	215	ALA	3.0
1	H	190	LEU	3.0
1	H	223	PHE	3.0
1	F	215	ALA	3.0
1	F	78	ILE	3.0
1	J	246	PHE	3.0
1	J	188	PHE	2.9
1	G	224	LEU	2.9
1	J	160	GLY	2.8
1	H	221	ALA	2.8
1	J	232	LEU	2.8
1	J	229	TRP	2.8
1	J	192	GLU	2.8
1	H	157	VAL	2.8
1	F	83	HIS	2.8
1	F	223	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	220	GLY	2.8
1	H	217	SER	2.8
1	F	218	VAL	2.7
1	K	151	LEU	2.7
1	H	139	CYS	2.7
1	F	224	LEU	2.7
1	G	211	VAL	2.7
1	L	183	PHE	2.7
1	H	267	MET	2.7
1	K	226	THR	2.7
1	J	223	PHE	2.7
1	G	245	VAL	2.7
1	K	225	TYR	2.6
1	I	188	PHE	2.6
1	G	186	GLU	2.6
1	J	235	ALA	2.6
1	F	245	VAL	2.6
1	B	215	ALA	2.6
1	G	217	SER	2.6
1	H	156	VAL	2.6
1	J	215	ALA	2.6
1	J	183	PHE	2.5
1	H	82	GLY	2.5
1	K	190	LEU	2.5
1	J	218	VAL	2.5
1	J	231	GLY	2.5
1	H	158	PHE	2.5
1	K	82	GLY	2.5
1	G	243	MET	2.5
1	G	247	TYR	2.5
1	C	234	GLU	2.5
1	L	215	ALA	2.4
1	H	180	PHE	2.4
1	I	247	TYR	2.4
1	H	226	THR	2.4
1	C	156	VAL	2.4
1	D	233	TYR	2.4
1	I	246	PHE	2.4
1	J	185	PRO	2.4
1	H	264	CYS	2.4
1	G	190	LEU	2.4
1	F	211	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	242	ARG	2.3
1	C	82	GLY	2.3
1	F	257	MET	2.3
1	J	184	GLY	2.3
1	J	190	LEU	2.3
1	G	227	ASP	2.3
1	G	182	HIS	2.3
1	B	77	GLN	2.3
1	I	183	PHE	2.3
1	G	159	VAL	2.3
1	G	215	ALA	2.2
1	G	235	ALA	2.2
1	G	228	VAL	2.2
1	B	235	ALA	2.2
1	F	227	ASP	2.2
1	J	250	TYR	2.2
1	E	246	PHE	2.2
1	C	183	PHE	2.2
1	H	146	PRO	2.2
1	I	224	LEU	2.2
1	F	256	MET	2.2
1	C	160	GLY	2.2
1	G	157	VAL	2.2
1	C	229	TRP	2.2
1	L	179	ASN	2.2
1	F	214	ASP	2.1
1	K	178	MET	2.1
1	C	275	GLY	2.1
1	D	231	GLY	2.1
1	H	181	VAL	2.1
1	L	146	PRO	2.1
1	G	287	ASN	2.1
1	I	243	MET	2.1
1	K	245	VAL	2.1
1	H	290	CYS	2.1
1	L	182	HIS	2.1
1	H	248	PRO	2.1
1	F	250	TYR	2.1
1	G	273	THR	2.1
1	A	79	GLN	2.1
1	F	155	LYS	2.1
1	L	154	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	141	MET	2.1
1	F	234	GLU	2.1
1	I	214	ASP	2.1
1	E	185	PRO	2.1
1	E	214	ASP	2.1
1	A	215	ALA	2.1
1	D	214	ASP	2.0
1	F	158	PHE	2.0
1	F	228	VAL	2.0
1	K	183	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	340	5/5	0.79	0.33	4.20	105,110,199,203	0
2	SO4	K	340	5/5	0.82	0.34	3.51	103,105,182,190	0
2	SO4	H	340	5/5	0.81	0.28	2.26	142,151,175,178	0
2	SO4	G	340	5/5	0.95	0.33	2.07	71,84,109,111	0
2	SO4	E	341	5/5	0.96	0.24	1.12	70,86,138,148	0
2	SO4	I	341	5/5	0.82	0.27	0.83	131,176,179,182	0
2	SO4	D	340	5/5	0.83	0.26	0.80	52,115,167,222	0
2	SO4	F	341	5/5	0.89	0.25	0.77	59,123,192,197	0
2	SO4	L	340	5/5	0.98	0.34	0.74	63,83,85,137	0
2	SO4	C	340	5/5	0.92	0.22	0.71	64,118,199,217	0
2	SO4	B	341	5/5	0.94	0.26	0.55	61,66,126,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	E	342	5/5	0.80	0.26	0.54	133,143,177,213	0
2	SO4	L	342	5/5	0.86	0.30	0.38	129,163,183,197	0
2	SO4	E	340	5/5	0.91	0.24	0.10	86,112,144,146	0
2	SO4	I	340	5/5	0.85	0.21	-0.04	97,135,192,204	0
2	SO4	J	340	5/5	0.90	0.19	-0.20	127,150,178,179	0
2	SO4	C	341	5/5	0.92	0.24	-0.27	159,176,191,193	0
2	SO4	G	342	5/5	0.96	0.20	-0.36	112,127,168,206	0
2	SO4	J	341	5/5	0.92	0.22	-0.37	42,180,185,214	0
2	SO4	B	340	5/5	0.94	0.25	-0.62	56,90,126,172	0
2	SO4	G	341	5/5	0.91	0.17	-1.13	134,152,174,175	0
2	SO4	L	341	5/5	0.96	0.18	-1.14	101,122,174,199	0
2	SO4	H	341	5/5	0.95	0.14	-1.54	68,151,194,196	0
2	SO4	F	340	5/5	0.93	0.15	-1.73	102,138,146,182	0
2	SO4	B	342	5/5	0.74	0.30	-	115,143,184,221	0
2	SO4	A	341	5/5	0.82	0.24	-	83,129,161,178	0
2	SO4	D	341	5/5	0.93	0.21	-	61,140,158,170	0

## 6.5 Other polymers

There are no such residues in this entry.