



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:53 AM 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 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/ValidationPDFNotes.html>

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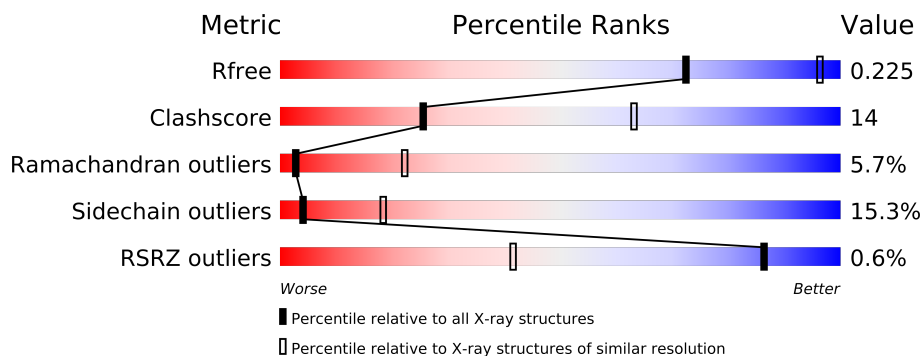
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	359	
1	B	359	
1	C	359	
1	D	359	
1	E	359	
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 that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	340	-	X
2	SO4	E	341	-	X
2	SO4	E	342	-	X

## 2 Entry composition

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

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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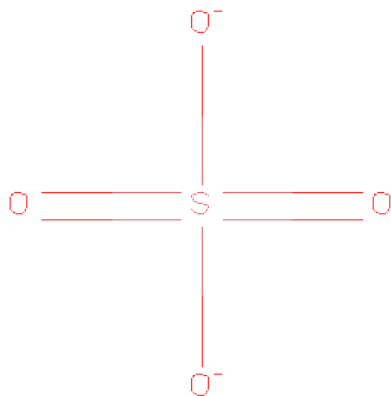
Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
I	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
I	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
I	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
I	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
I	-1	SER	-	EXPRESSION TAG	UNP Q837U7
I	0	HIS	-	EXPRESSION TAG	UNP Q837U7
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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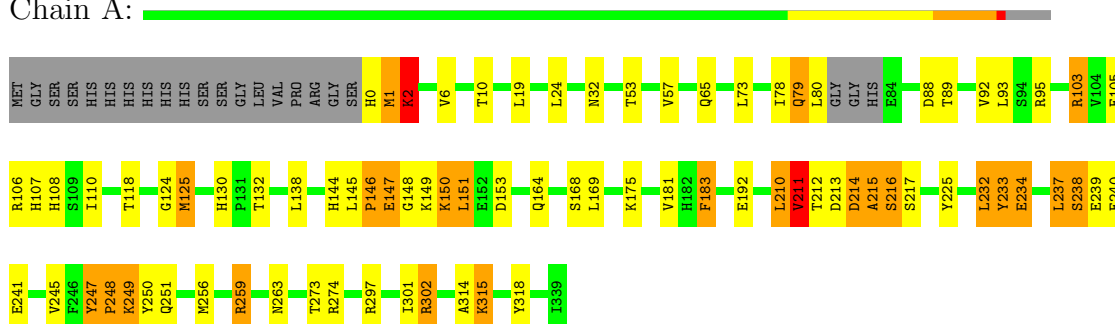
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

### 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.

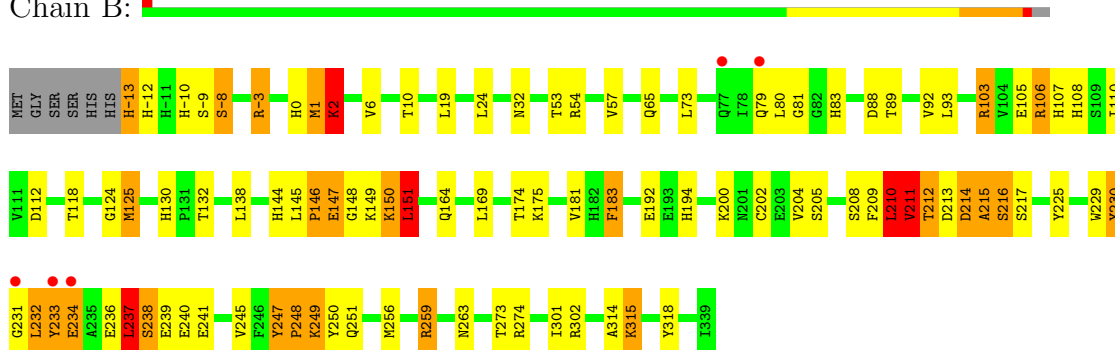
#### • Molecule 1: Putrescine carbamoyltransferase

Chain A:



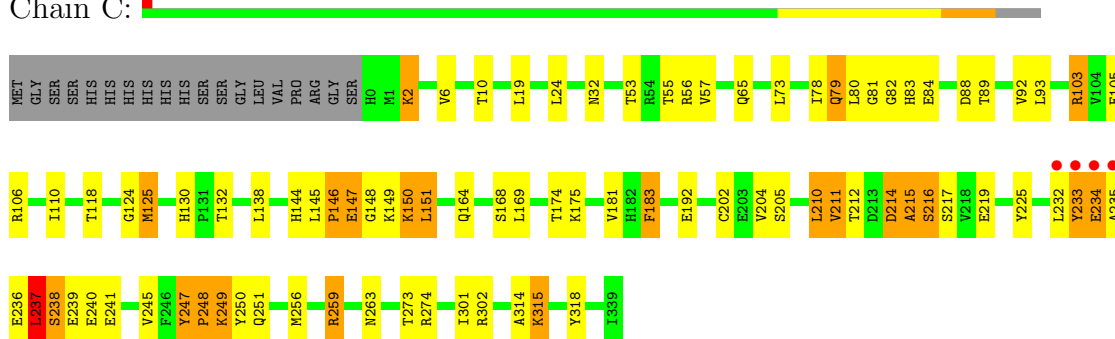
#### • Molecule 1: Putrescine carbamoyltransferase

Chain B:

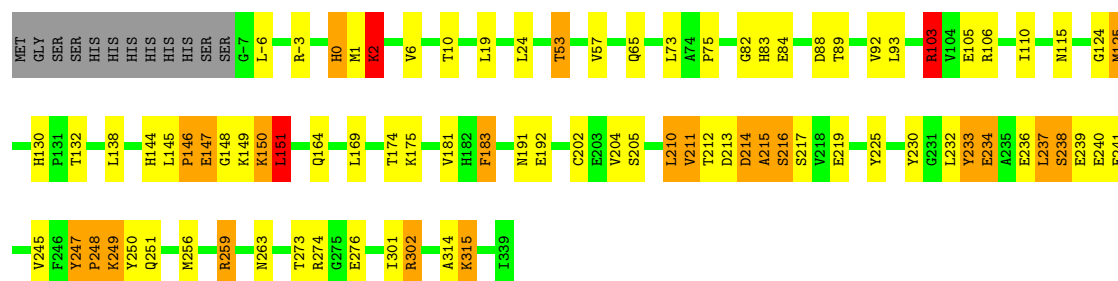


#### • Molecule 1: Putrescine carbamoyltransferase

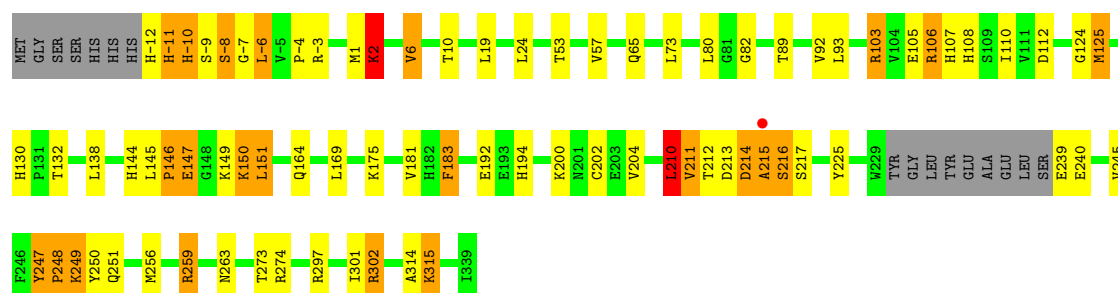
Chain C:



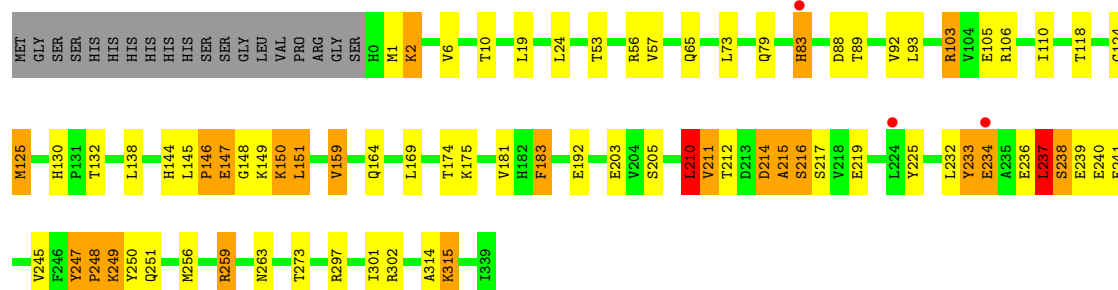
#### • Molecule 1: Putrescine carbamoyltransferase

Chain D: 

- Molecule 1: Putrescine carbamoyltransferase

Chain E: 

- Molecule 1: Putrescine carbamoyltransferase

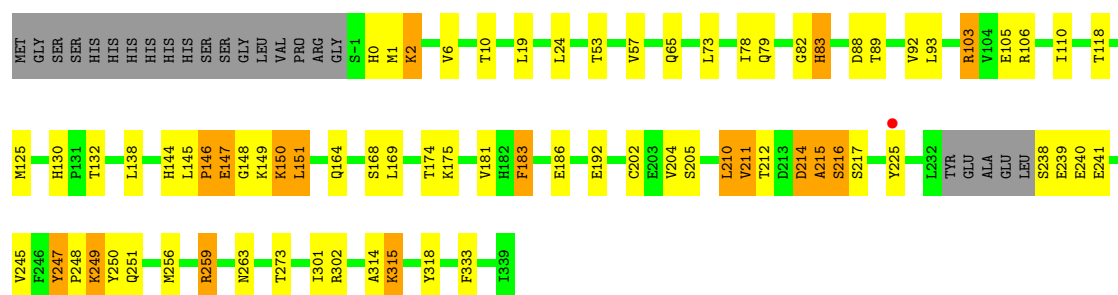
Chain F: 

- Molecule 1: Putrescine carbamoyltransferase

Chain G: 

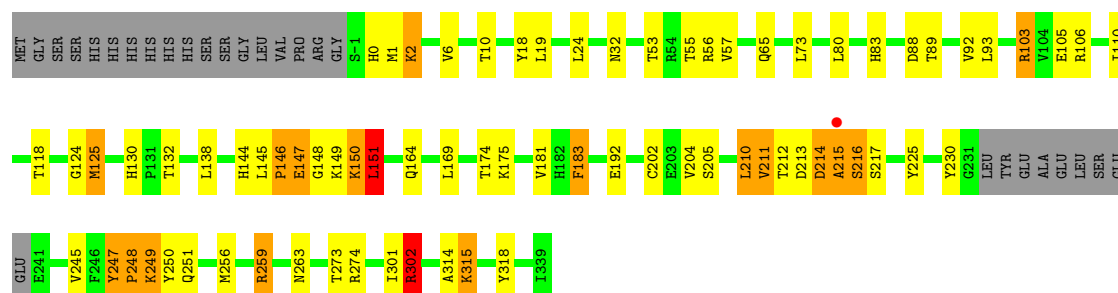
- Molecule 1: Putrescine carbamoyltransferase

Chain H: 



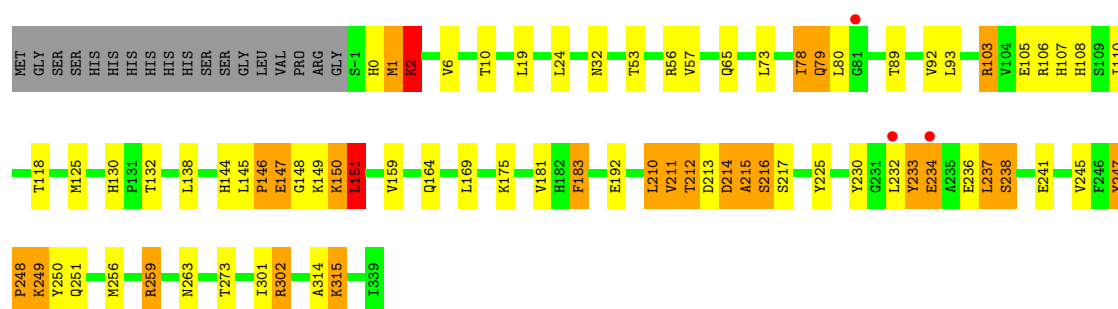
• Molecule 1: Putrescine carbamoyltransferase

Chain I:



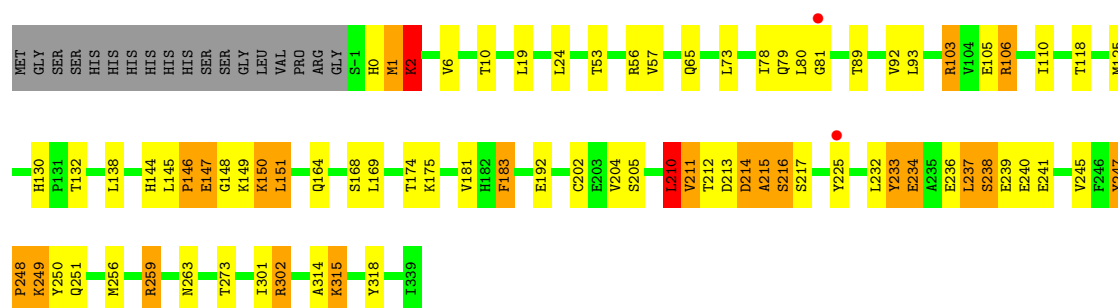
• Molecule 1: Putrescine carbamoyltransferase

Chain J:



• Molecule 1: Putrescine carbamoyltransferase

Chain K:



• Molecule 1: Putrescine carbamoyltransferase

Chain L:





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	273.86Å 87.79Å 241.30Å 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 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.190 , 0.234 0.178 , 0.225	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> )	0.29 , 45.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2642	0	0	45	0
1	B	2766	0	0	64	0
1	C	2659	0	0	38	0
1	D	2707	0	0	40	0
1	E	2694	0	0	55	0
1	F	2664	0	0	33	2
1	G	2660	0	0	34	0
1	H	2631	0	0	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2606	0	0	31	0
1	J	2651	0	0	34	0
1	K	2656	0	0	34	2
1	L	2671	0	0	39	0
2	A	10	0	0	2	0
2	B	15	0	0	3	0
2	C	10	0	0	1	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	3	0
All	All	32142	0	0	437	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (437) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:106:ARG:NH2	1:E:112:ASP:OD2	1.89	1.03
1:B:233:TYR:N	1:E:-11:HIS:CD2	2.36	0.93
1:B:233:TYR:N	1:E:-11:HIS:CG	2.43	0.87
1:A:214:ASP:O	1:A:216:SER:N	2.10	0.84
1:E:183:PHE:CD2	1:E:183:PHE:C	2.51	0.83
1:A:95:ARG:NH2	2:A:341:SO4:O3	2.11	0.83
1:K:79:GLN:O	1:K:81:GLY:N	2.12	0.82
1:B:214:ASP:O	1:B:216:SER:N	2.14	0.81
1:E:-8:SER:OG	1:E:-7:GLY:N	2.11	0.81
1:C:183:PHE:CD2	1:C:183:PHE:C	2.54	0.81
1:B:231:GLY:O	1:E:-11:HIS:CD2	2.34	0.80
1:D:214:ASP:O	1:D:216:SER:N	2.14	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:C:214:ASP:O	1:C:216:SER:N	2.15	0.79
1:D:215:ALA:O	1:D:259:ARG:NH2	2.16	0.79
1:F:183:PHE:CD2	1:F:183:PHE:C	2.55	0.79
1:J:183:PHE:C	1:J:183:PHE:CD2	2.55	0.79
1:C:79:GLN:O	1:C:81:GLY:N	2.16	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:183:PHE:C	1:D:183:PHE:CD2	2.55	0.78
1:K:183:PHE:C	1:K:183:PHE:CD2	2.55	0.78
1:H:183:PHE:C	1:H:183:PHE:CD2	2.56	0.78
1:I:214:ASP:O	1:I:216:SER:N	2.16	0.78
1:G:214:ASP:O	1:G:216:SER:N	2.17	0.78
1:L:183:PHE:C	1:L:183:PHE:CD2	2.57	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:A:183:PHE:C	1:A:183:PHE:CD2	2.55	0.78
1:L:214:ASP:O	1:L:216:SER:N	2.16	0.78
1:G:183:PHE:C	1:G:183:PHE:CD2	2.55	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:J:214:ASP:O	1:J:216:SER:N	2.18	0.76
1:B:183:PHE:CD2	1:B:183:PHE:C	2.54	0.76
1:B:215:ALA:O	1:B:259:ARG:NH2	2.19	0.76
1:A:183:PHE:O	1:A:183:PHE:CD2	2.39	0.76
1:D:183:PHE:O	1:D:183:PHE:CD2	2.40	0.76
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:I:183:PHE:C	1:I:183:PHE:CD2	2.57	0.75
1:L:103:ARG:NH2	2:L:341:SO4:O2	2.21	0.74
1:K:215:ALA:O	1:K:259:ARG:NH2	2.20	0.74
1:G:215:ALA:O	1:G:259:ARG:NH2	2.21	0.74
1:C:183:PHE:CD2	1:C:183:PHE:O	2.40	0.74
1:I:215:ALA:O	1:I:259:ARG:NH2	2.20	0.74
1:F:83:HIS:ND1	1:F:83:HIS:N	2.33	0.74
1:F:214:ASP:O	1:F:216:SER:N	2.21	0.73
1:A:210:LEU:CD1	1:A:211:VAL:N	2.52	0.73
1:B:-9:SER:O	1:B:-8:SER:O	2.07	0.72
1:A:249:LYS:O	1:A:251:GLN:N	2.23	0.72
1:F:215:ALA:O	1:F:259:ARG:NH2	2.23	0.72
1:E:210:LEU:CD1	1:E:211:VAL:N	2.53	0.71
1:H:249:LYS:O	1:H:251:GLN:N	2.22	0.71
1:K:183:PHE:O	1:K:183:PHE:CD2	2.43	0.71
1:F:249:LYS:O	1:F:251:GLN:N	2.23	0.71
1:C:249:LYS:O	1:C:251:GLN:N	2.24	0.71
1:D:-3:ARG:N	1:D:115:ASN:OD1	2.23	0.71
1:J:215:ALA:O	1:J:259:ARG:NH2	2.24	0.71
1:J:249:LYS:O	1:J:251:GLN:N	2.23	0.70
1:F:183:PHE:O	1:F:183:PHE:CD2	2.44	0.70
1:G:183:PHE:O	1:G:183:PHE:CD2	2.43	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:215:ALA:O	1:L:259:ARG:NH2	2.24	0.70
1:L:79:GLN:O	1:L:81:GLY:N	2.25	0.70
1:I:249:LYS:O	1:I:251:GLN:N	2.25	0.69
1:H:183:PHE:O	1:H:183:PHE:CD2	2.45	0.69
1:G:249:LYS:O	1:G:251:GLN:N	2.24	0.69
1:L:183:PHE:O	1:L:183:PHE:CD2	2.45	0.69
1:L:79:GLN:C	1:L:81:GLY:N	2.47	0.68
1:E:249:LYS:O	1:E:251:GLN:N	2.26	0.68
1:I:183:PHE:O	1:I:183:PHE:CD2	2.46	0.68
1:J:183:PHE:O	1:J:183:PHE:CD2	2.46	0.68
1:A:215:ALA:O	1:A:259:ARG:NH2	2.28	0.67
1:H:259:ARG:NH1	1:H:259:ARG:CG	2.57	0.67
1:B:249:LYS:O	1:B:251:GLN:N	2.27	0.67
1:E:259:ARG:NH1	1:E:259:ARG:CG	2.57	0.67
1:K:249:LYS:O	1:K:251:GLN:N	2.29	0.66
1:L:249:LYS:O	1:L:251:GLN:N	2.28	0.66
1:D:210:LEU:CD1	1:D:211:VAL:N	2.59	0.66
1:I:259:ARG:CG	1:I:259:ARG:NH1	2.59	0.66
1:A:237:LEU:O	1:A:238:SER:O	2.13	0.66
1:B:259:ARG:NH1	1:B:259:ARG:CG	2.59	0.65
1:E:103:ARG:NH1	1:E:103:ARG:CG	2.60	0.65
1:F:259:ARG:NH1	1:F:259:ARG:CG	2.59	0.65
1:H:318:TYR:CD1	1:I:32:ASN:C	2.69	0.65
1:J:259:ARG:CG	1:J:259:ARG:NH1	2.60	0.64
1:B:210:LEU:CD1	1:B:211:VAL:N	2.60	0.64
1:G:210:LEU:CD1	1:G:211:VAL:N	2.61	0.64
1:B:314:ALA:O	1:B:315:LYS:CB	2.44	0.64
1:C:259:ARG:NH1	1:C:259:ARG:CG	2.61	0.64
1:F:238:SER:CB	1:F:241:GLU:CB	2.75	0.64
1:A:183:PHE:CG	1:A:214:ASP:OD2	2.52	0.63
1:G:259:ARG:CG	1:G:259:ARG:NH1	2.60	0.63
1:G:79:GLN:O	1:G:81:GLY:N	2.32	0.63
1:I:103:ARG:NH1	1:I:103:ARG:CG	2.61	0.63
1:B:103:ARG:CG	1:B:103:ARG:NH1	2.62	0.63
1:K:259:ARG:NH1	1:K:259:ARG:CG	2.61	0.63
1:C:210:LEU:CD1	1:C:211:VAL:N	2.62	0.63
1:A:238:SER:CB	1:A:241:GLU:CB	2.77	0.62
1:L:259:ARG:CG	1:L:259:ARG:NH1	2.62	0.62
1:L:52:SER:OG	2:L:342:SO4:O2	2.16	0.62
1:F:103:ARG:NH1	1:F:103:ARG:CG	2.62	0.62
1:B:231:GLY:O	1:E:-11:HIS:CA	2.48	0.62
1:J:210:LEU:CD1	1:J:211:VAL:N	2.62	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:103:ARG:NH1	1:C:103:ARG:CG	2.62	0.62
1:E:183:PHE:CG	1:E:214:ASP:OD2	2.53	0.62
1:D:259:ARG:NH1	1:D:259:ARG:CG	2.62	0.62
1:K:103:ARG:CG	1:K:103:ARG:NH1	2.62	0.62
1:I:55:THR:OG1	2:I:341:SO4:O2	2.16	0.62
1:A:259:ARG:CG	1:A:259:ARG:NH1	2.60	0.62
1:G:103:ARG:CG	1:G:103:ARG:NH1	2.62	0.62
1:A:103:ARG:NH1	1:A:103:ARG:CG	2.63	0.62
1:G:314:ALA:O	1:G:315:LYS:CB	2.48	0.61
1:D:249:LYS:O	1:D:251:GLN:N	2.32	0.61
1:H:238:SER:CB	1:H:241:GLU:CB	2.79	0.61
1:L:238:SER:CB	1:L:241:GLU:CB	2.79	0.61
1:D:238:SER:CB	1:D:241:GLU:CB	2.79	0.61
1:K:237:LEU:O	1:K:238:SER:O	2.19	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:C:79:GLN:O	1:C:82:GLY:N	2.34	0.61
1:H:210:LEU:CD1	1:H:211:VAL:N	2.64	0.61
1:A:183:PHE:CD2	1:A:214:ASP:OD2	2.54	0.60
1:C:238:SER:CB	1:C:241:GLU:CB	2.80	0.60
1:E:314:ALA:O	1:E:315:LYS:CB	2.48	0.60
1:H:103:ARG:NH1	1:H:103:ARG:CG	2.65	0.60
1:B:200:LYS:NZ	1:E:200:LYS:NZ	2.49	0.60
1:J:103:ARG:NH1	1:J:103:ARG:CG	2.65	0.60
1:H:314:ALA:O	1:H:315:LYS:CB	2.49	0.60
1:K:183:PHE:CD2	1:K:214:ASP:OD2	2.55	0.60
1:K:210:LEU:CD1	1:K:211:VAL:N	2.65	0.60
1:J:238:SER:CB	1:J:241:GLU:CB	2.80	0.60
1:F:210:LEU:CD1	1:F:211:VAL:N	2.65	0.60
1:L:103:ARG:CG	1:L:103:ARG:NH1	2.65	0.59
1:H:183:PHE:CD2	1:H:214:ASP:OD2	2.55	0.59
1:I:314:ALA:O	1:I:315:LYS:CB	2.49	0.59
1:K:238:SER:CB	1:K:241:GLU:CB	2.81	0.59
1:C:183:PHE:CD2	1:C:214:ASP:OD2	2.56	0.59
1:G:274:ARG:NH2	1:I:88:ASP:OD1	2.35	0.59
1:E:183:PHE:CD2	1:E:214:ASP:OD2	2.56	0.59
1:K:314:ALA:O	1:K:315:LYS:CB	2.51	0.59
1:C:314:ALA:O	1:C:315:LYS:CB	2.51	0.58
1:J:314:ALA:O	1:J:315:LYS:CB	2.50	0.58
1:D:314:ALA:O	1:D:315:LYS:CB	2.51	0.58
1:I:210:LEU:CD1	1:I:211:VAL:N	2.67	0.58
1:E:-12:HIS:O	1:E:-11:HIS:CG	2.57	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:183:PHE:CD2	1:B:214:ASP:OD2	2.57	0.57
1:D:183:PHE:CD2	1:D:214:ASP:OD2	2.57	0.57
1:L:314:ALA:O	1:L:315:LYS:CB	2.51	0.57
1:B:-13:HIS:CE1	1:E:106:ARG:NE	2.72	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:L:210:LEU:CD1	1:L:211:VAL:N	2.68	0.57
1:A:314:ALA:O	1:A:315:LYS:CB	2.49	0.57
1:G:238:SER:CB	1:G:241:GLU:CB	2.82	0.57
1:J:78:ILE:CG1	1:J:79:GLN:N	2.67	0.57
1:J:237:LEU:O	1:J:238:SER:O	2.22	0.57
1:J:183:PHE:CD2	1:J:214:ASP:OD2	2.58	0.56
1:B:238:SER:CB	1:B:241:GLU:CB	2.82	0.56
1:D:88:ASP:OD1	1:E:274:ARG:NH2	2.38	0.56
1:K:147:GLU:O	1:K:149:LYS:N	2.37	0.56
1:G:183:PHE:CD2	1:G:214:ASP:OD2	2.58	0.56
1:J:183:PHE:CG	1:J:214:ASP:OD2	2.59	0.55
1:B:108:HIS:CD2	1:E:108:HIS:CD2	2.95	0.55
1:B:112:ASP:OD2	1:E:106:ARG:NH2	2.40	0.55
1:F:183:PHE:CG	1:F:214:ASP:OD2	2.60	0.55
1:D:103:ARG:CG	1:D:103:ARG:NH1	2.69	0.55
1:C:82:GLY:O	1:C:84:GLU:N	2.40	0.55
1:B:214:ASP:O	1:B:215:ALA:C	2.45	0.54
1:F:183:PHE:CD2	1:F:214:ASP:OD2	2.60	0.54
1:A:183:PHE:CD1	1:A:214:ASP:OD2	2.61	0.54
1:H:88:ASP:OD1	1:I:274:ARG:NH2	2.41	0.54
1:C:214:ASP:O	1:C:215:ALA:C	2.45	0.54
1:G:235:ALA:O	1:G:236:GLU:CB	2.54	0.54
1:H:247:TYR:O	1:H:247:TYR:CD1	2.61	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:D:183:PHE:CG	1:D:214:ASP:OD2	2.60	0.54
1:I:183:PHE:CG	1:I:214:ASP:OD2	2.61	0.54
1:G:236:GLU:C	1:G:238:SER:N	2.61	0.54
1:I:183:PHE:CD2	1:I:214:ASP:OD2	2.61	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:J:147:GLU:O	1:J:149:LYS:N	2.41	0.53
1:A:214:ASP:O	1:A:215:ALA:C	2.46	0.53
1:C:147:GLU:O	1:C:149:LYS:N	2.41	0.53
1:K:236:GLU:O	1:K:237:LEU:C	2.47	0.53
1:J:236:GLU:O	1:J:237:LEU:O	2.25	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:183:PHE:CD1	1:E:214:ASP:OD2	2.62	0.53
1:E:-11:HIS:O	1:E:-10:HIS:O	2.27	0.52
1:E:214:ASP:O	1:E:215:ALA:C	2.47	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:147:GLU:O	1:L:149:LYS:N	2.42	0.52
1:J:214:ASP:O	1:J:215:ALA:C	2.47	0.52
1:L:183:PHE:CD2	1:L:214:ASP:OD2	2.62	0.52
1:F:314:ALA:O	1:F:315:LYS:CB	2.56	0.52
1:L:214:ASP:O	1:L:215:ALA:C	2.47	0.52
1:L:150:LYS:O	1:L:151:LEU:CB	2.57	0.52
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:G:236:GLU:O	1:G:238:SER:N	2.43	0.51
1:D:247:TYR:CD1	1:D:247:TYR:O	2.63	0.51
1:E:147:GLU:O	1:E:149:LYS:N	2.44	0.51
1:E:-12:HIS:O	1:E:-11:HIS:ND1	2.43	0.51
1:F:147:GLU:O	1:F:149:LYS:N	2.44	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:D:230:TYR:OH	1:F:83:HIS:NE2	2.44	0.51
1:B:150:LYS:O	1:B:151:LEU:CB	2.59	0.51
1:B:-3:ARG:CA	1:B:-3:ARG:NE	2.74	0.51
1:F:247:TYR:O	1:F:247:TYR:CD1	2.64	0.51
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
1:E:247:TYR:O	1:E:247:TYR:CD1	2.63	0.50
1:F:214:ASP:O	1:F:215:ALA:C	2.50	0.50
1:J:232:LEU:O	1:J:234:GLU:N	2.45	0.50
1:L:232:LEU:O	1:L:234:GLU:N	2.44	0.50
1:A:147:GLU:O	1:A:149:LYS:N	2.45	0.50
1:G:214:ASP:O	1:G:215:ALA:C	2.50	0.50
1:I:247:TYR:O	1:I:247:TYR:CD1	2.65	0.50
1:J:247:TYR:O	1:J:247:TYR:CD1	2.65	0.50
1:D:274:ARG:NH2	1:F:88:ASP:OD1	2.45	0.50
1:E:150:LYS:O	1:E:151:LEU:CB	2.59	0.50
1:C:150:LYS:O	1:C:151:LEU:CB	2.60	0.50
1:H:150:LYS:O	1:H:151:LEU:CB	2.59	0.50
1:B:54:ARG:NH2	2:B:342:SO4:O3	2.44	0.49
1:D:0:HIS:N	1:D:0:HIS:ND1	2.60	0.49
1:A:0:HIS:O	1:A:1:MET:C	2.49	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:232:LEU:O	1:G:234:GLU:N	2.45	0.49
1:C:247:TYR:CD1	1:C:247:TYR:O	2.65	0.49
1:G:150:LYS:O	1:G:151:LEU:CB	2.59	0.49
1:B:231:GLY:O	1:E:-11:HIS:CG	2.65	0.49
1:K:150:LYS:O	1:K:151:LEU:CB	2.60	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: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:B:247:TYR:O	1:B:248:PRO:O	2.30	0.49
1:B:232:LEU:CA	1:E:-11:HIS:CB	2.91	0.49
1:H:214:ASP:O	1:H:215:ALA:C	2.51	0.49
1:J:150:LYS:O	1:J:151:LEU:CB	2.60	0.49
1:A:150:LYS:O	1:A:151:LEU:CB	2.60	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:K:232:LEU:O	1:K:234:GLU:N	2.46	0.49
1:B:-13:HIS:CE1	1:E:106:ARG:CD	2.96	0.49
1:I:150:LYS:O	1:I:151:LEU:CB	2.60	0.49
1:B:236:GLU:O	1:B:238:SER:N	2.46	0.48
1:C:235:ALA:C	1:C:237:LEU:N	2.66	0.48
1:K:247:TYR:O	1:K:247:TYR:CD1	2.66	0.48
1:A:79:GLN:O	1:A:80:LEU:C	2.51	0.48
1:B:145:LEU:O	1:B:146:PRO:O	2.30	0.48
1:A:215:ALA:CB	1:A:259:ARG:NE	2.77	0.48
1:D:215:ALA:CB	1:D:259:ARG:NE	2.77	0.48
1:F:232:LEU:O	1:F:234:GLU:N	2.46	0.48
1:B:213:ASP:O	1:B:213:ASP:CG	2.52	0.48
1:A:210:LEU:CD1	1:A:211:VAL:CA	2.91	0.48
1:A:247:TYR:O	1:A:247:TYR:CG	2.67	0.48
1:B:247:TYR:O	1:B:247:TYR:CD1	2.67	0.48
1:J:78:ILE:O	1:J:80:LEU:N	2.47	0.47
1:A:247:TYR:O	1:A:248:PRO:O	2.31	0.47
1:K:318:TYR:CD1	1:L:32:ASN:C	2.87	0.47
1:G:247:TYR:CD1	1:G:247:TYR:O	2.67	0.47
1:D:232:LEU:O	1:D:234:GLU:N	2.47	0.47
1:F:150:LYS:O	1:F:151:LEU:CB	2.62	0.47
1:A:144:HIS:C	1:A:146:PRO:CD	2.83	0.47
1:B:183:PHE:CD1	1:B:214:ASP:OD2	2.68	0.47
1:E:210:LEU:CD1	1:E:211:VAL:CA	2.91	0.47
1:K:247:TYR:O	1:K:248:PRO:O	2.32	0.47
1:C:232:LEU:O	1:C:234:GLU:N	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:232:LEU:O	1:A:234:GLU:N	2.48	0.47
1:B:106:ARG:NH2	1:E:112:ASP:CG	2.63	0.47
1:D:124:GLY:O	1:D:125:MET:CB	2.62	0.46
1:C:247:TYR:O	1:C:248:PRO:O	2.33	0.46
1:G:1:MET:O	1:G:2:LYS:CB	2.63	0.46
1:H:82:GLY:O	1:H:83:HIS:CB	2.63	0.46
1:H:183:PHE:CD1	1:H:214:ASP:OD2	2.69	0.46
1:K:247:TYR:O	1:K:247:TYR:CG	2.68	0.46
1:A:88:ASP:OD1	1:B:274:ARG:NH2	2.49	0.46
1:I:215:ALA:CB	1:I:259:ARG:NE	2.80	0.45
1:B:318:TYR:CD1	1:C:32:ASN:C	2.90	0.45
1:H:333:PHE:CZ	1:I:18:TYR:CE1	3.05	0.45
1:C:215:ALA:CB	1:C:259:ARG:NE	2.80	0.45
1:G:247:TYR:O	1:G:248:PRO:O	2.35	0.45
1:J:247:TYR:CG	1:J:247:TYR:O	2.69	0.45
1:K:213:ASP:O	1:K:213:ASP:CG	2.55	0.45
1:B:79:GLN:O	1:B:81:GLY:N	2.50	0.45
1:B:215:ALA:CB	1:B:259:ARG:NE	2.79	0.45
1:B:194:HIS:NE2	1:E:-8:SER:CB	2.80	0.45
1:F:247:TYR:O	1:F:248:PRO:O	2.35	0.45
1:A:32:ASN:C	1:C:318:TYR:CD1	2.90	0.45
1:D:82:GLY:O	1:D:84:GLU:N	2.50	0.45
1:F:247:TYR:CG	1:F:247:TYR:O	2.70	0.44
1:I:144:HIS:C	1:I:146:PRO:CD	2.85	0.44
1:E:144:HIS:C	1:E:146:PRO:CD	2.85	0.44
1:C:247:TYR:CG	1:C:247:TYR:O	2.70	0.44
1:B:247:TYR:O	1:B:247:TYR:CG	2.70	0.44
1:K:145:LEU:O	1:K:146:PRO:O	2.34	0.44
1:E:247:TYR:O	1:E:247:TYR:CG	2.70	0.44
1:E:213:ASP:O	1:E:213:ASP:CG	2.55	0.44
1:A:274:ARG:NH2	1:C:88:ASP:OD1	2.50	0.44
1:E:215:ALA:CB	1:E:259:ARG:NE	2.81	0.44
1:D:219:GLU:OE2	1:D:259:ARG:NH1	2.51	0.44
1:E:124:GLY:O	1:E:125:MET:CB	2.65	0.44
1:B:202:CYS:C	1:B:204:VAL:N	2.70	0.44
1:H:215:ALA:CB	1:H:259:ARG:NE	2.81	0.44
1:G:32:ASN:C	1:I:318:TYR:CD1	2.91	0.44
1:A:215:ALA:O	1:L:115:ASN:OD1	2.35	0.44
1:E:107:HIS:O	1:E:108:HIS:C	2.56	0.44
1:L:202:CYS:C	1:L:204:VAL:N	2.71	0.44
1:L:247:TYR:O	1:L:247:TYR:CG	2.70	0.44
1:A:183:PHE:CE2	1:A:214:ASP:OD2	2.70	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:145:LEU:O	1:H:146:PRO:O	2.36	0.44
1:G:215:ALA:CB	1:G:259:ARG:NE	2.81	0.43
1:I:145:LEU:O	1:I:146:PRO:O	2.36	0.43
1:G:124:GLY:O	1:G:125:MET:CB	2.67	0.43
1:B:232:LEU:O	1:B:234:GLU:N	2.50	0.43
1:C:183:PHE:CD1	1:C:214:ASP:OD2	2.71	0.43
1:C:219:GLU:OE2	1:C:259:ARG:NH1	2.51	0.43
1:J:247:TYR:O	1:J:248:PRO:O	2.36	0.43
1:L:174:THR:O	1:L:205:SER:OG	2.37	0.43
1:C:124:GLY:O	1:C:125:MET:CB	2.66	0.43
1:C:144:HIS:C	1:C:146:PRO:CD	2.86	0.43
1:F:145:LEU:O	1:F:146:PRO:O	2.37	0.43
1:K:215:ALA:CB	1:K:259:ARG:NE	2.82	0.43
1:D:210:LEU:CD1	1:D:211:VAL:CA	2.96	0.43
1:F:144:HIS:C	1:F:146:PRO:CD	2.86	0.43
1:A:318:TYR:CD1	1:B:32:ASN:C	2.92	0.43
1:I:302:ARG:NH1	1:I:302:ARG:CG	2.81	0.43
1:E:145:LEU:O	1:E:146:PRO:O	2.36	0.43
1:J:213:ASP:CG	1:J:213:ASP:O	2.56	0.43
1:L:144:HIS:C	1:L:146:PRO:CD	2.87	0.43
1:E:247:TYR:O	1:E:248:PRO:O	2.37	0.43
1:B:194:HIS:CE1	1:E:-8:SER:CB	3.02	0.43
1:L:124:GLY:O	1:L:125:MET:CB	2.67	0.43
1:A:213:ASP:O	1:A:213:ASP:CG	2.57	0.43
1:E:-7:GLY:O	1:E:-6:LEU:CB	2.66	0.43
1:I:247:TYR:O	1:I:247:TYR:CG	2.72	0.43
1:G:202:CYS:C	1:G:204:VAL:N	2.71	0.43
1:L:237:LEU:O	1:L:238:SER:C	2.57	0.43
1:K:144:HIS:C	1:K:146:PRO:CD	2.87	0.43
1:H:144:HIS:C	1:H:146:PRO:CD	2.87	0.43
1:A:124:GLY:O	1:A:125:MET:CB	2.66	0.43
1:J:302:ARG:CG	1:J:302:ARG:NH1	2.82	0.43
1:F:174:THR:O	1:F:205:SER:OG	2.36	0.43
1:J:215:ALA:CB	1:J:259:ARG:NE	2.82	0.42
1:B:209:PHE:N	1:B:209:PHE:CD1	2.87	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:J:144:HIS:C	1:J:146:PRO:CD	2.88	0.42
1:H:174:THR:O	1:H:205:SER:OG	2.38	0.42
1:J:1:MET:O	1:J:2:LYS:CB	2.67	0.42
1:F:124:GLY:O	1:F:125:MET:CB	2.67	0.42
1:L:215:ALA:CB	1:L:259:ARG:NE	2.83	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:215:ALA:CB	1:F:259:ARG:NE	2.83	0.42
1:H:247:TYR:O	1:H:247:TYR:CG	2.72	0.42
1:K:302:ARG:CG	1:K:302:ARG:NH1	2.81	0.42
1:D:174:THR:O	1:D:205:SER:OG	2.38	0.42
1:J:232:LEU:O	1:J:233:TYR:C	2.58	0.42
1:G:144:HIS:C	1:G:146:PRO:CD	2.88	0.42
1:G:247:TYR:O	1:G:247:TYR:CG	2.72	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:G:174:THR:O	1:G:205:SER:OG	2.38	0.42
1:L:145:LEU:O	1:L:146:PRO:O	2.36	0.42
1:I:202:CYS:C	1:I:204:VAL:N	2.73	0.42
1:D:1:MET:O	1:D:2:LYS:CB	2.67	0.42
1:A:95:ARG:NH2	2:A:341:SO4:S	2.93	0.42
1:L:1:MET:O	1:L:2:LYS:CB	2.67	0.42
1:D:145:LEU:O	1:D:146:PRO:O	2.38	0.42
1:A:297:ARG:CG	1:A:297:ARG:NH1	2.82	0.42
1:B:208:SER:C	1:B:209:PHE:CD1	2.93	0.42
1:B:1:MET:O	1:B:2:LYS:CB	2.68	0.42
1:C:202:CYS:C	1:C:204:VAL:N	2.73	0.42
1:A:151:LEU:C	1:A:153:ASP:N	2.73	0.41
1:A:145:LEU:N	1:A:146:PRO:CD	2.83	0.41
1:L:107:HIS:O	1:L:108:HIS:C	2.58	0.41
1:G:213:ASP:O	1:G:213:ASP:CG	2.58	0.41
1:B:88:ASP:OD1	1:C:274:ARG:NH2	2.53	0.41
1:I:124:GLY:O	1:I:125:MET:CB	2.68	0.41
1:B:210:LEU:CD1	1:B:211:VAL:CA	2.98	0.41
1:B:211:VAL:CG1	1:B:212:THR:N	2.80	0.41
1:L:232:LEU:O	1:L:233:TYR:C	2.58	0.41
1:B:144:HIS:C	1:B:146:PRO:CD	2.88	0.41
1:D:247:TYR:O	1:D:247:TYR:CG	2.73	0.41
1:E:1:MET:O	1:E:2:LYS:CB	2.69	0.41
1:B:103:ARG:NH2	2:B:341:SO4:O1	2.54	0.41
1:E:183:PHE:CE2	1:E:214:ASP:OD2	2.73	0.41
1:B:183:PHE:CE2	1:B:214:ASP:OD2	2.74	0.41
1:K:183:PHE:CE2	1:K:214:ASP:OD2	2.73	0.41
1:K:232:LEU:O	1:K:233:TYR:C	2.58	0.41
1:E:4:PRO:CG	1:E:6:VAL:CG2	2.99	0.41
1:J:32:ASN:C	1:L:318:TYR:CD1	2.94	0.41
1:I:174:THR:O	1:I:205:SER:OG	2.39	0.41
1:A:145:LEU:O	1:A:146:PRO:O	2.39	0.41
1:D:144:HIS:C	1:D:146:PRO:CD	2.89	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:302:ARG:NH1	1:D:302:ARG:CG	2.84	0.41
1:B:107:HIS:O	1:B:108:HIS:C	2.58	0.41
1:C:55:THR:OG1	2:C:340:SO4:O3	2.38	0.41
1:A:302:ARG:CG	1:A:302:ARG:NH1	2.84	0.41
1:I:213:ASP:CG	1:I:213:ASP:O	2.58	0.41
1:J:107:HIS:O	1:J:108:HIS:C	2.58	0.41
1:D:202:CYS:C	1:D:204:VAL:N	2.73	0.41
1:B:231:GLY:C	1:E:-11:HIS:CD2	2.92	0.41
1:F:219:GLU:OE2	1:F:259:ARG:NH1	2.54	0.41
1:D:232:LEU:O	1:D:233:TYR:C	2.59	0.41
1:A:232:LEU:O	1:A:233:TYR:C	2.58	0.41
1:E:202:CYS:C	1:E:204:VAL:N	2.73	0.41
1:F:236:GLU:O	1:F:237:LEU:C	2.59	0.41
1:H:202:CYS:C	1:H:204:VAL:N	2.74	0.41
1:C:174:THR:O	1:C:205:SER:OG	2.38	0.41
1:B:124:GLY:O	1:B:125:MET:CB	2.69	0.41
1:F:297:ARG:NH1	2:F:341:SO4:O3	2.54	0.41
1:K:1:MET:O	1:K:2:LYS:CB	2.69	0.41
1:J:183:PHE:CD1	1:J:214:ASP:OD2	2.74	0.41
1:D:247:TYR:O	1:D:248:PRO:O	2.39	0.41
1:E:297:ARG:NH1	1:E:297:ARG:CG	2.82	0.41
1:K:174:THR:O	1:K:205:SER:OG	2.39	0.41
1:L:302:ARG:CG	1:L:302:ARG:NH1	2.84	0.40
1:J:211:VAL:CG1	1:J:212:THR:N	2.84	0.40
1:D:251:GLN:CG	1:D:276:GLU:O	2.69	0.40
1:D:213:ASP:O	1:D:213:ASP:CG	2.60	0.40
1:B:232:LEU:CD1	1:B:232:LEU:N	2.85	0.40
1:C:82:GLY:C	1:C:84:GLU:N	2.74	0.40
1:B:-9:SER:CB	1:E:194:HIS:CE1	3.05	0.40
1:F:159:VAL:CB	1:F:183:PHE:CE2	3.05	0.40
1:L:297:ARG:NH1	2:L:341:SO4:O1	2.54	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:D:53:THR:OG1	1:F:79:GLN:CG	2.69	0.40
1:B:229:TRP:O	1:B:230:TYR:C	2.60	0.40
1:A:215:ALA:CB	1:L:115:ASN:CB	3.00	0.40
1:K:202:CYS:C	1:K:204:VAL:N	2.74	0.40
1:B:174:THR:O	1:B:205:SER:OG	2.39	0.40
1:A:107:HIS:O	1:A:108:HIS:C	2.58	0.40
1:D:191:ASN:CB	1:H:186:GLU:CG	2.99	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	Distance(Å)	Clash(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

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/359 (93%)	288 (86%)	25 (8%)	20 (6%)	2	20
1	B	351/359 (98%)	303 (86%)	26 (7%)	22 (6%)	2	18
1	C	338/359 (94%)	288 (85%)	27 (8%)	23 (7%)	2	15
1	D	345/359 (96%)	295 (86%)	32 (9%)	18 (5%)	3	25
1	E	339/359 (94%)	294 (87%)	26 (8%)	19 (6%)	3	23
1	F	338/359 (94%)	291 (86%)	29 (9%)	18 (5%)	3	24
1	G	339/359 (94%)	291 (86%)	27 (8%)	21 (6%)	2	19
1	H	332/359 (92%)	283 (85%)	32 (10%)	17 (5%)	3	25
1	I	328/359 (91%)	286 (87%)	25 (8%)	17 (5%)	3	25
1	J	339/359 (94%)	290 (86%)	29 (9%)	20 (6%)	2	20
1	K	339/359 (94%)	293 (86%)	26 (8%)	20 (6%)	2	20
1	L	339/359 (94%)	289 (85%)	32 (9%)	18 (5%)	3	24
All	All	4060/4308 (94%)	3491 (86%)	336 (8%)	233 (6%)	3	22

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	4	18
1	B	302/313 (96%)	252 (83%)	50 (17%)	3	14
1	C	289/313 (92%)	245 (85%)	44 (15%)	4	19
1	D	294/313 (94%)	250 (85%)	44 (15%)	4	19
1	E	296/313 (95%)	255 (86%)	41 (14%)	5	24
1	F	291/313 (93%)	245 (84%)	46 (16%)	4	16
1	G	289/313 (92%)	245 (85%)	44 (15%)	4	19
1	H	288/313 (92%)	244 (85%)	44 (15%)	4	18
1	I	286/313 (91%)	243 (85%)	43 (15%)	4	19
1	J	287/313 (92%)	242 (84%)	45 (16%)	4	17
1	K	288/313 (92%)	243 (84%)	45 (16%)	4	17
1	L	292/313 (93%)	248 (85%)	44 (15%)	4	19
All	All	3490/3756 (93%)	2956 (85%)	534 (15%)	4	18

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
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

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Mol	Chain	Res	Type
1	A	301	ILE
1	A	302	ARG
1	B	-13	HIS
1	B	-12	HIS
1	B	-3	ARG
1	B	0	HIS
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

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Mol	Chain	Res	Type
1	B	238	SER
1	B	239	GLU
1	B	240	GLU
1	B	245	VAL
1	B	256	MET
1	B	259	ARG
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

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Mol	Chain	Res	Type
1	C	217	SER
1	C	225	TYR
1	C	237	LEU
1	C	239	GLU
1	C	240	GLU
1	C	245	VAL
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

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Mol	Chain	Res	Type
1	D	192	GLU
1	D	210	LEU
1	D	212	THR
1	D	217	SER
1	D	225	TYR
1	D	239	GLU
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

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Mol	Chain	Res	Type
1	E	210	LEU
1	E	212	THR
1	E	217	SER
1	E	225	TYR
1	E	239	GLU
1	E	240	GLU
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

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Mol	Chain	Res	Type
1	F	181	VAL
1	F	183	PHE
1	F	192	GLU
1	F	210	LEU
1	F	212	THR
1	F	217	SER
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

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Mol	Chain	Res	Type
1	G	175	LYS
1	G	181	VAL
1	G	183	PHE
1	G	192	GLU
1	G	210	LEU
1	G	211	VAL
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

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Mol	Chain	Res	Type
1	H	150	LYS
1	H	164	GLN
1	H	168	SER
1	H	169	LEU
1	H	175	LYS
1	H	181	VAL
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

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Mol	Chain	Res	Type
1	I	132	THR
1	I	138	LEU
1	I	147	GLU
1	I	150	LYS
1	I	151	LEU
1	I	164	GLN
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

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Mol	Chain	Res	Type
1	J	118	THR
1	J	130	HIS
1	J	132	THR
1	J	138	LEU
1	J	147	GLU
1	J	150	LYS
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

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Mol	Chain	Res	Type
1	K	106	ARG
1	K	110	ILE
1	K	118	THR
1	K	130	HIS
1	K	132	THR
1	K	138	LEU
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

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Mol	Chain	Res	Type
1	L	92	VAL
1	L	93	LEU
1	L	103	ARG
1	L	105	GLU
1	L	106	ARG
1	L	110	ILE
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. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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	0.16	0	6,6,6	0.29	0
2	SO4	A	341	-	4,4,4	0.12	0	6,6,6	0.35	0
2	SO4	B	340	-	4,4,4	0.21	0	6,6,6	0.40	0
2	SO4	B	341	-	4,4,4	0.24	0	6,6,6	0.41	0
2	SO4	B	342	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	C	340	-	4,4,4	0.12	0	6,6,6	0.13	0
2	SO4	C	341	-	4,4,4	0.17	0	6,6,6	0.17	0
2	SO4	D	340	-	4,4,4	0.32	0	6,6,6	0.47	0
2	SO4	D	341	-	4,4,4	0.18	0	6,6,6	0.13	0
2	SO4	E	340	-	4,4,4	0.05	0	6,6,6	0.21	0
2	SO4	E	341	-	4,4,4	0.17	0	6,6,6	0.14	0
2	SO4	E	342	-	4,4,4	0.12	0	6,6,6	0.28	0
2	SO4	F	340	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	F	341	-	4,4,4	0.09	0	6,6,6	0.23	0
2	SO4	G	340	-	4,4,4	0.27	0	6,6,6	0.28	0
2	SO4	G	341	-	4,4,4	0.16	0	6,6,6	0.22	0
2	SO4	G	342	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	H	340	-	4,4,4	0.18	0	6,6,6	0.29	0
2	SO4	H	341	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	I	340	-	4,4,4	0.13	0	6,6,6	0.08	0
2	SO4	I	341	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	J	340	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	J	341	-	4,4,4	0.16	0	6,6,6	0.18	0
2	SO4	K	340	-	4,4,4	0.24	0	6,6,6	0.61	0
2	SO4	L	340	-	4,4,4	0.22	0	6,6,6	0.25	0
2	SO4	L	341	-	4,4,4	0.11	0	6,6,6	0.12	0
2	SO4	L	342	-	4,4,4	0.15	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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 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%)	-0.15	0 100 100	41, 74, 137, 219	0
1	B	353/359 (98%)	0.00	5 (1%) 72 22	39, 69, 144, 211	0
1	C	340/359 (94%)	-0.02	4 (1%) 75 26	43, 75, 141, 207	0
1	D	347/359 (96%)	-0.12	0 100 100	40, 74, 137, 208	0
1	E	343/359 (95%)	-0.17	1 (0%) 91 58	34, 67, 127, 209	0
1	F	340/359 (94%)	0.02	3 (0%) 81 32	38, 82, 147, 224	0
1	G	341/359 (94%)	-0.05	1 (0%) 91 58	46, 76, 144, 209	0
1	H	336/359 (93%)	-0.04	1 (0%) 91 58	44, 80, 141, 208	0
1	I	332/359 (92%)	-0.04	1 (0%) 91 58	44, 76, 136, 208	0
1	J	341/359 (94%)	-0.00	3 (0%) 81 32	46, 81, 147, 224	0
1	K	341/359 (94%)	-0.08	2 (0%) 86 41	46, 80, 148, 210	0
1	L	341/359 (94%)	0.00	3 (0%) 81 32	38, 79, 149, 238	0
All	All	4092/4308 (94%)	-0.05	24 (0%) 86 41	34, 76, 144, 238	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	GLU	5.2
1	C	234	GLU	3.3
1	B	233	TYR	3.2
1	B	79	GLN	3.2
1	J	234	GLU	3.1
1	B	231	GLY	3.0
1	J	81	GLY	2.7
1	C	232	LEU	2.5
1	G	246	PHE	2.4
1	L	82	GLY	2.4
1	F	83	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	225	TYR	2.3
1	I	215	ALA	2.3
1	J	232	LEU	2.2
1	K	81	GLY	2.2
1	L	211	VAL	2.2
1	C	233	TYR	2.2
1	E	215	ALA	2.2
1	L	79	GLN	2.2
1	F	234	GLU	2.1
1	C	235	ALA	2.0
1	K	225	TYR	2.0
1	B	77	GLN	2.0
1	F	224	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	A	340	5/5	0.41	7.44	105,110,199,203	0
2	SO4	E	342	5/5	0.33	2.49	133,143,177,213	0
2	SO4	E	341	5/5	0.27	2.14	70,86,138,148	0
2	SO4	G	340	5/5	0.29	1.94	71,84,109,111	0
2	SO4	K	340	5/5	0.31	1.93	103,105,182,190	0
2	SO4	J	340	5/5	0.28	1.45	127,150,178,179	0
2	SO4	A	341	5/5	0.22	1.42	83,129,161,178	0
2	SO4	D	340	5/5	0.26	1.30	52,115,167,222	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	H	340	5/5	0.22	0.96	142,151,175,178	0
2	SO4	L	340	5/5	0.35	0.85	63,83,85,137	0
2	SO4	C	340	5/5	0.22	0.72	64,118,199,217	0
2	SO4	F	341	5/5	0.23	0.55	59,123,192,197	0
2	SO4	G	342	5/5	0.20	0.55	112,127,168,206	0
2	SO4	I	340	5/5	0.23	0.44	97,135,192,204	0
2	SO4	L	342	5/5	0.30	0.41	129,163,183,197	0
2	SO4	B	341	5/5	0.27	0.38	61,66,126,155	0
2	SO4	I	341	5/5	0.23	0.22	131,176,179,182	0
2	SO4	J	341	5/5	0.31	0.15	42,180,185,214	0
2	SO4	B	342	5/5	0.27	-0.05	115,143,184,221	0
2	SO4	E	340	5/5	0.21	-0.14	86,112,144,146	0
2	SO4	C	341	5/5	0.28	-0.16	159,176,191,193	0
2	SO4	G	341	5/5	0.18	-0.59	134,152,174,175	0
2	SO4	L	341	5/5	0.19	-0.77	101,122,174,199	0
2	SO4	D	341	5/5	0.18	-0.97	61,140,158,170	0
2	SO4	B	340	5/5	0.27	-1.26	56,90,126,172	0
2	SO4	H	341	5/5	0.13	-1.37	68,151,194,196	0
2	SO4	F	340	5/5	0.14	-1.61	102,138,146,182	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.