



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 02:58 pm BST

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

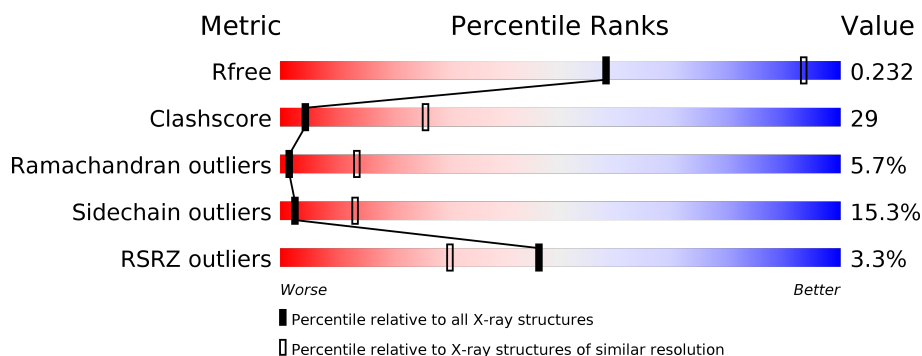
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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></div> <div>50% 32% 12% • 6%</div> </div>
1	B	359	<div> <div>2%</div> <div>51% 33% 13% • •</div> </div>
1	C	359	<div> <div>2%</div> <div>51% 31% 12% • 5%</div> </div>
1	D	359	<div> <div>0%</div> <div>53% 32% 11% • •</div> </div>
1	E	359	<div> <div>0%</div> <div>52% 32% 11% • •</div> </div>
1	F	359	<div> <div>7%</div> <div>52% 31% 11% • 5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain				
1	G	359	6%	50%	33%	11%	5%
1	H	359	5%	51%	31%	11%	6%
1	I	359	2%	50%	31%	10%	8%
1	J	359	6%	50%	33%	12%	5%
1	K	359	3%	49%	34%	11%	5%
1	L	359	3%	52%	31%	11%	5%

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

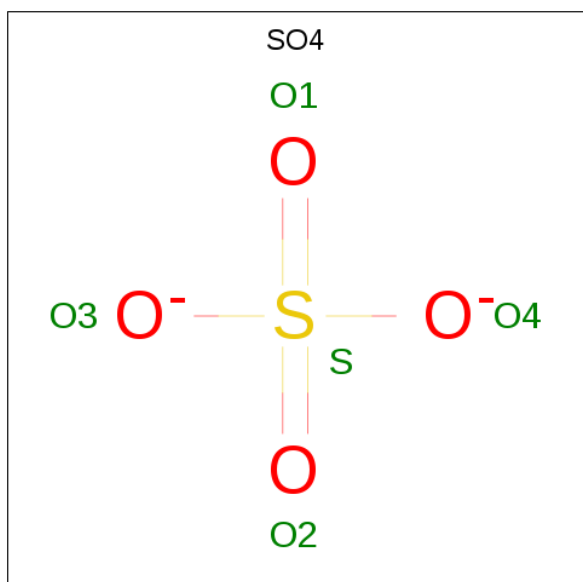
Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	EXPRESSION TAG	UNP Q837U7
I	-5	VAL	-	EXPRESSION TAG	UNP Q837U7
I	-4	PRO	-	EXPRESSION TAG	UNP Q837U7
I	-3	ARG	-	EXPRESSION TAG	UNP Q837U7
I	-2	GLY	-	EXPRESSION TAG	UNP Q837U7
I	-1	SER	-	EXPRESSION TAG	UNP Q837U7
I	0	HIS	-	EXPRESSION TAG	UNP Q837U7
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

Continued on next page...

Continued from previous page...

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: O₄S).



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

Continued on next page...

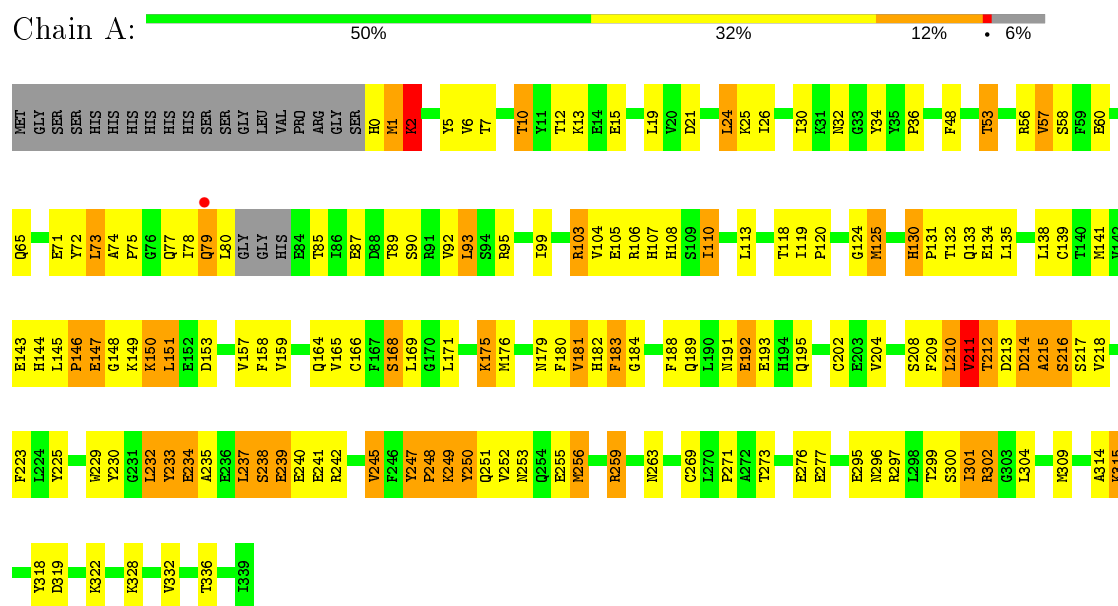
Continued from previous page...

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

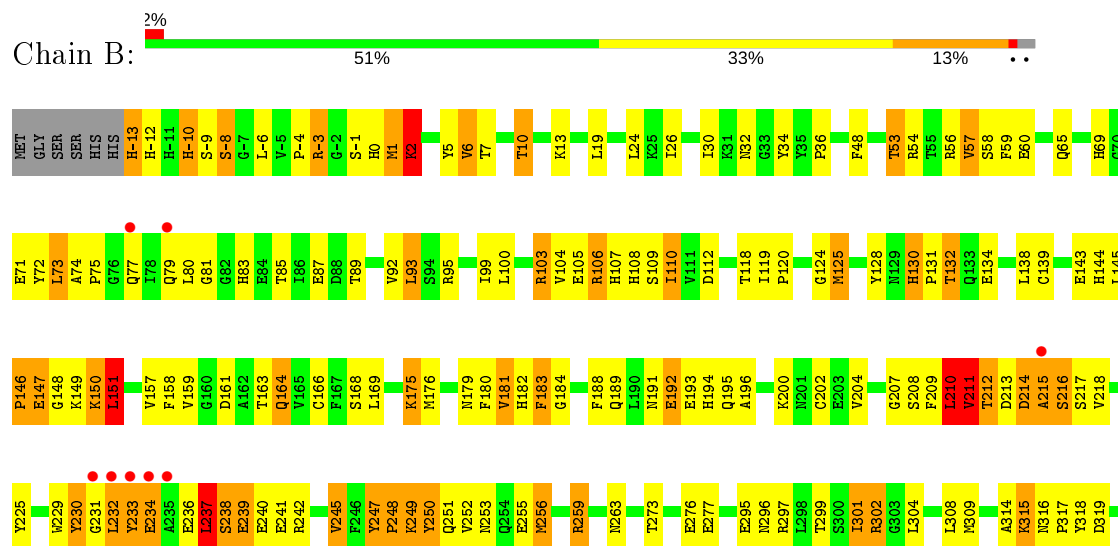
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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

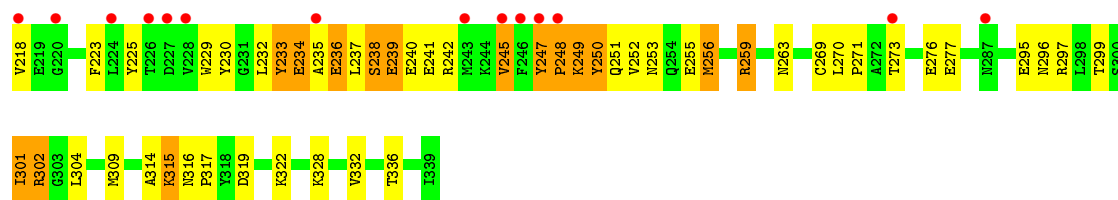


• Molecule 1: Putrescine carbamoyltransferase

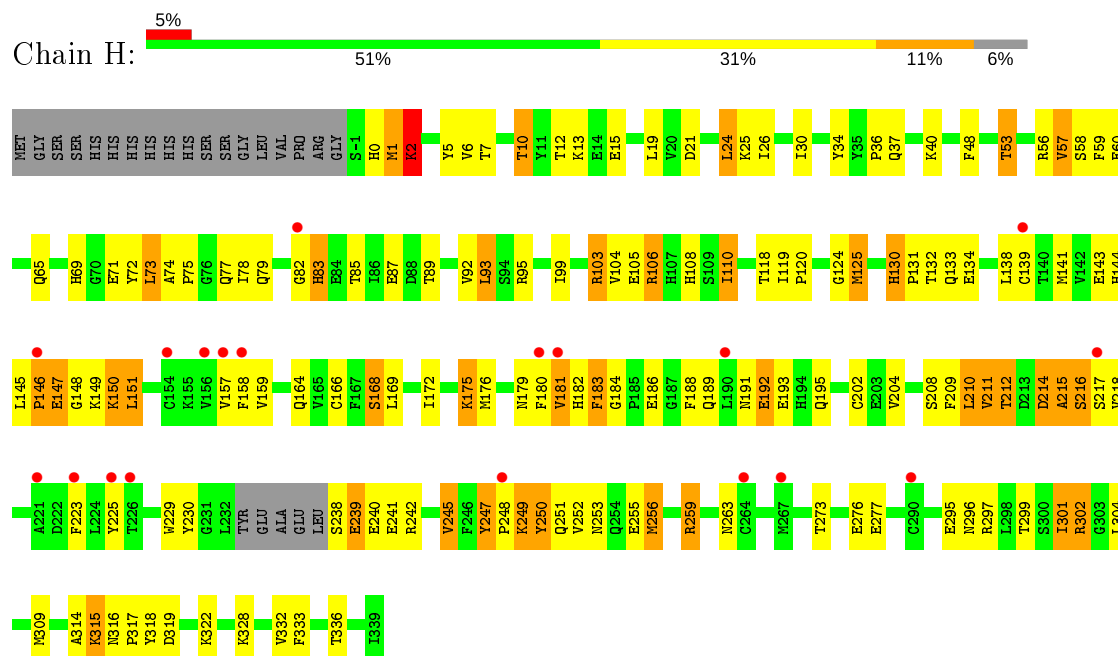




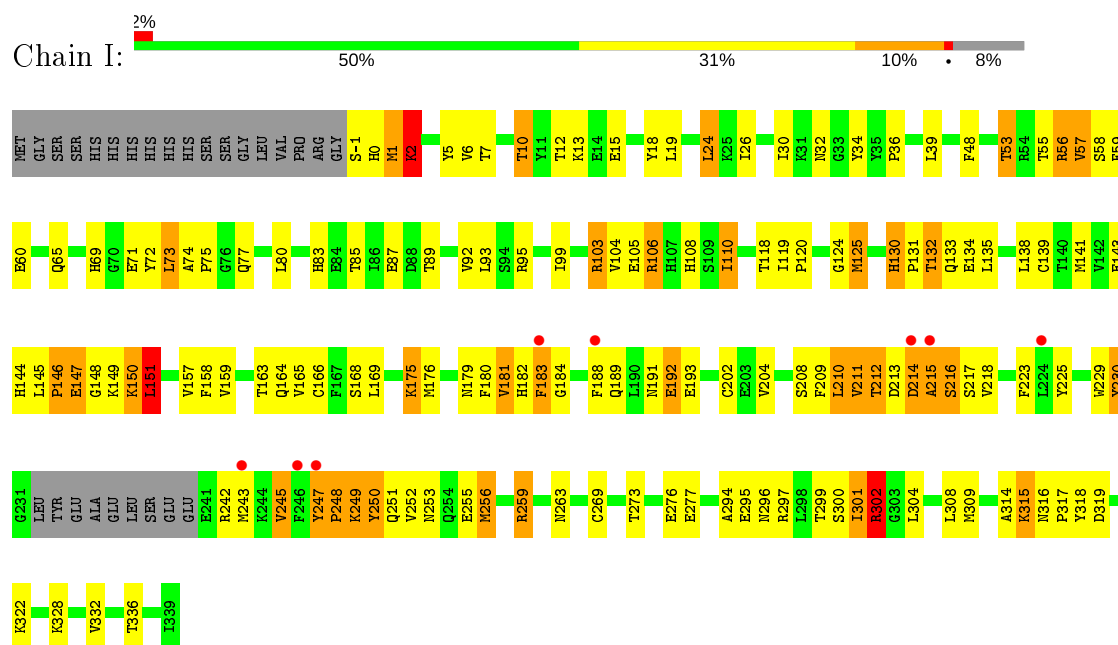




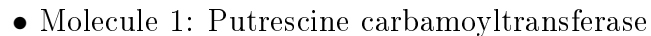
• Molecule 1: Putrescine carbamoyltransferase

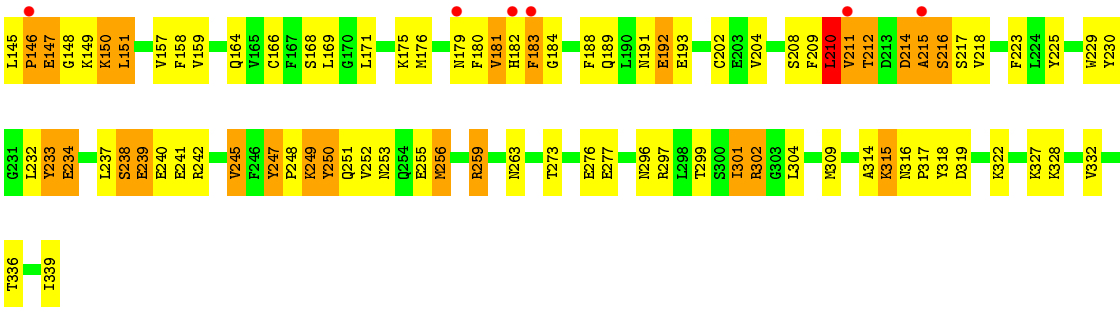


• Molecule 1: Putrescine carbamoyltransferase



• Molecule 1: Putrescine carbamoyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.190 , 0.234 0.183 , 0.232	Depositor DCC
R_{free} test set	2000 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32142	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The worst 5 of 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

There are no chirality outliers.

5 of 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

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

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%)	1	12
1	B	351/359 (98%)	303 (86%)	26 (7%)	22 (6%)	1	10
1	C	338/359 (94%)	288 (85%)	27 (8%)	23 (7%)	1	9
1	D	345/359 (96%)	295 (86%)	32 (9%)	18 (5%)	2	15
1	E	339/359 (94%)	294 (87%)	26 (8%)	19 (6%)	2	14
1	F	338/359 (94%)	291 (86%)	29 (9%)	18 (5%)	2	15
1	G	339/359 (94%)	291 (86%)	27 (8%)	21 (6%)	1	11
1	H	332/359 (92%)	283 (85%)	32 (10%)	17 (5%)	2	15
1	I	328/359 (91%)	286 (87%)	25 (8%)	17 (5%)	2	15
1	J	339/359 (94%)	290 (86%)	29 (9%)	20 (6%)	1	12
1	K	339/359 (94%)	293 (86%)	26 (8%)	20 (6%)	1	12
1	L	339/359 (94%)	289 (85%)	32 (9%)	18 (5%)	2	15
All	All	4060/4308 (94%)	3491 (86%)	336 (8%)	233 (6%)	1	14

5 of 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

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%)	2	13
1	B	302/313 (96%)	252 (83%)	50 (17%)	2	10
1	C	289/313 (92%)	245 (85%)	44 (15%)	3	13
1	D	294/313 (94%)	250 (85%)	44 (15%)	3	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	296/313 (95%)	255 (86%)	41 (14%)	3	16
1	F	291/313 (93%)	245 (84%)	46 (16%)	2	12
1	G	289/313 (92%)	245 (85%)	44 (15%)	3	13
1	H	288/313 (92%)	244 (85%)	44 (15%)	2	13
1	I	286/313 (91%)	243 (85%)	43 (15%)	3	14
1	J	287/313 (92%)	242 (84%)	45 (16%)	2	12
1	K	288/313 (92%)	243 (84%)	45 (16%)	2	12
1	L	292/313 (93%)	248 (85%)	44 (15%)	3	14
All	All	3490/3756 (93%)	2956 (85%)	534 (15%)	2	13

5 of 534 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	110	ILE
1	G	210	LEU
1	L	6	VAL
1	F	159	VAL
1	G	6	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	50	GLN
1	E	108	HIS
1	I	50	GLN
1	E	-11	HIS
1	H	50	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	B	342	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	I	340	-	4,4,4	0.17	0	6,6,6	0.08	0
2	SO4	B	341	-	4,4,4	0.08	0	6,6,6	0.32	0
2	SO4	I	341	-	4,4,4	0.15	0	6,6,6	0.21	0
2	SO4	F	340	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	A	341	-	4,4,4	0.15	0	6,6,6	0.34	0
2	SO4	L	342	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	J	341	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	D	341	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	F	341	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	E	340	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	B	340	-	4,4,4	0.11	0	6,6,6	0.42	0
2	SO4	A	340	-	4,4,4	0.11	0	6,6,6	0.28	0
2	SO4	C	341	-	4,4,4	0.12	0	6,6,6	0.12	0
2	SO4	E	341	-	4,4,4	0.19	0	6,6,6	0.23	0
2	SO4	L	341	-	4,4,4	0.12	0	6,6,6	0.09	0
2	SO4	E	342	-	4,4,4	0.10	0	6,6,6	0.28	0
2	SO4	H	341	-	4,4,4	0.11	0	6,6,6	0.13	0
2	SO4	G	341	-	4,4,4	0.09	0	6,6,6	0.19	0
2	SO4	J	340	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	L	340	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	K	340	-	4,4,4	0.26	0	6,6,6	0.33	0
2	SO4	D	340	-	4,4,4	0.14	0	6,6,6	0.43	0
2	SO4	C	340	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	G	342	-	4,4,4	0.16	0	6,6,6	0.17	0
2	SO4	H	340	-	4,4,4	0.17	0	6,6,6	0.16	0
2	SO4	G	340	-	4,4,4	0.16	0	6,6,6	0.35	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	B	342	SO4	1	0
2	B	341	SO4	1	0
2	I	341	SO4	1	0
2	A	341	SO4	1	0
2	L	342	SO4	1	0
2	F	341	SO4	1	0
2	L	341	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 [i](#)

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

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, 95th 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 ²)	Q<0.9
1	A	337/359 (93%)	-0.11	1 (0%) 94 92	41, 74, 137, 219	0
1	B	353/359 (98%)	-0.02	8 (2%) 60 47	39, 69, 144, 211	0
1	C	340/359 (94%)	-0.03	7 (2%) 63 49	43, 75, 141, 207	0
1	D	347/359 (96%)	-0.08	3 (0%) 84 75	40, 74, 137, 208	0
1	E	343/359 (95%)	-0.09	3 (0%) 84 75	34, 67, 127, 209	0
1	F	340/359 (94%)	0.21	26 (7%) 13 7	38, 82, 147, 224	0
1	G	341/359 (94%)	0.16	23 (6%) 17 10	46, 76, 144, 209	0
1	H	336/359 (93%)	0.21	19 (5%) 23 13	44, 80, 141, 208	0
1	I	332/359 (92%)	-0.01	8 (2%) 59 44	44, 76, 136, 208	0
1	J	341/359 (94%)	0.11	21 (6%) 20 11	46, 81, 147, 224	0
1	K	341/359 (94%)	0.04	9 (2%) 56 40	46, 80, 148, 210	0
1	L	341/359 (94%)	-0.00	9 (2%) 56 40	38, 79, 149, 238	0
All	All	4092/4308 (94%)	0.03	137 (3%) 46 30	34, 76, 144, 238	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	GLU	5.3
1	B	231	GLY	4.6
1	J	81	GLY	4.5
1	B	233	TYR	4.5
1	G	218	VAL	4.4

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	SO4	B	342	5/5	0.74	0.30	115,143,184,221	0
2	SO4	A	340	5/5	0.78	0.33	105,110,199,203	0
2	SO4	E	342	5/5	0.80	0.26	133,143,177,213	0
2	SO4	H	340	5/5	0.81	0.28	142,151,175,178	0
2	SO4	A	341	5/5	0.82	0.24	83,129,161,178	0
2	SO4	K	340	5/5	0.82	0.34	103,105,182,190	0
2	SO4	I	341	5/5	0.82	0.27	131,176,179,182	0
2	SO4	D	340	5/5	0.83	0.26	52,115,167,222	0
2	SO4	I	340	5/5	0.85	0.21	97,135,192,204	0
2	SO4	L	342	5/5	0.86	0.30	129,163,183,197	0
2	SO4	F	341	5/5	0.89	0.25	59,123,192,197	0
2	SO4	J	340	5/5	0.90	0.19	127,150,178,179	0
2	SO4	E	340	5/5	0.91	0.24	86,112,144,146	0
2	SO4	G	341	5/5	0.91	0.17	134,152,174,175	0
2	SO4	J	341	5/5	0.92	0.22	42,180,185,214	0
2	SO4	C	340	5/5	0.92	0.22	64,118,199,217	0
2	SO4	C	341	5/5	0.92	0.24	159,176,191,193	0
2	SO4	D	341	5/5	0.93	0.21	61,140,158,170	0
2	SO4	F	340	5/5	0.93	0.15	102,138,146,182	0
2	SO4	B	340	5/5	0.94	0.25	56,90,126,172	0
2	SO4	B	341	5/5	0.94	0.26	61,66,126,155	0
2	SO4	H	341	5/5	0.95	0.14	68,151,194,196	0
2	SO4	G	340	5/5	0.95	0.33	71,84,109,111	0
2	SO4	G	342	5/5	0.96	0.20	112,127,168,206	0
2	SO4	L	341	5/5	0.96	0.18	101,122,174,199	0
2	SO4	E	341	5/5	0.96	0.24	70,86,138,148	0
2	SO4	L	340	5/5	0.98	0.34	63,83,85,137	0

6.5 Other polymers [i](#)

There are no such residues in this entry.