



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 3TXX / pdb_00003txx
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

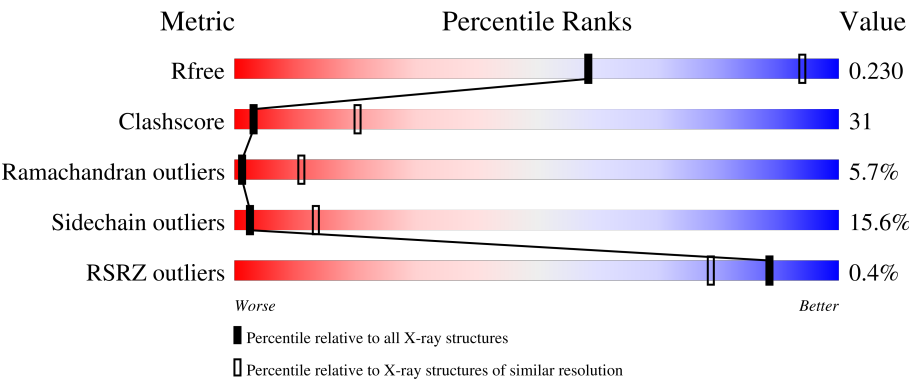
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 of 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	% 48%32%13%6%
1	B	359	% 48%35%14%..
1	C	359	48%33%12%5%
1	D	359	% 49%34%12%..
1	E	359	50%32%12%..

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Mol	Chain	Length	Quality of chain
1	F	359	51%31%12%5%
1	G	359	48%34%11%5%
1	H	359	49%33%11%6%
1	I	359	%48%33%11%8%
1	J	359	49%33%11%5%
1	K	359	49%34%11%5%
1	L	359	51%31%12%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

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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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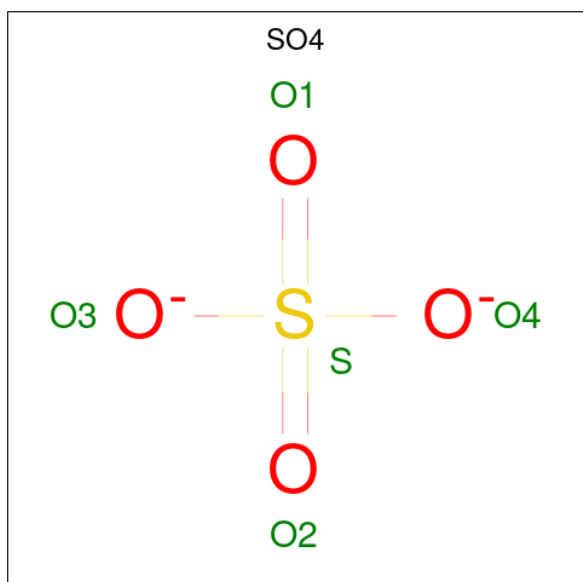
Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	expression tag	UNP Q837U7
I	-5	VAL	-	expression tag	UNP Q837U7
I	-4	PRO	-	expression tag	UNP Q837U7
I	-3	ARG	-	expression tag	UNP Q837U7
I	-2	GLY	-	expression tag	UNP Q837U7
I	-1	SER	-	expression tag	UNP Q837U7
I	0	HIS	-	expression tag	UNP Q837U7
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 (CCD ID: 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		

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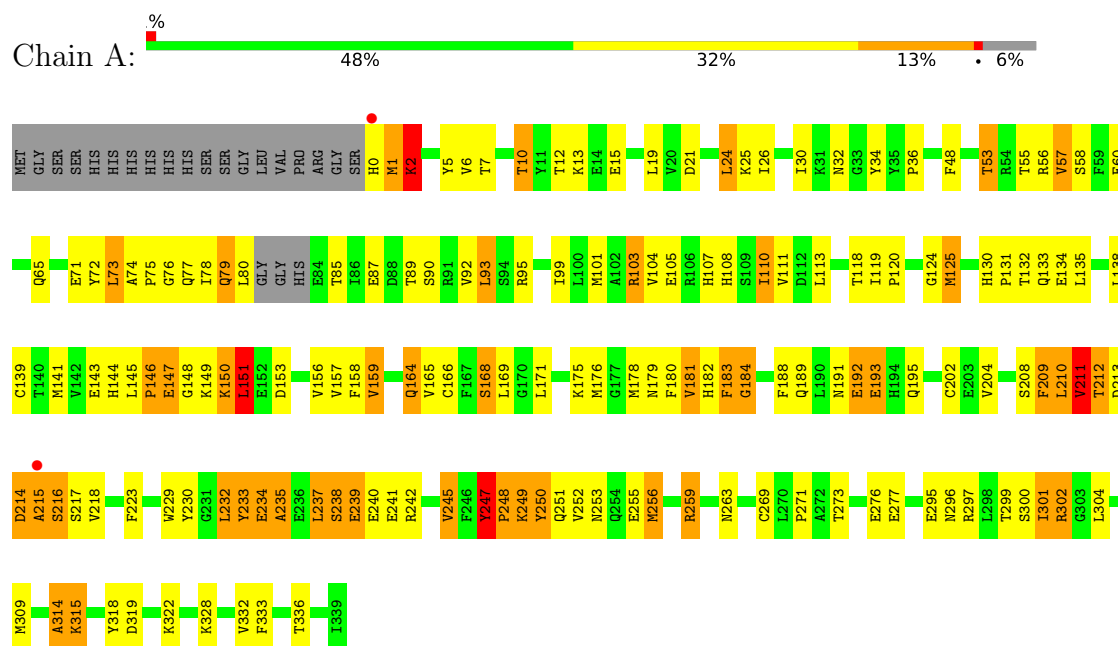
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

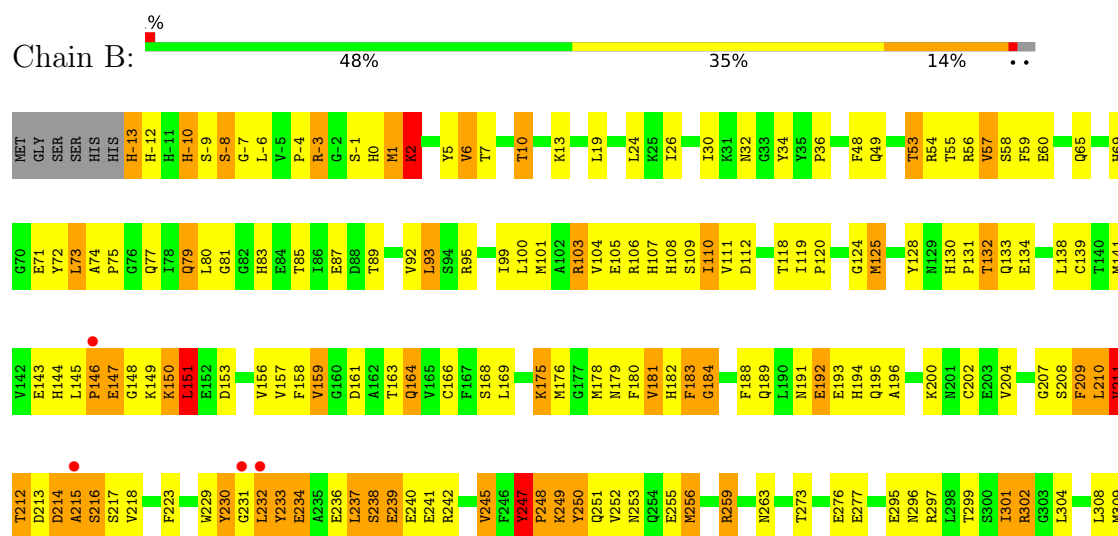
3 Residue-property plots

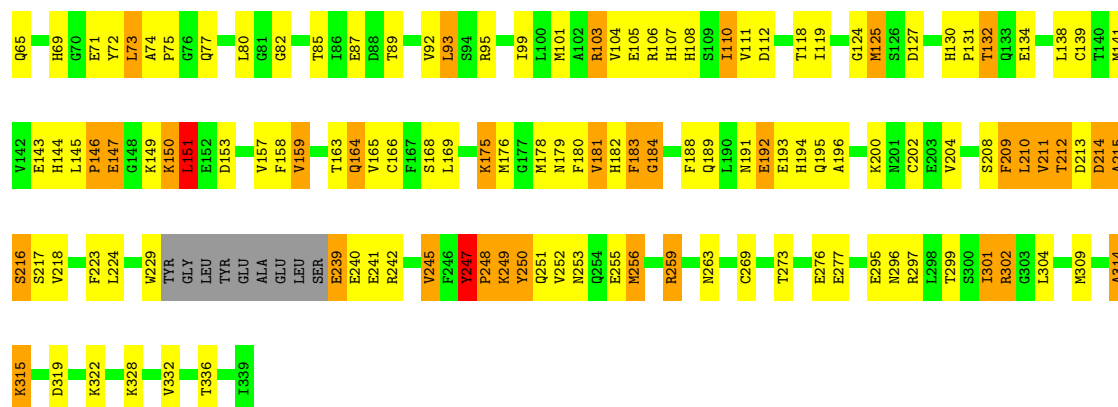
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Putrescine carbamoyltransferase



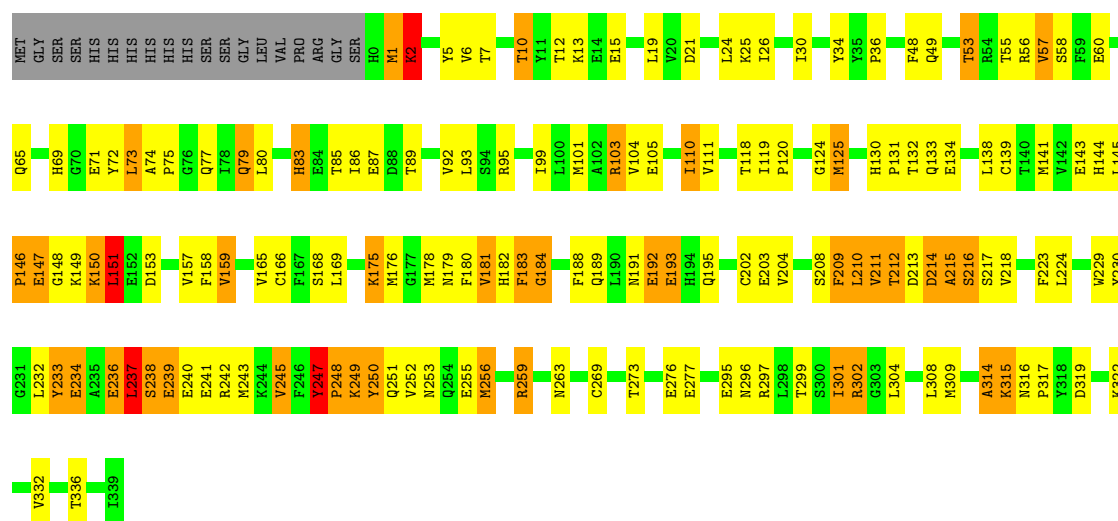
• Molecule 1: Putrescine carbamoyltransferase





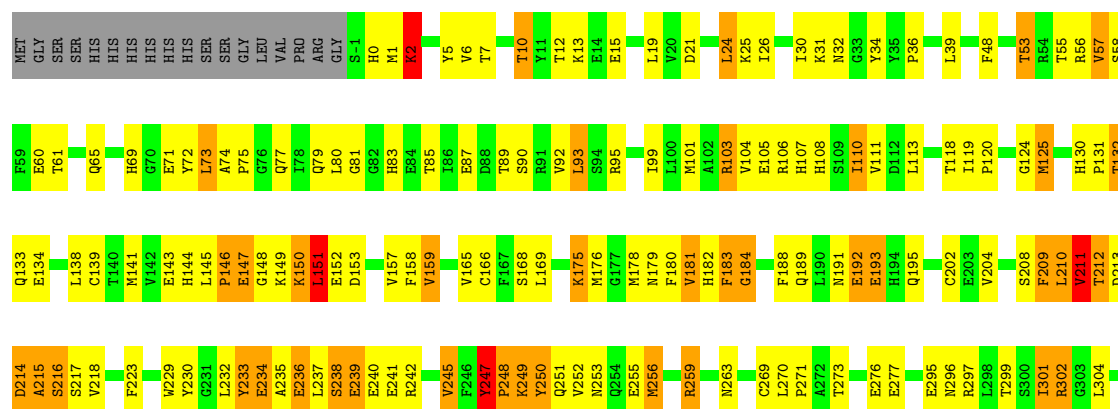
• Molecule 1: Putrescine carbamoyltransferase

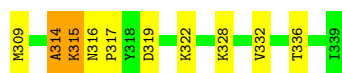
Chain F: 51% 31% 12% • 5%



• Molecule 1: Putrescine carbamoyltransferase

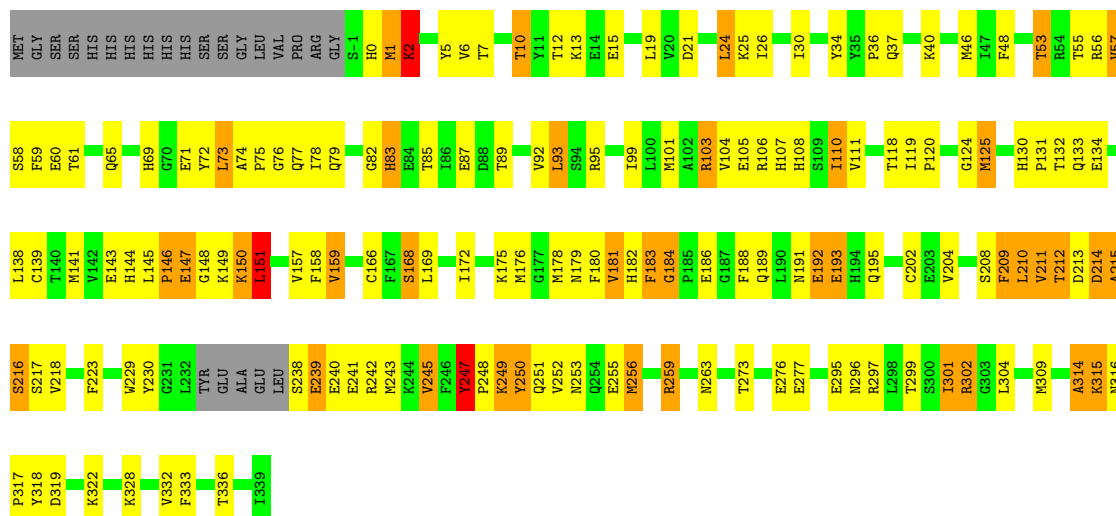
Chain G: 48% 34% 11% • 5%





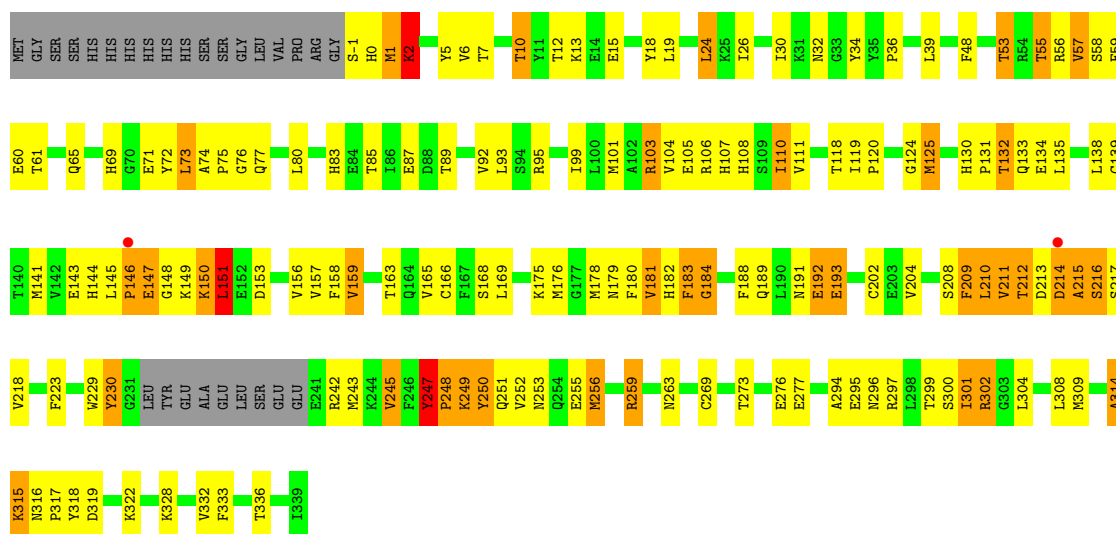
• Molecule 1: Putrescine carbamoyltransferase

Chain H: 49% 33% 11% • 6%



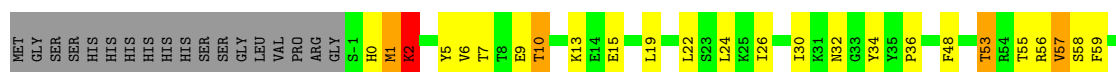
• Molecule 1: Putrescine carbamoyltransferase

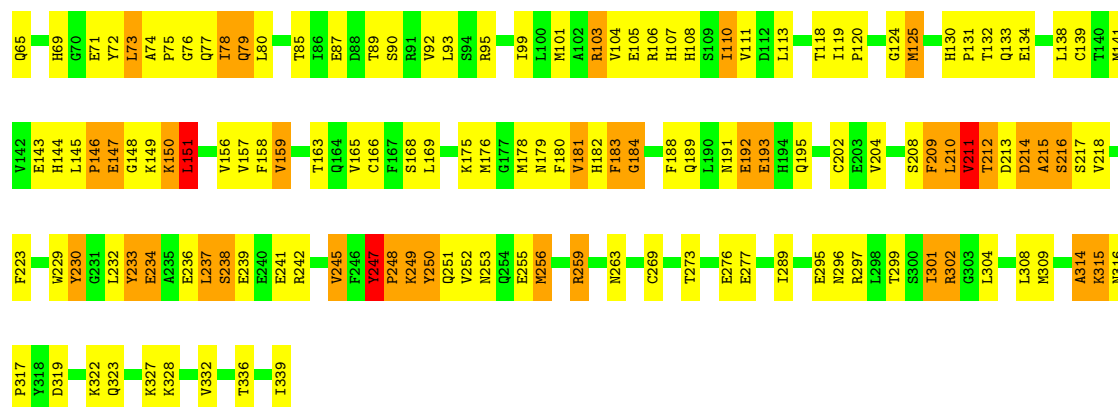
Chain I: 48% 33% 11% • 8%



• Molecule 1: Putrescine carbamoyltransferase

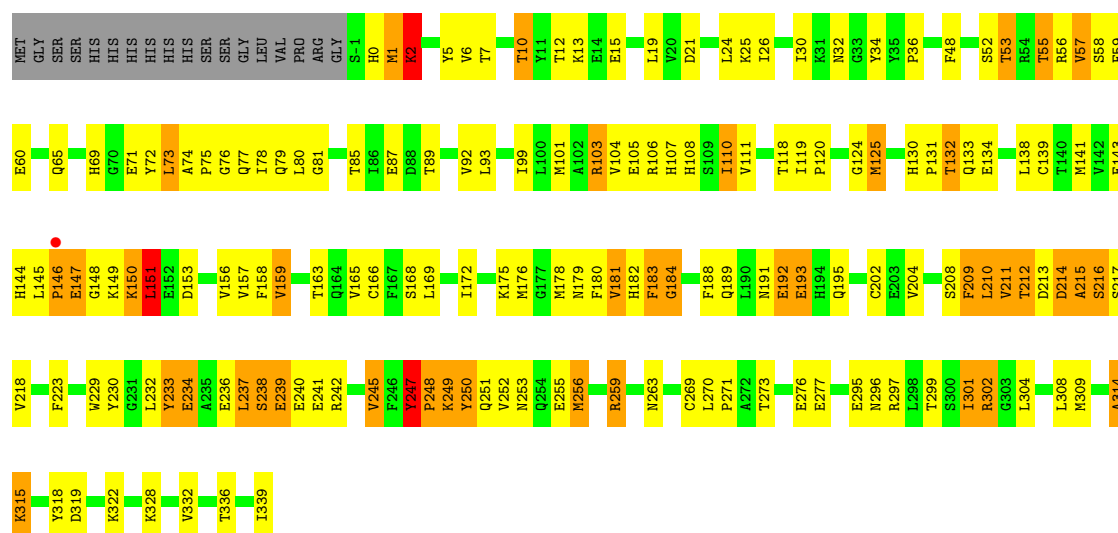
Chain J: 49% 33% 11% • 5%





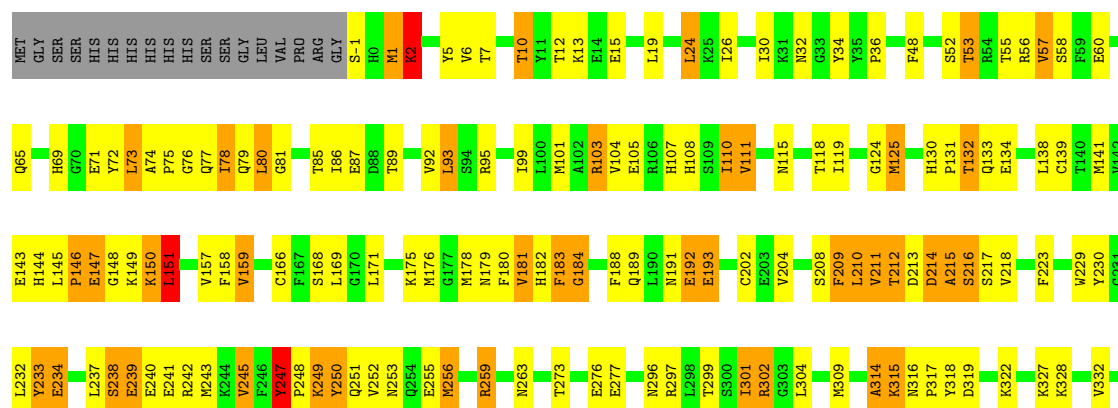
• Molecule 1: Putrescine carbamoyltransferase

Chain K: 49% 34% 11% • 5%



• Molecule 1: Putrescine carbamoyltransferase

Chain L: 51% 31% 12% • 5%





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 48.17 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (48.17-3.20) 91.5 (48.17-3.20)	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 0.180 , 0.230	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)	0.32 , 91.7	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	0.59	0/2687	0.95	7/3626 (0.2%)
1	B	0.65	0/2818	0.99	9/3803 (0.2%)
1	C	0.56	0/2705	0.94	7/3650 (0.2%)
1	D	0.63	0/2755	0.99	11/3718 (0.3%)
1	E	0.67	0/2743	1.02	10/3699 (0.3%)
1	F	0.55	0/2710	0.94	9/3656 (0.2%)
1	G	0.54	0/2706	0.93	6/3651 (0.2%)
1	H	0.53	0/2676	0.93	6/3608 (0.2%)
1	I	0.54	0/2651	0.94	6/3574 (0.2%)
1	J	0.54	0/2697	0.92	6/3640 (0.2%)
1	K	0.55	0/2702	0.93	6/3646 (0.2%)
1	L	0.56	0/2718	0.94	6/3667 (0.2%)
All	All	0.58	0/32568	0.95	89/43938 (0.2%)

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 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	-5	VAL	CA-C-N	10.95	130.91	119.85
1	E	-5	VAL	C-N-CA	10.95	130.91	119.85
1	F	236	GLU	N-CA-C	-10.13	100.07	111.71
1	D	209	PHE	N-CA-C	9.33	122.70	108.52
1	H	209	PHE	N-CA-C	9.32	122.68	108.52

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	181	0
1	B	2766	0	2678	225	0
1	C	2659	0	2575	176	0
1	D	2707	0	2625	173	0
1	E	2694	0	2614	217	0
1	F	2664	0	2586	157	2
1	G	2660	0	2569	158	0
1	H	2631	0	2549	149	0
1	I	2606	0	2536	153	0
1	J	2651	0	2564	166	0
1	K	2656	0	2563	160	2
1	L	2671	0	2592	171	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

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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	1961	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 31.

The worst 5 of 1961 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	10
1	B	351/359 (98%)	303 (86%)	26 (7%)	22 (6%)	1	8
1	C	338/359 (94%)	288 (85%)	27 (8%)	23 (7%)	1	7
1	D	345/359 (96%)	295 (86%)	32 (9%)	18 (5%)	1	12
1	E	339/359 (94%)	294 (87%)	26 (8%)	19 (6%)	1	11
1	F	338/359 (94%)	291 (86%)	29 (9%)	18 (5%)	1	12
1	G	339/359 (94%)	291 (86%)	27 (8%)	21 (6%)	1	9
1	H	332/359 (92%)	283 (85%)	32 (10%)	17 (5%)	1	13
1	I	328/359 (91%)	286 (87%)	25 (8%)	17 (5%)	1	12
1	J	339/359 (94%)	290 (86%)	29 (9%)	20 (6%)	1	10
1	K	339/359 (94%)	293 (86%)	26 (8%)	20 (6%)	1	10
1	L	339/359 (94%)	289 (85%)	32 (9%)	18 (5%)	1	12
All	All	4060/4308 (94%)	3491 (86%)	336 (8%)	233 (6%)	1	11

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%)	242 (84%)	46 (16%)	2	13
1	B	302/313 (96%)	252 (83%)	50 (17%)	2	11
1	C	289/313 (92%)	244 (84%)	45 (16%)	2	13
1	D	294/313 (94%)	248 (84%)	46 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	296/313 (95%)	250 (84%)	46 (16%)	2	14
1	F	291/313 (93%)	246 (84%)	45 (16%)	2	14
1	G	289/313 (92%)	243 (84%)	46 (16%)	2	13
1	H	288/313 (92%)	242 (84%)	46 (16%)	2	13
1	I	286/313 (91%)	243 (85%)	43 (15%)	3	15
1	J	287/313 (92%)	243 (85%)	44 (15%)	3	14
1	K	288/313 (92%)	244 (85%)	44 (15%)	3	14
1	L	292/313 (93%)	247 (85%)	45 (15%)	2	14
All	All	3490/3756 (93%)	2944 (84%)	546 (16%)	2	13

5 of 546 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	24	LEU
1	K	118	THR
1	K	19	LEU
1	L	111	VAL
1	E	19	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	133	GLN
1	L	37	GLN
1	E	41	ASN
1	E	37	GLN
1	L	41	ASN

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 oligosaccharides 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	I	340	-	4,4,4	0.28	0	6,6,6	0.10	0
2	SO4	G	341	-	4,4,4	0.20	0	6,6,6	0.19	0
2	SO4	D	340	-	4,4,4	0.24	0	6,6,6	0.41	0
2	SO4	C	341	-	4,4,4	0.22	0	6,6,6	0.11	0
2	SO4	A	341	-	4,4,4	0.26	0	6,6,6	0.26	0
2	SO4	A	340	-	4,4,4	0.22	0	6,6,6	0.27	0
2	SO4	H	340	-	4,4,4	0.28	0	6,6,6	0.21	0
2	SO4	L	341	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	L	342	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	342	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	E	341	-	4,4,4	0.30	0	6,6,6	0.22	0
2	SO4	B	341	-	4,4,4	0.16	0	6,6,6	0.30	0
2	SO4	E	340	-	4,4,4	0.25	0	6,6,6	0.22	0
2	SO4	B	340	-	4,4,4	0.20	0	6,6,6	0.40	0
2	SO4	F	341	-	4,4,4	0.26	0	6,6,6	0.20	0
2	SO4	E	342	-	4,4,4	0.22	0	6,6,6	0.27	0
2	SO4	J	341	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	G	340	-	4,4,4	0.25	0	6,6,6	0.37	0
2	SO4	H	341	-	4,4,4	0.22	0	6,6,6	0.13	0
2	SO4	C	340	-	4,4,4	0.24	0	6,6,6	0.15	0
2	SO4	J	340	-	4,4,4	0.26	0	6,6,6	0.15	0
2	SO4	F	340	-	4,4,4	0.24	0	6,6,6	0.15	0
2	SO4	G	342	-	4,4,4	0.26	0	6,6,6	0.13	0
2	SO4	I	341	-	4,4,4	0.25	0	6,6,6	0.23	0
2	SO4	K	340	-	4,4,4	0.37	0	6,6,6	0.38	0
2	SO4	L	340	-	4,4,4	0.28	0	6,6,6	0.19	0
2	SO4	D	341	-	4,4,4	0.26	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

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

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, 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%)	-0.45	2 (0%) 85 73	41, 74, 137, 219	0
1	B	353/359 (98%)	-0.38	4 (1%) 78 61	39, 69, 144, 211	0
1	C	340/359 (94%)	-0.48	1 (0%) 90 81	43, 75, 141, 207	0
1	D	347/359 (96%)	-0.30	5 (1%) 73 54	40, 74, 137, 208	0
1	E	343/359 (95%)	-0.40	0 100 100	34, 67, 127, 209	0
1	F	340/359 (94%)	-0.39	0 100 100	38, 82, 147, 224	0
1	G	341/359 (94%)	-0.50	0 100 100	46, 76, 144, 209	0
1	H	336/359 (93%)	-0.46	0 100 100	44, 80, 141, 208	0
1	I	332/359 (92%)	-0.46	2 (0%) 85 73	44, 76, 136, 208	0
1	J	341/359 (94%)	-0.36	0 100 100	46, 81, 147, 224	0
1	K	341/359 (94%)	-0.43	1 (0%) 90 81	46, 80, 148, 210	0
1	L	341/359 (94%)	-0.36	0 100 100	38, 79, 149, 238	0
All	All	4092/4308 (94%)	-0.41	15 (0%) 88 79	34, 76, 144, 238	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	231	GLY	3.7
1	A	0	HIS	3.0
1	B	232	LEU	2.8
1	A	215	ALA	2.6
1	D	214	ASP	2.5

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 [i](#)

There are no oligosaccharides 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	H	340	5/5	0.70	0.12	142,151,175,178	0
2	SO4	A	340	5/5	0.72	0.09	105,110,199,203	0
2	SO4	B	342	5/5	0.73	0.09	115,143,184,221	0
2	SO4	L	342	5/5	0.75	0.08	129,163,183,197	0
2	SO4	E	342	5/5	0.77	0.11	133,143,177,213	0
2	SO4	C	341	5/5	0.79	0.07	159,176,191,193	0
2	SO4	I	340	5/5	0.81	0.07	97,135,192,204	0
2	SO4	D	340	5/5	0.82	0.12	52,115,167,222	0
2	SO4	F	340	5/5	0.83	0.13	102,138,146,182	0
2	SO4	C	340	5/5	0.83	0.18	64,118,199,217	0
2	SO4	A	341	5/5	0.84	0.14	83,129,161,178	0
2	SO4	F	341	5/5	0.84	0.13	59,123,192,197	0
2	SO4	J	340	5/5	0.84	0.09	127,150,178,179	0
2	SO4	G	341	5/5	0.84	0.07	134,152,174,175	0
2	SO4	I	341	5/5	0.85	0.09	131,176,179,182	0
2	SO4	K	340	5/5	0.87	0.09	103,105,182,190	0
2	SO4	L	341	5/5	0.87	0.13	101,122,174,199	0
2	SO4	H	341	5/5	0.87	0.06	68,151,194,196	0
2	SO4	J	341	5/5	0.89	0.08	42,180,185,214	0
2	SO4	G	342	5/5	0.89	0.08	112,127,168,206	0
2	SO4	B	341	5/5	0.90	0.10	61,66,126,155	0
2	SO4	E	340	5/5	0.92	0.10	86,112,144,146	0
2	SO4	E	341	5/5	0.92	0.10	70,86,138,148	0
2	SO4	G	340	5/5	0.93	0.07	71,84,109,111	0
2	SO4	D	341	5/5	0.93	0.12	61,140,158,170	0
2	SO4	B	340	5/5	0.93	0.12	56,90,126,172	0
2	SO4	L	340	5/5	0.98	0.05	63,83,85,137	0

6.5 Other polymers [i](#)

There are no such residues in this entry.