



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:32 AM UTC

PDB ID : 6D63 / pdb\_00006d63  
Title : The structure of AtzH: a little known member of the atrazine breakdown pathway  
Authors : Peat, T.S.; Newman, J.; Scott, C.; Esquirol, L.  
Deposited on : 2018-04-19  
Resolution : 2.30 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](mailto: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>.

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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

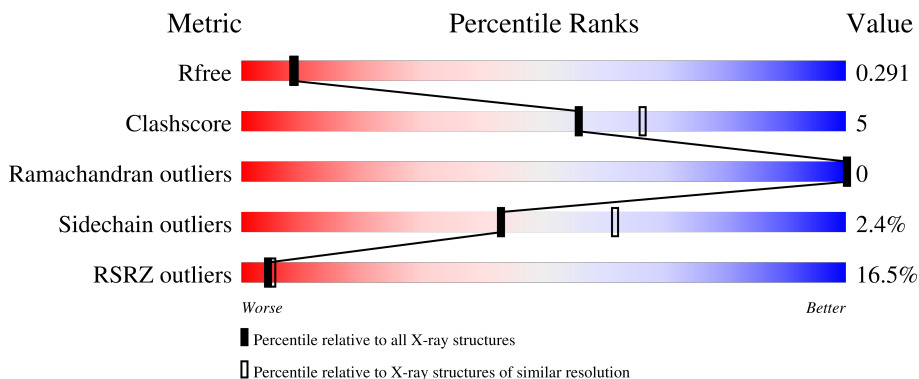
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.



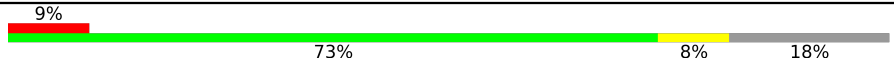
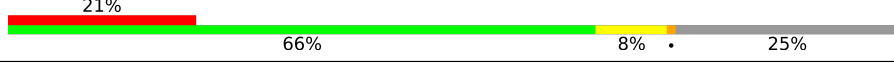
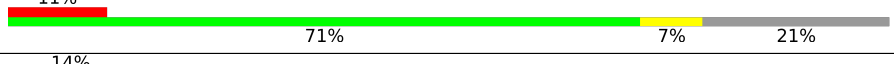
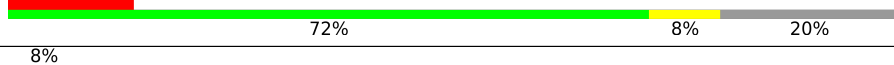

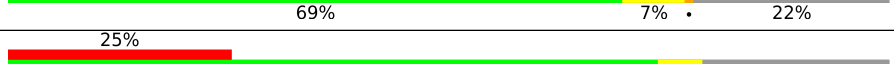
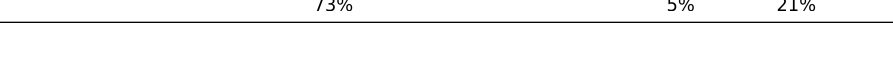
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	154	
1	B	154	
1	C	154	
1	D	154	
1	E	154	

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Mol	Chain	Length	Quality of chain
1	F	154	
1	G	154	
1	H	154	
1	I	154	
1	J	154	
1	K	154	
1	L	154	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	6JN	B	201	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12009 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 atzH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	127	1010	638	187	183	2	0	1	0
1	B	128	1023	647	185	189	2	0	1	0
1	C	125	1000	634	181	183	2	0	0	0
1	D	115	925	585	168	170	2	0	0	0
1	E	119	956	604	174	176	2	0	1	0
1	F	126	1002	635	182	184	1	0	1	0
1	G	115	892	571	158	162	1	0	0	0
1	H	121	963	609	172	180	2	0	0	0
1	I	123	975	618	176	179	2	0	1	0
1	J	129	1033	654	188	190	1	0	1	0
1	K	120	954	605	172	175	2	0	1	0
1	L	121	958	607	172	177	2	0	0	0

There are 312 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP A0A0V8SMU2
A	-20	GLY	-	expression tag	UNP A0A0V8SMU2
A	-19	SER	-	expression tag	UNP A0A0V8SMU2
A	-18	SER	-	expression tag	UNP A0A0V8SMU2
A	-17	HIS	-	expression tag	UNP A0A0V8SMU2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	expression tag	UNP A0A0V8SMU2
A	-15	HIS	-	expression tag	UNP A0A0V8SMU2
A	-14	HIS	-	expression tag	UNP A0A0V8SMU2
A	-13	HIS	-	expression tag	UNP A0A0V8SMU2
A	-12	HIS	-	expression tag	UNP A0A0V8SMU2
A	-11	HIS	-	expression tag	UNP A0A0V8SMU2
A	-10	SER	-	expression tag	UNP A0A0V8SMU2
A	-9	SER	-	expression tag	UNP A0A0V8SMU2
A	-8	GLY	-	expression tag	UNP A0A0V8SMU2
A	-7	LEU	-	expression tag	UNP A0A0V8SMU2
A	-6	VAL	-	expression tag	UNP A0A0V8SMU2
A	-5	PRO	-	expression tag	UNP A0A0V8SMU2
A	-4	ARG	-	expression tag	UNP A0A0V8SMU2
A	-3	GLY	-	expression tag	UNP A0A0V8SMU2
A	-2	SER	-	expression tag	UNP A0A0V8SMU2
A	-1	HIS	-	expression tag	UNP A0A0V8SMU2
A	0	HIS	-	expression tag	UNP A0A0V8SMU2
A	1	MET	-	expression tag	UNP A0A0V8SMU2
A	2	LEU	-	expression tag	UNP A0A0V8SMU2
A	3	GLU	-	expression tag	UNP A0A0V8SMU2
A	73	LYS	ARG	engineered mutation	UNP A0A0V8SMU2
B	-21	MET	-	initiating methionine	UNP A0A0V8SMU2
B	-20	GLY	-	expression tag	UNP A0A0V8SMU2
B	-19	SER	-	expression tag	UNP A0A0V8SMU2
B	-18	SER	-	expression tag	UNP A0A0V8SMU2
B	-17	HIS	-	expression tag	UNP A0A0V8SMU2
B	-16	HIS	-	expression tag	UNP A0A0V8SMU2
B	-15	HIS	-	expression tag	UNP A0A0V8SMU2
B	-14	HIS	-	expression tag	UNP A0A0V8SMU2
B	-13	HIS	-	expression tag	UNP A0A0V8SMU2
B	-12	HIS	-	expression tag	UNP A0A0V8SMU2
B	-11	HIS	-	expression tag	UNP A0A0V8SMU2
B	-10	SER	-	expression tag	UNP A0A0V8SMU2
B	-9	SER	-	expression tag	UNP A0A0V8SMU2
B	-8	GLY	-	expression tag	UNP A0A0V8SMU2
B	-7	LEU	-	expression tag	UNP A0A0V8SMU2
B	-6	VAL	-	expression tag	UNP A0A0V8SMU2
B	-5	PRO	-	expression tag	UNP A0A0V8SMU2
B	-4	ARG	-	expression tag	UNP A0A0V8SMU2
B	-3	GLY	-	expression tag	UNP A0A0V8SMU2
B	-2	SER	-	expression tag	UNP A0A0V8SMU2
B	-1	HIS	-	expression tag	UNP A0A0V8SMU2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP A0A0V8SMU2
B	1	MET	-	expression tag	UNP A0A0V8SMU2
B	2	LEU	-	expression tag	UNP A0A0V8SMU2
B	3	GLU	-	expression tag	UNP A0A0V8SMU2
B	73	LYS	ARG	engineered mutation	UNP A0A0V8SMU2
C	-21	MET	-	initiating methionine	UNP A0A0V8SMU2
C	-20	GLY	-	expression tag	UNP A0A0V8SMU2
C	-19	SER	-	expression tag	UNP A0A0V8SMU2
C	-18	SER	-	expression tag	UNP A0A0V8SMU2
C	-17	HIS	-	expression tag	UNP A0A0V8SMU2
C	-16	HIS	-	expression tag	UNP A0A0V8SMU2
C	-15	HIS	-	expression tag	UNP A0A0V8SMU2
C	-14	HIS	-	expression tag	UNP A0A0V8SMU2
C	-13	HIS	-	expression tag	UNP A0A0V8SMU2
C	-12	HIS	-	expression tag	UNP A0A0V8SMU2
C	-11	HIS	-	expression tag	UNP A0A0V8SMU2
C	-10	SER	-	expression tag	UNP A0A0V8SMU2
C	-9	SER	-	expression tag	UNP A0A0V8SMU2
C	-8	GLY	-	expression tag	UNP A0A0V8SMU2
C	-7	LEU	-	expression tag	UNP A0A0V8SMU2
C	-6	VAL	-	expression tag	UNP A0A0V8SMU2
C	-5	PRO	-	expression tag	UNP A0A0V8SMU2
C	-4	ARG	-	expression tag	UNP A0A0V8SMU2
C	-3	GLY	-	expression tag	UNP A0A0V8SMU2
C	-2	SER	-	expression tag	UNP A0A0V8SMU2
C	-1	HIS	-	expression tag	UNP A0A0V8SMU2
C	0	HIS	-	expression tag	UNP A0A0V8SMU2
C	1	MET	-	expression tag	UNP A0A0V8SMU2
C	2	LEU	-	expression tag	UNP A0A0V8SMU2
C	3	GLU	-	expression tag	UNP A0A0V8SMU2
C	73	LYS	ARG	engineered mutation	UNP A0A0V8SMU2
D	-21	MET	-	initiating methionine	UNP A0A0V8SMU2
D	-20	GLY	-	expression tag	UNP A0A0V8SMU2
D	-19	SER	-	expression tag	UNP A0A0V8SMU2
D	-18	SER	-	expression tag	UNP A0A0V8SMU2
D	-17	HIS	-	expression tag	UNP A0A0V8SMU2
D	-16	HIS	-	expression tag	UNP A0A0V8SMU2
D	-15	HIS	-	expression tag	UNP A0A0V8SMU2
D	-14	HIS	-	expression tag	UNP A0A0V8SMU2
D	-13	HIS	-	expression tag	UNP A0A0V8SMU2
D	-12	HIS	-	expression tag	UNP A0A0V8SMU2
D	-11	HIS	-	expression tag	UNP A0A0V8SMU2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	SER	-	expression tag	UNP A0A0V8SMU2
D	-9	SER	-	expression tag	UNP A0A0V8SMU2
D	-8	GLY	-	expression tag	UNP A0A0V8SMU2
D	-7	LEU	-	expression tag	UNP A0A0V8SMU2
D	-6	VAL	-	expression tag	UNP A0A0V8SMU2
D	-5	PRO	-	expression tag	UNP A0A0V8SMU2
D	-4	ARG	-	expression tag	UNP A0A0V8SMU2
D	-3	GLY	-	expression tag	UNP A0A0V8SMU2
D	-2	SER	-	expression tag	UNP A0A0V8SMU2
D	-1	HIS	-	expression tag	UNP A0A0V8SMU2
D	0	HIS	-	expression tag	UNP A0A0V8SMU2
D	1	MET	-	expression tag	UNP A0A0V8SMU2
D	2	LEU	-	expression tag	UNP A0A0V8SMU2
D	3	GLU	-	expression tag	UNP A0A0V8SMU2
D	73	LYS	ARG	engineered mutation	UNP A0A0V8SMU2
E	-21	MET	-	initiating methionine	UNP A0A0V8SMU2
E	-20	GLY	-	expression tag	UNP A0A0V8SMU2
E	-19	SER	-	expression tag	UNP A0A0V8SMU2
E	-18	SER	-	expression tag	UNP A0A0V8SMU2
E	-17	HIS	-	expression tag	UNP A0A0V8SMU2
E	-16	HIS	-	expression tag	UNP A0A0V8SMU2
E	-15	HIS	-	expression tag	UNP A0A0V8SMU2
E	-14	HIS	-	expression tag	UNP A0A0V8SMU2
E	-13	HIS	-	expression tag	UNP A0A0V8SMU2
E	-12	HIS	-	expression tag	UNP A0A0V8SMU2
E	-11	HIS	-	expression tag	UNP A0A0V8SMU2
E	-10	SER	-	expression tag	UNP A0A0V8SMU2
E	-9	SER	-	expression tag	UNP A0A0V8SMU2
E	-8	GLY	-	expression tag	UNP A0A0V8SMU2
E	-7	LEU	-	expression tag	UNP A0A0V8SMU2
E	-6	VAL	-	expression tag	UNP A0A0V8SMU2
E	-5	PRO	-	expression tag	UNP A0A0V8SMU2
E	-4	ARG	-	expression tag	UNP A0A0V8SMU2
E	-3	GLY	-	expression tag	UNP A0A0V8SMU2
E	-2	SER	-	expression tag	UNP A0A0V8SMU2
E	-1	HIS	-	expression tag	UNP A0A0V8SMU2
E	0	HIS	-	expression tag	UNP A0A0V8SMU2
E	1	MET	-	expression tag	UNP A0A0V8SMU2
E	2	LEU	-	expression tag	UNP A0A0V8SMU2
E	3	GLU	-	expression tag	UNP A0A0V8SMU2
E	73	LYS	ARG	engineered mutation	UNP A0A0V8SMU2
F	-21	MET	-	initiating methionine	UNP A0A0V8SMU2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-20	GLY	-	expression tag	UNP A0A0V8SMU2
F	-19	SER	-	expression tag	UNP A0A0V8SMU2
F	-18	SER	-	expression tag	UNP A0A0V8SMU2
F	-17	HIS	-	expression tag	UNP A0A0V8SMU2
F	-16	HIS	-	expression tag	UNP A0A0V8SMU2
F	-15	HIS	-	expression tag	UNP A0A0V8SMU2
F	-14	HIS	-	expression tag	UNP A0A0V8SMU2
F	-13	HIS	-	expression tag	UNP A0A0V8SMU2
F	-12	HIS	-	expression tag	UNP A0A0V8SMU2
F	-11	HIS	-	expression tag	UNP A0A0V8SMU2
F	-10	SER	-	expression tag	UNP A0A0V8SMU2
F	-9	SER	-	expression tag	UNP A0A0V8SMU2
F	-8	GLY	-	expression tag	UNP A0A0V8SMU2
F	-7	LEU	-	expression tag	UNP A0A0V8SMU2
F	-6	VAL	-	expression tag	UNP A0A0V8SMU2
F	-5	PRO	-	expression tag	UNP A0A0V8SMU2
F	-4	ARG	-	expression tag	UNP A0A0V8SMU2
F	-3	GLY	-	expression tag	UNP A0A0V8SMU2
F	-2	SER	-	expression tag	UNP A0A0V8SMU2
F	-1	HIS	-	expression tag	UNP A0A0V8SMU2
F	0	HIS	-	expression tag	UNP A0A0V8SMU2
F	1	MET	-	expression tag	UNP A0A0V8SMU2
F	2	LEU	-	expression tag	UNP A0A0V8SMU2
F	3	GLU	-	expression tag	UNP A0A0V8SMU2
F	73	LYS	ARG	engineered mutation	UNP A0A0V8SMU2
G	-21	MET	-	initiating methionine	UNP A0A0V8SMU2
G	-20	GLY	-	expression tag	UNP A0A0V8SMU2
G	-19	SER	-	expression tag	UNP A0A0V8SMU2
G	-18	SER	-	expression tag	UNP A0A0V8SMU2
G	-17	HIS	-	expression tag	UNP A0A0V8SMU2
G	-16	HIS	-	expression tag	UNP A0A0V8SMU2
G	-15	HIS	-	expression tag	UNP A0A0V8SMU2
G	-14	HIS	-	expression tag	UNP A0A0V8SMU2
G	-13	HIS	-	expression tag	UNP A0A0V8SMU2
G	-12	HIS	-	expression tag	UNP A0A0V8SMU2
G	-11	HIS	-	expression tag	UNP A0A0V8SMU2
G	-10	SER	-	expression tag	UNP A0A0V8SMU2
G	-9	SER	-	expression tag	UNP A0A0V8SMU2
G	-8	GLY	-	expression tag	UNP A0A0V8SMU2
G	-7	LEU	-	expression tag	UNP A0A0V8SMU2
G	-6	VAL	-	expression tag	UNP A0A0V8SMU2
G	-5	PRO	-	expression tag	UNP A0A0V8SMU2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ARG	-	expression tag	UNP A0A0V8SMU2
G	-3	GLY	-	expression tag	UNP A0A0V8SMU2
G	-2	SER	-	expression tag	UNP A0A0V8SMU2
G	-1	HIS	-	expression tag	UNP A0A0V8SMU2
G	0	HIS	-	expression tag	UNP A0A0V8SMU2
G	1	MET	-	expression tag	UNP A0A0V8SMU2
G	2	LEU	-	expression tag	UNP A0A0V8SMU2
G	3	GLU	-	expression tag	UNP A0A0V8SMU2
G	73	LYS	ARG	engineered mutation	UNP A0A0V8SMU2
H	-21	MET	-	initiating methionine	UNP A0A0V8SMU2
H	-20	GLY	-	expression tag	UNP A0A0V8SMU2
H	-19	SER	-	expression tag	UNP A0A0V8SMU2
H	-18	SER	-	expression tag	UNP A0A0V8SMU2
H	-17	HIS	-	expression tag	UNP A0A0V8SMU2
H	-16	HIS	-	expression tag	UNP A0A0V8SMU2
H	-15	HIS	-	expression tag	UNP A0A0V8SMU2
H	-14	HIS	-	expression tag	UNP A0A0V8SMU2
H	-13	HIS	-	expression tag	UNP A0A0V8SMU2
H	-12	HIS	-	expression tag	UNP A0A0V8SMU2
H	-11	HIS	-	expression tag	UNP A0A0V8SMU2
H	-10	SER	-	expression tag	UNP A0A0V8SMU2
H	-9	SER	-	expression tag	UNP A0A0V8SMU2
H	-8	GLY	-	expression tag	UNP A0A0V8SMU2
H	-7	LEU	-	expression tag	UNP A0A0V8SMU2
H	-6	VAL	-	expression tag	UNP A0A0V8SMU2
H	-5	PRO	-	expression tag	UNP A0A0V8SMU2
H	-4	ARG	-	expression tag	UNP A0A0V8SMU2
H	-3	GLY	-	expression tag	UNP A0A0V8SMU2
H	-2	SER	-	expression tag	UNP A0A0V8SMU2
H	-1	HIS	-	expression tag	UNP A0A0V8SMU2
H	0	HIS	-	expression tag	UNP A0A0V8SMU2
H	1	MET	-	expression tag	UNP A0A0V8SMU2
H	2	LEU	-	expression tag	UNP A0A0V8SMU2
H	3	GLU	-	expression tag	UNP A0A0V8SMU2
H	73	LYS	ARG	engineered mutation	UNP A0A0V8SMU2
I	-21	MET	-	initiating methionine	UNP A0A0V8SMU2
I	-20	GLY	-	expression tag	UNP A0A0V8SMU2
I	-19	SER	-	expression tag	UNP A0A0V8SMU2
I	-18	SER	-	expression tag	UNP A0A0V8SMU2
I	-17	HIS	-	expression tag	UNP A0A0V8SMU2
I	-16	HIS	-	expression tag	UNP A0A0V8SMU2
I	-15	HIS	-	expression tag	UNP A0A0V8SMU2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-14	HIS	-	expression tag	UNP A0A0V8SMU2
I	-13	HIS	-	expression tag	UNP A0A0V8SMU2
I	-12	HIS	-	expression tag	UNP A0A0V8SMU2
I	-11	HIS	-	expression tag	UNP A0A0V8SMU2
I	-10	SER	-	expression tag	UNP A0A0V8SMU2
I	-9	SER	-	expression tag	UNP A0A0V8SMU2
I	-8	GLY	-	expression tag	UNP A0A0V8SMU2
I	-7	LEU	-	expression tag	UNP A0A0V8SMU2
I	-6	VAL	-	expression tag	UNP A0A0V8SMU2
I	-5	PRO	-	expression tag	UNP A0A0V8SMU2
I	-4	ARG	-	expression tag	UNP A0A0V8SMU2
I	-3	GLY	-	expression tag	UNP A0A0V8SMU2
I	-2	SER	-	expression tag	UNP A0A0V8SMU2
I	-1	HIS	-	expression tag	UNP A0A0V8SMU2
I	0	HIS	-	expression tag	UNP A0A0V8SMU2
I	1	MET	-	expression tag	UNP A0A0V8SMU2
I	2	LEU	-	expression tag	UNP A0A0V8SMU2
I	3	GLU	-	expression tag	UNP A0A0V8SMU2
I	73	LYS	ARG	engineered mutation	UNP A0A0V8SMU2
J	-21	MET	-	initiating methionine	UNP A0A0V8SMU2
J	-20	GLY	-	expression tag	UNP A0A0V8SMU2
J	-19	SER	-	expression tag	UNP A0A0V8SMU2
J	-18	SER	-	expression tag	UNP A0A0V8SMU2
J	-17	HIS	-	expression tag	UNP A0A0V8SMU2
J	-16	HIS	-	expression tag	UNP A0A0V8SMU2
J	-15	HIS	-	expression tag	UNP A0A0V8SMU2
J	-14	HIS	-	expression tag	UNP A0A0V8SMU2
J	-13	HIS	-	expression tag	UNP A0A0V8SMU2
J	-12	HIS	-	expression tag	UNP A0A0V8SMU2
J	-11	HIS	-	expression tag	UNP A0A0V8SMU2
J	-10	SER	-	expression tag	UNP A0A0V8SMU2
J	-9	SER	-	expression tag	UNP A0A0V8SMU2
J	-8	GLY	-	expression tag	UNP A0A0V8SMU2
J	-7	LEU	-	expression tag	UNP A0A0V8SMU2
J	-6	VAL	-	expression tag	UNP A0A0V8SMU2
J	-5	PRO	-	expression tag	UNP A0A0V8SMU2
J	-4	ARG	-	expression tag	UNP A0A0V8SMU2
J	-3	GLY	-	expression tag	UNP A0A0V8SMU2
J	-2	SER	-	expression tag	UNP A0A0V8SMU2
J	-1	HIS	-	expression tag	UNP A0A0V8SMU2
J	0	HIS	-	expression tag	UNP A0A0V8SMU2
J	1	MET	-	expression tag	UNP A0A0V8SMU2

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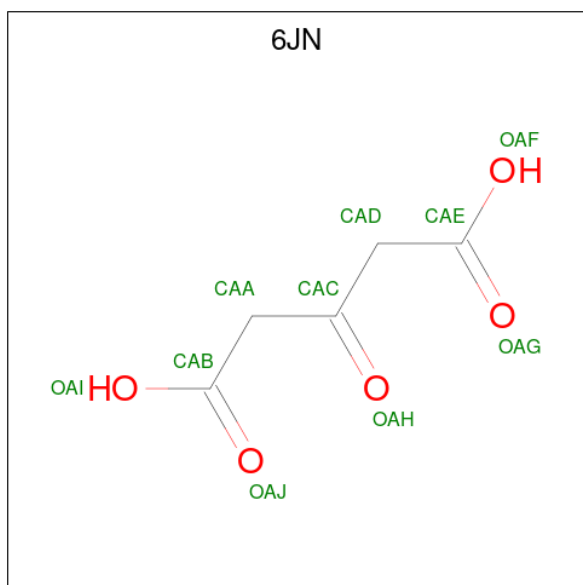
Chain	Residue	Modelled	Actual	Comment	Reference
J	2	LEU	-	expression tag	UNP A0A0V8SMU2
J	3	GLU	-	expression tag	UNP A0A0V8SMU2
J	73	LYS	ARG	engineered mutation	UNP A0A0V8SMU2
K	-21	MET	-	initiating methionine	UNP A0A0V8SMU2
K	-20	GLY	-	expression tag	UNP A0A0V8SMU2
K	-19	SER	-	expression tag	UNP A0A0V8SMU2
K	-18	SER	-	expression tag	UNP A0A0V8SMU2
K	-17	HIS	-	expression tag	UNP A0A0V8SMU2
K	-16	HIS	-	expression tag	UNP A0A0V8SMU2
K	-15	HIS	-	expression tag	UNP A0A0V8SMU2
K	-14	HIS	-	expression tag	UNP A0A0V8SMU2
K	-13	HIS	-	expression tag	UNP A0A0V8SMU2
K	-12	HIS	-	expression tag	UNP A0A0V8SMU2
K	-11	HIS	-	expression tag	UNP A0A0V8SMU2
K	-10	SER	-	expression tag	UNP A0A0V8SMU2
K	-9	SER	-	expression tag	UNP A0A0V8SMU2
K	-8	GLY	-	expression tag	UNP A0A0V8SMU2
K	-7	LEU	-	expression tag	UNP A0A0V8SMU2
K	-6	VAL	-	expression tag	UNP A0A0V8SMU2
K	-5	PRO	-	expression tag	UNP A0A0V8SMU2
K	-4	ARG	-	expression tag	UNP A0A0V8SMU2
K	-3	GLY	-	expression tag	UNP A0A0V8SMU2
K	-2	SER	-	expression tag	UNP A0A0V8SMU2
K	-1	HIS	-	expression tag	UNP A0A0V8SMU2
K	0	HIS	-	expression tag	UNP A0A0V8SMU2
K	1	MET	-	expression tag	UNP A0A0V8SMU2
K	2	LEU	-	expression tag	UNP A0A0V8SMU2
K	3	GLU	-	expression tag	UNP A0A0V8SMU2
K	73	LYS	ARG	engineered mutation	UNP A0A0V8SMU2
L	-21	MET	-	initiating methionine	UNP A0A0V8SMU2
L	-20	GLY	-	expression tag	UNP A0A0V8SMU2
L	-19	SER	-	expression tag	UNP A0A0V8SMU2
L	-18	SER	-	expression tag	UNP A0A0V8SMU2
L	-17	HIS	-	expression tag	UNP A0A0V8SMU2
L	-16	HIS	-	expression tag	UNP A0A0V8SMU2
L	-15	HIS	-	expression tag	UNP A0A0V8SMU2
L	-14	HIS	-	expression tag	UNP A0A0V8SMU2
L	-13	HIS	-	expression tag	UNP A0A0V8SMU2
L	-12	HIS	-	expression tag	UNP A0A0V8SMU2
L	-11	HIS	-	expression tag	UNP A0A0V8SMU2
L	-10	SER	-	expression tag	UNP A0A0V8SMU2
L	-9	SER	-	expression tag	UNP A0A0V8SMU2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-8	GLY	-	expression tag	UNP A0A0V8SMU2
L	-7	LEU	-	expression tag	UNP A0A0V8SMU2
L	-6	VAL	-	expression tag	UNP A0A0V8SMU2
L	-5	PRO	-	expression tag	UNP A0A0V8SMU2
L	-4	ARG	-	expression tag	UNP A0A0V8SMU2
L	-3	GLY	-	expression tag	UNP A0A0V8SMU2
L	-2	SER	-	expression tag	UNP A0A0V8SMU2
L	-1	HIS	-	expression tag	UNP A0A0V8SMU2
L	0	HIS	-	expression tag	UNP A0A0V8SMU2
L	1	MET	-	expression tag	UNP A0A0V8SMU2
L	2	LEU	-	expression tag	UNP A0A0V8SMU2
L	3	GLU	-	expression tag	UNP A0A0V8SMU2
L	73	LYS	ARG	engineered mutation	UNP A0A0V8SMU2

- Molecule 2 is 3-oxopentanedioic acid (CCD ID: 6JN) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>5</sub>).



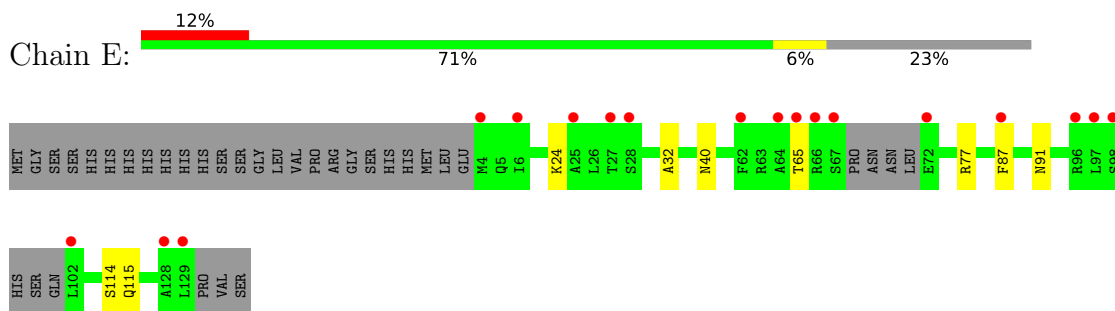
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		
2	J	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is water.

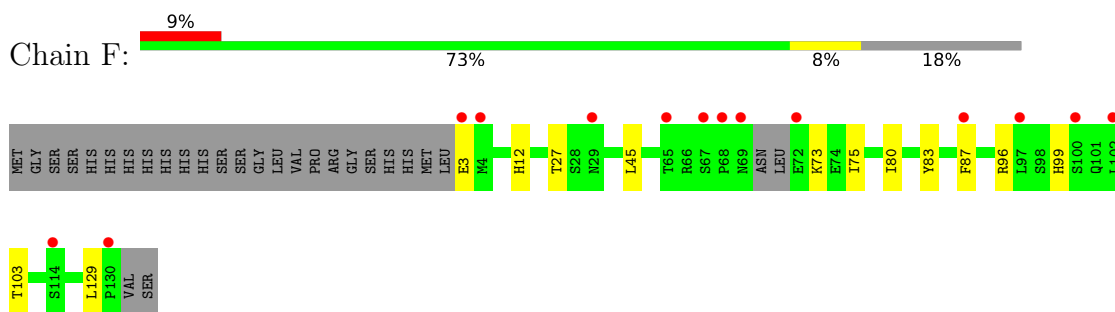
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	38	Total O 38 38	0	0
3	B	26	Total O 26 26	0	0
3	C	33	Total O 33 33	0	0
3	D	27	Total O 27 27	0	0
3	E	21	Total O 21 21	0	0
3	F	24	Total O 24 24	0	0
3	G	20	Total O 20 20	0	0
3	H	20	Total O 20 20	0	0
3	I	17	Total O 17 17	0	0
3	J	30	Total O 30 30	0	0
3	K	18	Total O 18 18	0	0
3	L	14	Total O 14 14	0	0



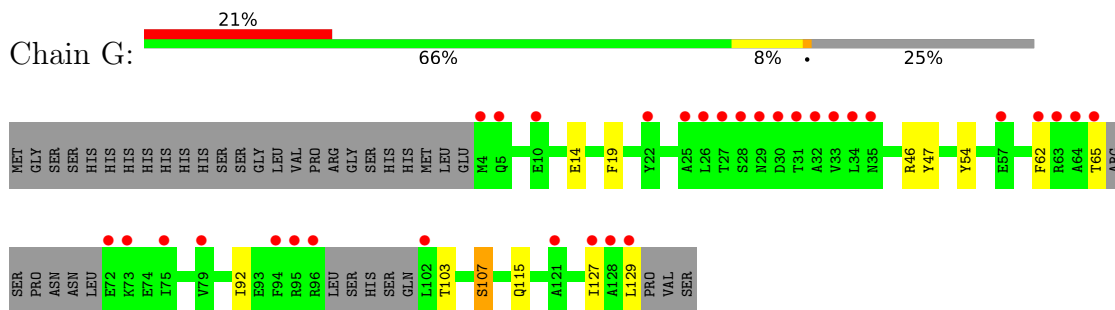
- Molecule 1: atzH



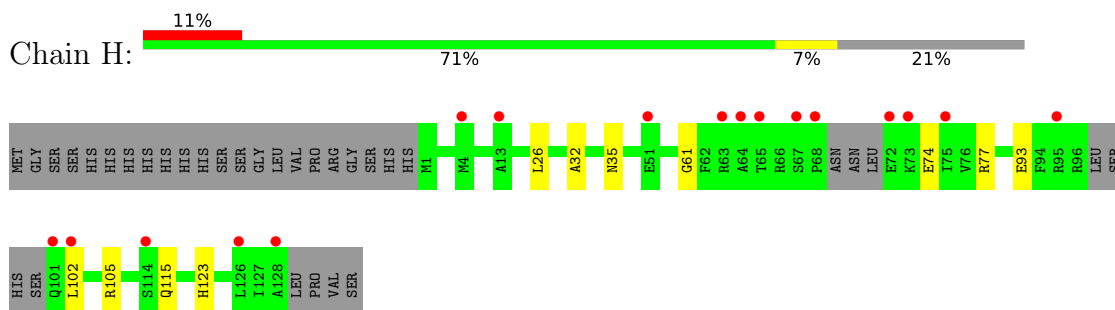
- Molecule 1: atzH



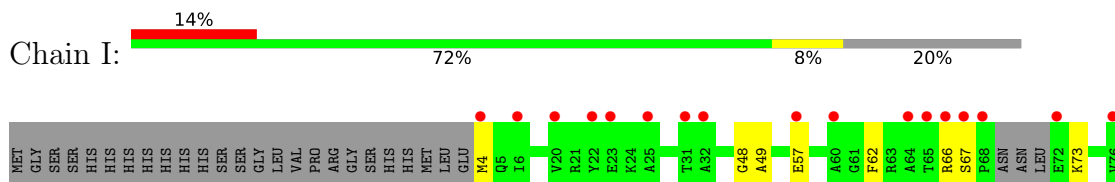
- Molecule 1: atzH



- Molecule 1: atzH

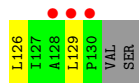
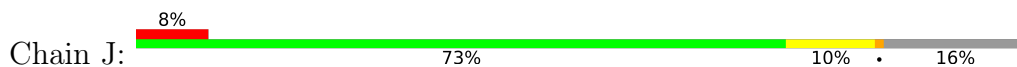


- Molecule 1: atzH

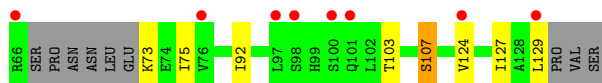
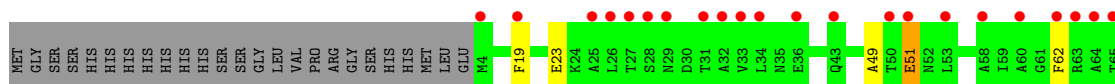




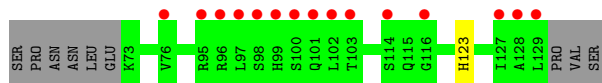
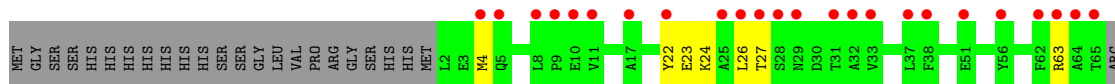
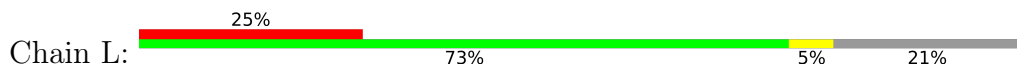
• Molecule 1: atzH



• Molecule 1: atzH



• Molecule 1: atzH



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.72Å 74.66Å 103.61Å 90.00° 96.69° 90.00°	Depositor
Resolution (Å)	50.10 – 2.30 50.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.10-2.30) 100.0 (50.10-2.30)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0218	Depositor
R, $R_{free}$	0.249 , 0.286 0.256 , 0.291	Depositor DCC
$R_{free}$ test set	3196 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtrriage
Anisotropy	0.280	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	12009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.81% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6JN

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	0.77	0/1032	0.75	0/1405
1	B	0.74	0/1045	0.69	0/1423
1	C	0.84	0/1020	0.85	3/1386 (0.2%)
1	D	0.85	1/943 (0.1%)	0.81	0/1279
1	E	0.65	0/974	0.71	0/1322
1	F	0.66	0/1025	0.76	0/1396
1	G	0.79	1/910 (0.1%)	0.76	0/1239
1	H	0.71	0/982	0.76	0/1334
1	I	0.74	0/996	0.77	0/1355
1	J	0.71	0/1057	0.79	0/1441
1	K	0.67	0/973	0.70	0/1324
1	L	0.68	0/978	0.69	0/1331
All	All	0.74	2/11935 (0.0%)	0.76	3/16235 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	14	GLU	C-O	-6.10	1.17	1.24
1	G	14	GLU	C-O	-5.92	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	ARG	CA-CB-CG	-5.53	103.04	114.10
1	C	99	HIS	N-CA-CB	-5.24	103.62	110.59
1	C	102	LEU	N-CA-CB	-5.01	102.49	110.06

There are no chirality outliers.

There are no planarity outliers.

## 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	1010	0	973	12	0
1	B	1023	0	991	4	0
1	C	1000	0	977	17	0
1	D	925	0	902	13	0
1	E	956	0	924	16	0
1	F	1002	0	956	13	0
1	G	892	0	848	10	0
1	H	963	0	933	13	0
1	I	975	0	929	9	0
1	J	1033	0	995	13	0
1	K	954	0	921	9	0
1	L	958	0	915	9	0
2	A	10	0	0	3	0
2	B	10	0	0	4	0
2	J	10	0	0	1	0
3	A	38	0	0	0	0
3	B	26	0	0	0	0
3	C	33	0	0	1	0
3	D	27	0	0	0	0
3	E	21	0	0	0	0
3	F	24	0	0	0	0
3	G	20	0	0	0	0
3	H	20	0	0	0	0
3	I	17	0	0	0	0
3	J	30	0	0	3	0
3	K	18	0	0	0	0
3	L	14	0	0	0	0
All	All	12009	0	11264	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 108 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:D:23:GLU:OE2	1:D:73:LYS:NZ	2.05	0.89
1:C:71:LEU:CD1	1:C:96:ARG:HE	1.86	0.86
1:E:114:SER:HB3	1:H:115:GLN:HG2	1.60	0.82
1:J:69:ASN:HB2	1:J:71:LEU:HD22	1.60	0.81
1:E:40:ASN:CG	1:H:32:ALA:HB2	2.06	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	126/154 (82%)	124 (98%)	2 (2%)	0	100	100
1	B	127/154 (82%)	125 (98%)	2 (2%)	0	100	100
1	C	121/154 (79%)	119 (98%)	2 (2%)	0	100	100
1	D	109/154 (71%)	108 (99%)	1 (1%)	0	100	100
1	E	114/154 (74%)	112 (98%)	2 (2%)	0	100	100
1	F	123/154 (80%)	121 (98%)	2 (2%)	0	100	100
1	G	109/154 (71%)	109 (100%)	0	0	100	100
1	H	115/154 (75%)	114 (99%)	1 (1%)	0	100	100
1	I	120/154 (78%)	118 (98%)	2 (2%)	0	100	100
1	J	128/154 (83%)	126 (98%)	2 (2%)	0	100	100
1	K	117/154 (76%)	116 (99%)	1 (1%)	0	100	100
1	L	117/154 (76%)	115 (98%)	2 (2%)	0	100	100
All	All	1426/1848 (77%)	1407 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	101/132 (76%)	100 (99%)	1 (1%)	68	82
1	B	105/132 (80%)	103 (98%)	2 (2%)	50	69
1	C	102/132 (77%)	102 (100%)	0	100	100
1	D	95/132 (72%)	93 (98%)	2 (2%)	47	66
1	E	97/132 (74%)	95 (98%)	2 (2%)	47	66
1	F	101/132 (76%)	99 (98%)	2 (2%)	48	67
1	G	86/132 (65%)	84 (98%)	2 (2%)	44	63
1	H	99/132 (75%)	95 (96%)	4 (4%)	28	42
1	I	97/132 (74%)	93 (96%)	4 (4%)	27	41
1	J	106/132 (80%)	101 (95%)	5 (5%)	23	35
1	K	96/132 (73%)	94 (98%)	2 (2%)	47	66
1	L	96/132 (73%)	94 (98%)	2 (2%)	47	66
All	All	1181/1584 (75%)	1153 (98%)	28 (2%)	43	62

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	102	LEU
1	L	63	ARG
1	I	96	ARG
1	K	51	GLU
1	I	73	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	85	HIS
1	I	85	HIS
1	L	99	HIS
1	K	85	HIS

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Mol	Chain	Res	Type
1	E	106	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

3 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	6JN	B	201	-	9,9,9	0.92	0	11,11,11	1.81	4 (36%)
2	6JN	A	201	-	9,9,9	1.00	0	11,11,11	2.80	5 (45%)
2	6JN	J	201	-	9,9,9	1.00	0	11,11,11	2.44	7 (63%)

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	6JN	B	201	-	-	4/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6JN	A	201	-	-	3/8/8/8	-
2	6JN	J	201	-	-	4/8/8/8	-

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	6JN	CAC-CAA-CAB	-5.36	101.61	112.32
2	A	201	6JN	OAF-CAE-OAG	4.44	134.75	123.33
2	A	201	6JN	OAG-CAE-CAD	-3.98	110.78	122.11
2	J	201	6JN	CAC-CAD-CAE	-3.51	105.30	112.32
2	J	201	6JN	OAI-CAB-OAJ	3.47	132.25	123.33

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	6JN	CAA-CAC-CAD-CAE
2	B	201	6JN	OAH-CAC-CAD-CAE
2	J	201	6JN	CAB-CAA-CAC-CAD
2	J	201	6JN	CAB-CAA-CAC-OAH
2	A	201	6JN	CAC-CAD-CAE-OAF

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	6JN	4	0
2	A	201	6JN	3	0
2	J	201	6JN	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, 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	127/154 (82%)	0.74	9 (7%) 22 24	8, 17, 34, 48	1 (0%)
1	B	128/154 (83%)	1.02	16 (12%) 8 9	9, 21, 61, 85	1 (0%)
1	C	125/154 (81%)	0.79	11 (8%) 15 17	10, 19, 38, 76	0
1	D	115/154 (74%)	1.12	21 (18%) 3 4	10, 20, 53, 68	0
1	E	119/154 (77%)	1.21	18 (15%) 5 6	8, 24, 53, 77	1 (0%)
1	F	126/154 (81%)	1.00	14 (11%) 10 11	8, 21, 48, 73	1 (0%)
1	G	115/154 (74%)	1.41	32 (27%) 1 1	11, 25, 64, 80	0
1	H	121/154 (78%)	1.13	17 (14%) 6 7	12, 22, 52, 80	0
1	I	123/154 (79%)	1.20	22 (17%) 3 4	7, 23, 53, 88	1 (0%)
1	J	129/154 (83%)	0.90	13 (10%) 12 14	7, 19, 47, 61	1 (0%)
1	K	120/154 (77%)	1.45	30 (25%) 2 2	11, 27, 60, 79	1 (0%)
1	L	121/154 (78%)	1.73	39 (32%) 1 1	15, 34, 65, 83	0
All	All	1469/1848 (79%)	1.14	242 (16%) 4 5	7, 22, 56, 88	7 (0%)

The worst 5 of 242 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	69	ASN	6.2
1	G	31	THR	6.2
1	E	67	SER	5.6
1	L	65	THR	5.6
1	H	68	PRO	5.6

### 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 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	6JN	B	201	10/10	0.75	0.20	54,58,62,71	0
2	6JN	A	201	10/10	0.76	0.17	25,30,31,33	0
2	6JN	J	201	10/10	0.81	0.13	26,32,36,39	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.