wwPDB X-ray Structure Validation Summary Report (i)

Sep 27, 2023 – 01:05 AM EDT

PDB ID	:	6D63
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

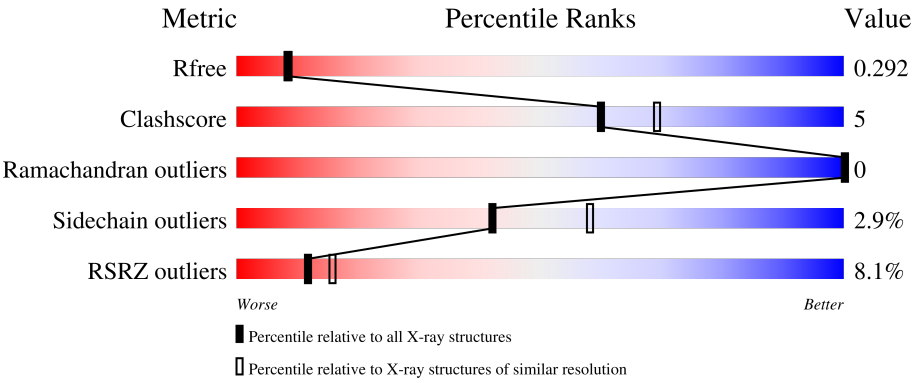
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 >=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 <=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	74% 8% 18%
1	B	154	6% 80% • • 17%
1	C	154	6% 72% 9% 19%
1	D	154	5% 64% 10% • 25%
1	E	154	5% 71% 6% 23%

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Mol	Chain	Length	Quality of chain
1	F	154	5% 73% 8% 18%
1	G	154	12% 65% 9% 25%
1	H	154	8% 72% 6% 21%
1	I	154	6% 73% 6% 20%
1	J	154	5% 72% 10% 16%
1	K	154	7% 68% 8% 22%
1	L	154	12% 73% 5% 21%

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	6JN	J	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
1	A	127	Total	C	N	O	S	0	1	0
			1010	638	187	183	2			
1	B	128	Total	C	N	O	S	0	1	0
			1023	647	185	189	2			
1	C	125	Total	C	N	O	S	0	0	0
			1000	634	181	183	2			
1	D	115	Total	C	N	O	S	0	0	0
			925	585	168	170	2			
1	E	119	Total	C	N	O	S	0	1	0
			956	604	174	176	2			
1	F	126	Total	C	N	O	S	0	1	0
			1002	635	182	184	1			
1	G	115	Total	C	N	O	S	0	0	0
			892	571	158	162	1			
1	H	121	Total	C	N	O	S	0	0	0
			963	609	172	180	2			
1	I	123	Total	C	N	O	S	0	1	0
			975	618	176	179	2			
1	J	129	Total	C	N	O	S	0	1	0
			1033	654	188	190	1			
1	K	120	Total	C	N	O	S	0	1	0
			954	605	172	175	2			
1	L	121	Total	C	N	O	S	0	0	0
			958	607	172	177	2			

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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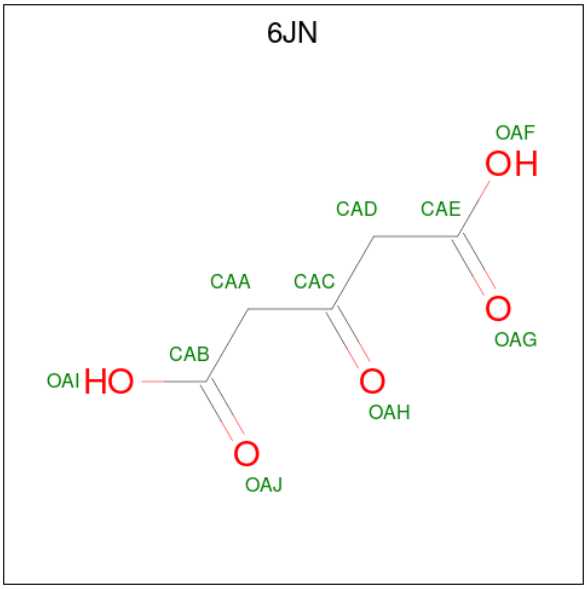
Chain	Residue	Modelled	Actual	Comment	Reference
L	-8	GLY	-	expression tag	UNP A0A0V8SMU2
L	-7	LEU	-	expression tag	UNP A0A0V8SMU2
L	-6	VAL	-	expression tag	UNP A0A0V8SMU2
L	-5	PRO	-	expression tag	UNP A0A0V8SMU2
L	-4	ARG	-	expression tag	UNP A0A0V8SMU2
L	-3	GLY	-	expression tag	UNP A0A0V8SMU2
L	-2	SER	-	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 (three-letter code: 6JN) (formula: $C_5H_6O_5$).



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.

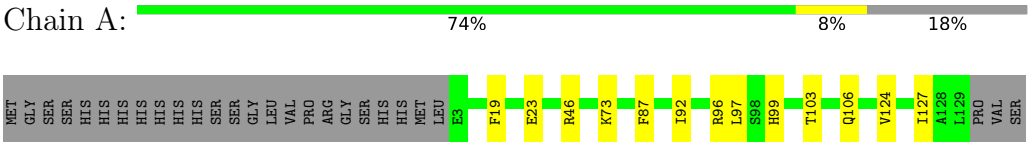
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	38	Total O 38 38	0	0
3	B	26	Total O 26 26	0	0
3	C	33	Total O 33 33	0	0
3	D	27	Total O 27 27	0	0
3	E	21	Total O 21 21	0	0
3	F	24	Total O 24 24	0	0
3	G	20	Total O 20 20	0	0
3	H	20	Total O 20 20	0	0
3	I	17	Total O 17 17	0	0
3	J	30	Total O 30 30	0	0
3	K	18	Total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

3 Residue-property plots (i)

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.

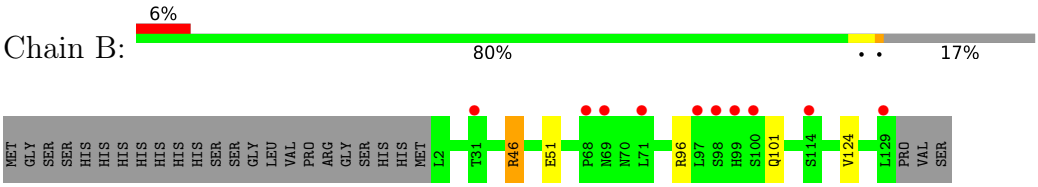
• Molecule 1: atzH

Chain A:



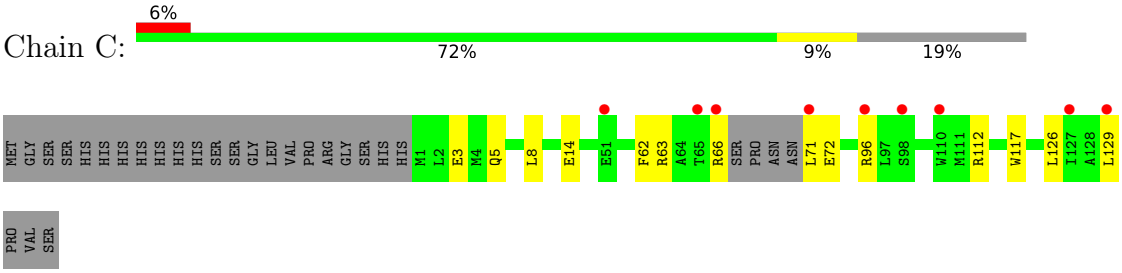
• Molecule 1: atzH

Chain B:



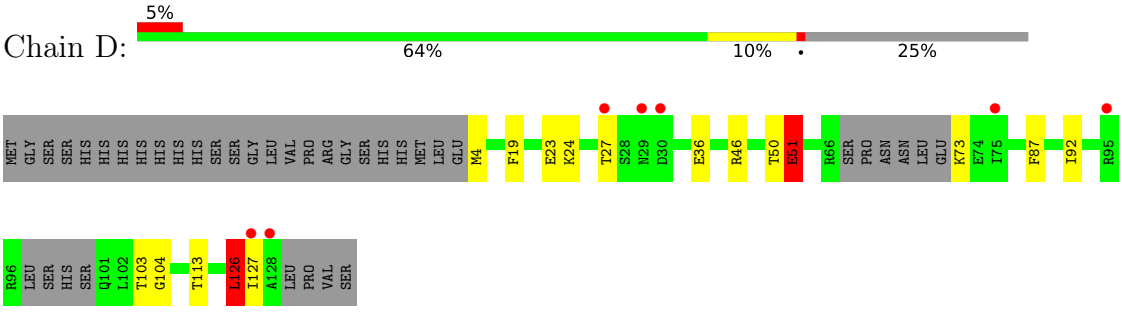
• Molecule 1: atzH

Chain C:



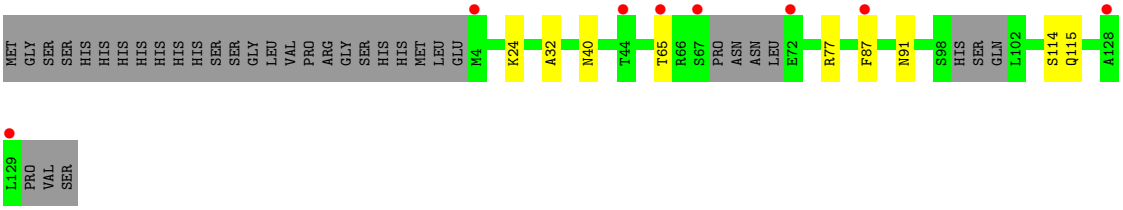
• Molecule 1: atzH

Chain D:



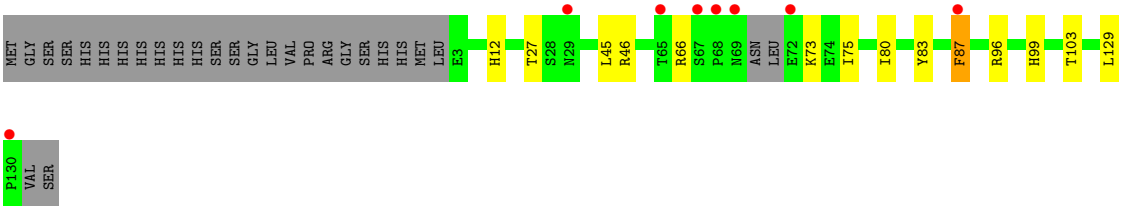
• Molecule 1: atzH

Chain E:



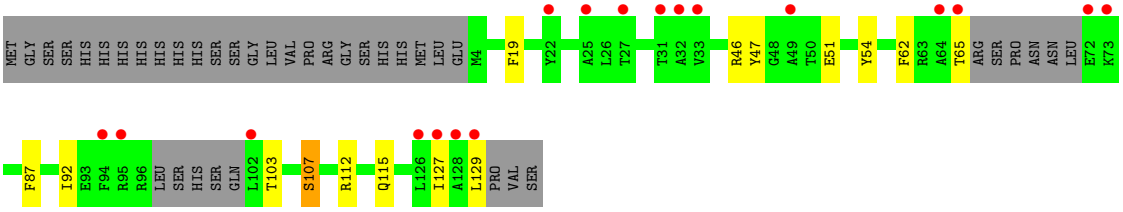
• Molecule 1: atzH

Chain F:



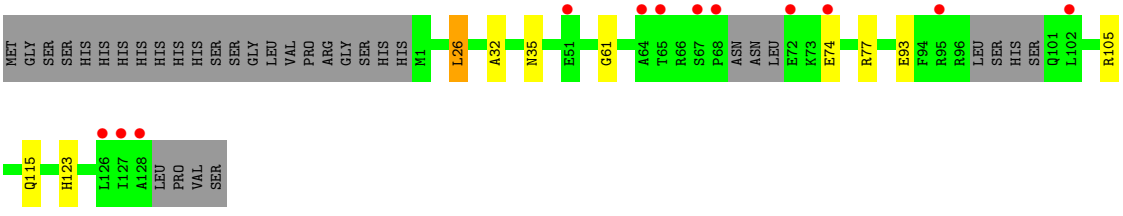
• Molecule 1: atzH

Chain G:



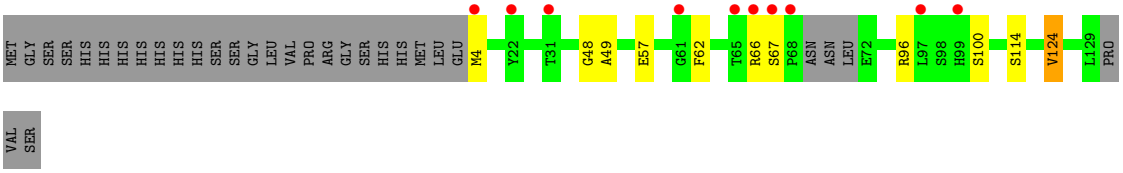
• Molecule 1: atzH

Chain H:

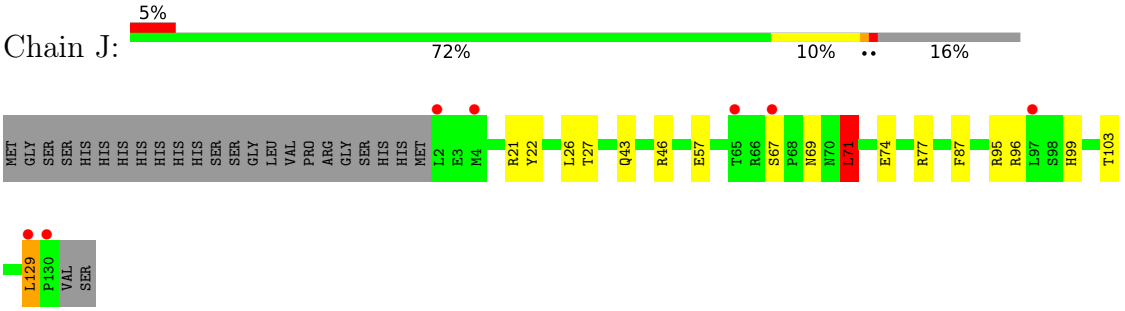


• Molecule 1: atzH

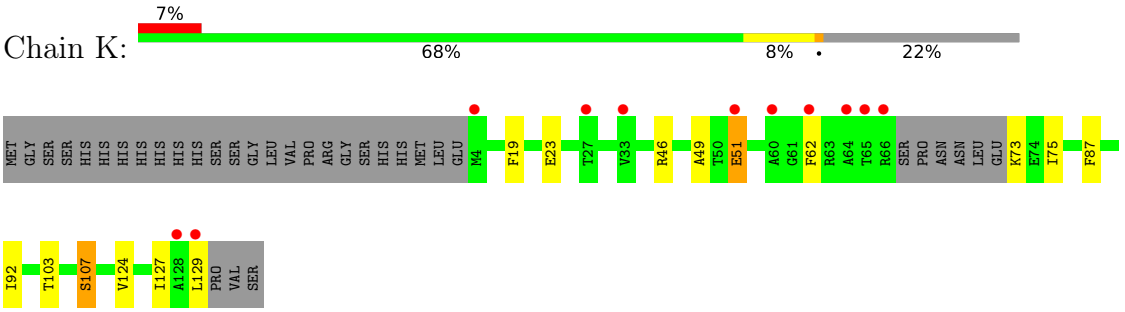
Chain I:



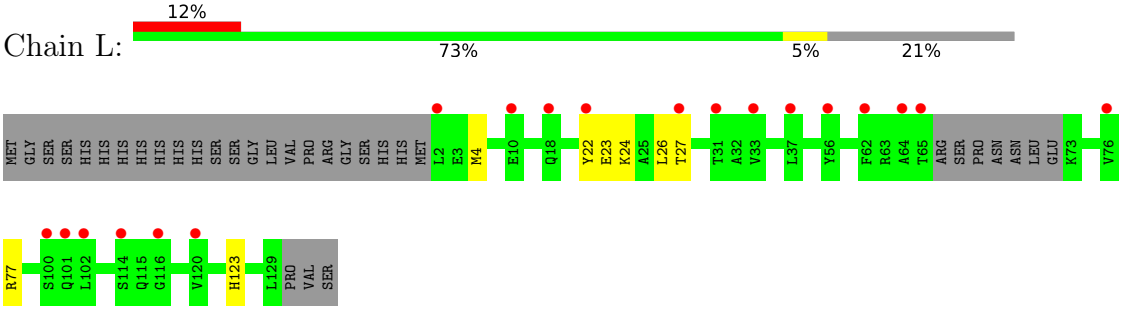
• Molecule 1: atzH



• 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, α, β, γ	99.72Å 74.66Å 103.61Å 90.00° 96.69° 90.00°	Depositor
Resolution (Å)	50.10 – 2.30 50.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.10-2.30) 100.0 (50.08-2.30)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.249 , 0.286 0.256 , 0.292	Depositor DCC
R_{free} test set	3196 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12009	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.59	0/1032	0.73	0/1405
1	B	0.59	0/1045	0.72	1/1423 (0.1%)
1	C	0.69	0/1020	0.77	0/1386
1	D	0.68	0/943	0.84	3/1279 (0.2%)
1	E	0.55	0/974	0.69	0/1322
1	F	0.57	0/1025	0.74	1/1396 (0.1%)
1	G	0.61	0/910	0.75	1/1239 (0.1%)
1	H	0.60	0/982	0.75	1/1334 (0.1%)
1	I	0.63	1/996 (0.1%)	0.75	0/1355
1	J	0.58	0/1057	0.77	3/1441 (0.2%)
1	K	0.56	0/973	0.67	0/1324
1	L	0.55	0/978	0.69	0/1331
All	All	0.60	1/11935 (0.0%)	0.74	10/16235 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	124	VAL	CB-CG1	-5.08	1.42	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	126	LEU	CB-CG-CD2	7.39	123.56	111.00
1	D	51	GLU	OE1-CD-OE2	-6.45	115.56	123.30
1	B	46	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	F	46	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	J	71	LEU	CA-CB-CG	5.30	127.49	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	10	0
1	B	1023	0	991	4	0
1	C	1000	0	977	16	0
1	D	925	0	902	13	0
1	E	956	0	924	15	0
1	F	1002	0	956	13	0
1	G	892	0	848	11	0
1	H	963	0	933	13	0
1	I	975	0	929	9	0
1	J	1033	0	995	12	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	105	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 105 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	0.76

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%)	76 87
1	B	105/132 (80%)	103 (98%)	2 (2%)	57 73
1	C	102/132 (77%)	102 (100%)	0	100 100
1	D	95/132 (72%)	91 (96%)	4 (4%)	30 42
1	E	97/132 (74%)	95 (98%)	2 (2%)	53 70
1	F	101/132 (76%)	97 (96%)	4 (4%)	31 44
1	G	86/132 (65%)	82 (95%)	4 (5%)	26 37
1	H	99/132 (75%)	96 (97%)	3 (3%)	41 57
1	I	97/132 (74%)	94 (97%)	3 (3%)	40 55
1	J	106/132 (80%)	99 (93%)	7 (7%)	16 22
1	K	96/132 (73%)	92 (96%)	4 (4%)	30 42
1	L	96/132 (73%)	94 (98%)	2 (2%)	53 70
All	All	1181/1584 (75%)	1145 (97%)	36 (3%)	42 57

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	87[B]	PHE
1	L	77	ARG
1	J	129	LEU
1	K	87	PHE
1	F	87[B]	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	12	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	A	201	-	9,9,9	1.05	0	11,11,11	2.78	5 (45%)
2	6JN	B	201	-	9,9,9	0.90	0	11,11,11	1.75	3 (27%)
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	A	201	-	-	3/8/8/8	-
2	6JN	B	201	-	-	5/8/8/8	-
2	6JN	J	201	-	-	6/8/8/8	-

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	6JN	CAC-CAA-CAB	-5.20	101.61	112.38
2	A	201	6JN	OAF-CAE-OAG	4.60	134.75	123.30
2	A	201	6JN	OAG-CAE-CAD	-3.87	110.78	122.08
2	J	201	6JN	OAI-CAB-OAJ	3.59	132.25	123.30
2	J	201	6JN	CAC-CAD-CAE	-3.41	105.30	112.38

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	6JN	OAH-CAC-CAD-CAE
2	J	201	6JN	CAC-CAA-CAB-OAI
2	J	201	6JN	CAB-CAA-CAC-OAH
2	J	201	6JN	CAC-CAA-CAB-OAJ
2	J	201	6JN	CAC-CAD-CAE-OAG

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	6JN	3	0
2	B	201	6JN	4	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	127/154 (82%)	0.31	0 100 100	8, 17, 34, 48	0
1	B	128/154 (83%)	0.60	10 (7%) 13 17	9, 21, 61, 85	0
1	C	125/154 (81%)	0.52	9 (7%) 15 20	10, 19, 38, 76	0
1	D	115/154 (74%)	0.58	7 (6%) 21 27	10, 20, 53, 68	0
1	E	119/154 (77%)	0.67	8 (6%) 17 23	13, 24, 53, 77	0
1	F	126/154 (81%)	0.56	8 (6%) 20 25	13, 21, 48, 73	0
1	G	115/154 (74%)	1.02	18 (15%) 2 2	11, 25, 64, 80	0
1	H	121/154 (78%)	0.75	12 (9%) 7 10	12, 22, 52, 80	0
1	I	123/154 (79%)	0.67	10 (8%) 12 16	13, 23, 53, 88	0
1	J	129/154 (83%)	0.46	7 (5%) 25 32	8, 19, 47, 61	0
1	K	120/154 (77%)	0.76	11 (9%) 9 12	13, 27, 60, 79	0
1	L	121/154 (78%)	1.13	19 (15%) 2 2	15, 34, 65, 83	0
All	All	1469/1848 (79%)	0.66	119 (8%) 12 16	8, 22, 56, 88	0

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	67	SER	6.4
1	G	102	LEU	5.8
1	L	64	ALA	5.6
1	E	129	LEU	5.1
1	K	65	THR	5.1

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 monosaccharides 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^{th} 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	6JN	B	201	10/10	0.74	0.27	54,58,62,71	0
2	6JN	A	201	10/10	0.83	0.23	25,30,31,33	0
2	6JN	J	201	10/10	0.86	0.17	26,32,36,39	0

6.5 Other polymers (i)

There are no such residues in this entry.