



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 12:30 AM BST

PDB ID : 4V1Y  
Title : The structure of the hexameric atrazine chlorohydrolase, AtzA  
Authors : Peat, T.S.; Newman, J.; Balotra, S.; Lucent, D.; Warden, A.C.; Scott, C.  
Deposited on : 2014-10-04  
Resolution : 2.80 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.

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

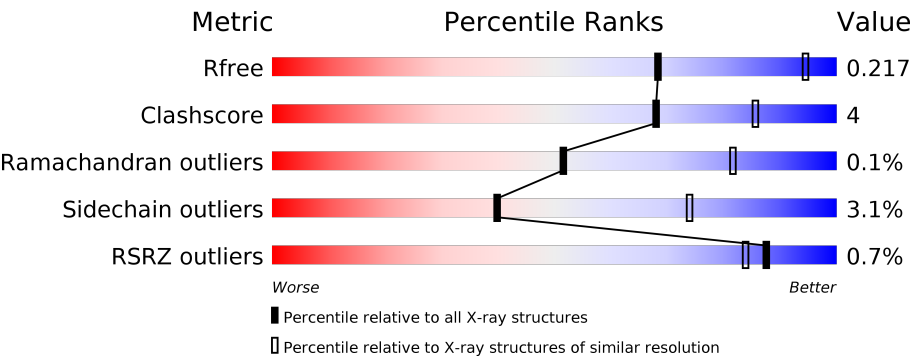
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

# 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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	494	<div><div>2%</div><div><div></div><div>88%</div><div>6%</div><div></div></div><div></div></div>
1	B	494	<div><div></div><div><div></div><div>85%</div><div>10%</div><div></div></div><div></div></div>
1	C	494	<div><div>2%</div><div><div></div><div>87%</div><div>8%</div><div></div></div><div></div></div>
1	D	494	<div><div></div><div><div></div><div>89%</div><div>6%</div><div></div></div><div></div></div>
1	E	494	<div><div></div><div><div></div><div>88%</div><div>7%</div><div></div></div><div></div></div>
1	F	494	<div><div></div><div><div></div><div>87%</div><div>8%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	494	 87% 7% . .
1	H	494	 87% 8% .
1	I	494	 86% 9% . .
1	J	494	 86% 9% . .
1	K	494	 87% 9% . .
1	L	494	 87% 8% . .

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
3	EDO	B	1475	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 44883 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 ATRAZINE CHLOROXYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	5	0
			3725	2323	687	691	24			
1	B	474	Total	C	N	O	S	0	5	0
			3735	2329	690	691	25			
1	C	473	Total	C	N	O	S	0	2	0
			3695	2308	680	683	24			
1	D	474	Total	C	N	O	S	0	2	0
			3704	2312	681	686	25			
1	E	474	Total	C	N	O	S	0	5	0
			3732	2329	688	690	25			
1	F	474	Total	C	N	O	S	0	3	0
			3710	2315	683	688	24			
1	G	474	Total	C	N	O	S	0	4	0
			3719	2320	683	690	26			
1	H	472	Total	C	N	O	S	0	4	0
			3707	2313	683	687	24			
1	I	474	Total	C	N	O	S	0	3	0
			3712	2318	683	686	25			
1	J	473	Total	C	N	O	S	0	3	0
			3705	2312	682	687	24			
1	K	474	Total	C	N	O	S	0	7	0
			3749	2338	692	693	26			
1	L	474	Total	C	N	O	S	0	4	0
			3719	2320	685	690	24			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P72156
A	-18	GLY	-	expression tag	UNP P72156
A	-17	SER	-	expression tag	UNP P72156
A	-16	SER	-	expression tag	UNP P72156
A	-15	HIS	-	expression tag	UNP P72156

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P72156
A	-13	HIS	-	expression tag	UNP P72156
A	-12	HIS	-	expression tag	UNP P72156
A	-11	HIS	-	expression tag	UNP P72156
A	-10	HIS	-	expression tag	UNP P72156
A	-9	SER	-	expression tag	UNP P72156
A	-8	SER	-	expression tag	UNP P72156
A	-7	GLY	-	expression tag	UNP P72156
A	-6	LEU	-	expression tag	UNP P72156
A	-5	VAL	-	expression tag	UNP P72156
A	-4	PRO	-	expression tag	UNP P72156
A	-3	ARG	-	expression tag	UNP P72156
A	-2	GLY	-	expression tag	UNP P72156
A	-1	SER	-	expression tag	UNP P72156
A	0	HIS	-	expression tag	UNP P72156
B	-19	MET	-	expression tag	UNP P72156
B	-18	GLY	-	expression tag	UNP P72156
B	-17	SER	-	expression tag	UNP P72156
B	-16	SER	-	expression tag	UNP P72156
B	-15	HIS	-	expression tag	UNP P72156
B	-14	HIS	-	expression tag	UNP P72156
B	-13	HIS	-	expression tag	UNP P72156
B	-12	HIS	-	expression tag	UNP P72156
B	-11	HIS	-	expression tag	UNP P72156
B	-10	HIS	-	expression tag	UNP P72156
B	-9	SER	-	expression tag	UNP P72156
B	-8	SER	-	expression tag	UNP P72156
B	-7	GLY	-	expression tag	UNP P72156
B	-6	LEU	-	expression tag	UNP P72156
B	-5	VAL	-	expression tag	UNP P72156
B	-4	PRO	-	expression tag	UNP P72156
B	-3	ARG	-	expression tag	UNP P72156
B	-2	GLY	-	expression tag	UNP P72156
B	-1	SER	-	expression tag	UNP P72156
B	0	HIS	-	expression tag	UNP P72156
C	-19	MET	-	expression tag	UNP P72156
C	-18	GLY	-	expression tag	UNP P72156
C	-17	SER	-	expression tag	UNP P72156
C	-16	SER	-	expression tag	UNP P72156
C	-15	HIS	-	expression tag	UNP P72156
C	-14	HIS	-	expression tag	UNP P72156
C	-13	HIS	-	expression tag	UNP P72156

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP P72156
C	-11	HIS	-	expression tag	UNP P72156
C	-10	HIS	-	expression tag	UNP P72156
C	-9	SER	-	expression tag	UNP P72156
C	-8	SER	-	expression tag	UNP P72156
C	-7	GLY	-	expression tag	UNP P72156
C	-6	LEU	-	expression tag	UNP P72156
C	-5	VAL	-	expression tag	UNP P72156
C	-4	PRO	-	expression tag	UNP P72156
C	-3	ARG	-	expression tag	UNP P72156
C	-2	GLY	-	expression tag	UNP P72156
C	-1	SER	-	expression tag	UNP P72156
C	0	HIS	-	expression tag	UNP P72156
D	-19	MET	-	expression tag	UNP P72156
D	-18	GLY	-	expression tag	UNP P72156
D	-17	SER	-	expression tag	UNP P72156
D	-16	SER	-	expression tag	UNP P72156
D	-15	HIS	-	expression tag	UNP P72156
D	-14	HIS	-	expression tag	UNP P72156
D	-13	HIS	-	expression tag	UNP P72156
D	-12	HIS	-	expression tag	UNP P72156
D	-11	HIS	-	expression tag	UNP P72156
D	-10	HIS	-	expression tag	UNP P72156
D	-9	SER	-	expression tag	UNP P72156
D	-8	SER	-	expression tag	UNP P72156
D	-7	GLY	-	expression tag	UNP P72156
D	-6	LEU	-	expression tag	UNP P72156
D	-5	VAL	-	expression tag	UNP P72156
D	-4	PRO	-	expression tag	UNP P72156
D	-3	ARG	-	expression tag	UNP P72156
D	-2	GLY	-	expression tag	UNP P72156
D	-1	SER	-	expression tag	UNP P72156
D	0	HIS	-	expression tag	UNP P72156
E	-19	MET	-	expression tag	UNP P72156
E	-18	GLY	-	expression tag	UNP P72156
E	-17	SER	-	expression tag	UNP P72156
E	-16	SER	-	expression tag	UNP P72156
E	-15	HIS	-	expression tag	UNP P72156
E	-14	HIS	-	expression tag	UNP P72156
E	-13	HIS	-	expression tag	UNP P72156
E	-12	HIS	-	expression tag	UNP P72156
E	-11	HIS	-	expression tag	UNP P72156

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP P72156
E	-9	SER	-	expression tag	UNP P72156
E	-8	SER	-	expression tag	UNP P72156
E	-7	GLY	-	expression tag	UNP P72156
E	-6	LEU	-	expression tag	UNP P72156
E	-5	VAL	-	expression tag	UNP P72156
E	-4	PRO	-	expression tag	UNP P72156
E	-3	ARG	-	expression tag	UNP P72156
E	-2	GLY	-	expression tag	UNP P72156
E	-1	SER	-	expression tag	UNP P72156
E	0	HIS	-	expression tag	UNP P72156
F	-19	MET	-	expression tag	UNP P72156
F	-18	GLY	-	expression tag	UNP P72156
F	-17	SER	-	expression tag	UNP P72156
F	-16	SER	-	expression tag	UNP P72156
F	-15	HIS	-	expression tag	UNP P72156
F	-14	HIS	-	expression tag	UNP P72156
F	-13	HIS	-	expression tag	UNP P72156
F	-12	HIS	-	expression tag	UNP P72156
F	-11	HIS	-	expression tag	UNP P72156
F	-10	HIS	-	expression tag	UNP P72156
F	-9	SER	-	expression tag	UNP P72156
F	-8	SER	-	expression tag	UNP P72156
F	-7	GLY	-	expression tag	UNP P72156
F	-6	LEU	-	expression tag	UNP P72156
F	-5	VAL	-	expression tag	UNP P72156
F	-4	PRO	-	expression tag	UNP P72156
F	-3	ARG	-	expression tag	UNP P72156
F	-2	GLY	-	expression tag	UNP P72156
F	-1	SER	-	expression tag	UNP P72156
F	0	HIS	-	expression tag	UNP P72156
G	-19	MET	-	expression tag	UNP P72156
G	-18	GLY	-	expression tag	UNP P72156
G	-17	SER	-	expression tag	UNP P72156
G	-16	SER	-	expression tag	UNP P72156
G	-15	HIS	-	expression tag	UNP P72156
G	-14	HIS	-	expression tag	UNP P72156
G	-13	HIS	-	expression tag	UNP P72156
G	-12	HIS	-	expression tag	UNP P72156
G	-11	HIS	-	expression tag	UNP P72156
G	-10	HIS	-	expression tag	UNP P72156
G	-9	SER	-	expression tag	UNP P72156

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	expression tag	UNP P72156
G	-7	GLY	-	expression tag	UNP P72156
G	-6	LEU	-	expression tag	UNP P72156
G	-5	VAL	-	expression tag	UNP P72156
G	-4	PRO	-	expression tag	UNP P72156
G	-3	ARG	-	expression tag	UNP P72156
G	-2	GLY	-	expression tag	UNP P72156
G	-1	SER	-	expression tag	UNP P72156
G	0	HIS	-	expression tag	UNP P72156
H	-19	MET	-	expression tag	UNP P72156
H	-18	GLY	-	expression tag	UNP P72156
H	-17	SER	-	expression tag	UNP P72156
H	-16	SER	-	expression tag	UNP P72156
H	-15	HIS	-	expression tag	UNP P72156
H	-14	HIS	-	expression tag	UNP P72156
H	-13	HIS	-	expression tag	UNP P72156
H	-12	HIS	-	expression tag	UNP P72156
H	-11	HIS	-	expression tag	UNP P72156
H	-10	HIS	-	expression tag	UNP P72156
H	-9	SER	-	expression tag	UNP P72156
H	-8	SER	-	expression tag	UNP P72156
H	-7	GLY	-	expression tag	UNP P72156
H	-6	LEU	-	expression tag	UNP P72156
H	-5	VAL	-	expression tag	UNP P72156
H	-4	PRO	-	expression tag	UNP P72156
H	-3	ARG	-	expression tag	UNP P72156
H	-2	GLY	-	expression tag	UNP P72156
H	-1	SER	-	expression tag	UNP P72156
H	0	HIS	-	expression tag	UNP P72156
I	-19	MET	-	expression tag	UNP P72156
I	-18	GLY	-	expression tag	UNP P72156
I	-17	SER	-	expression tag	UNP P72156
I	-16	SER	-	expression tag	UNP P72156
I	-15	HIS	-	expression tag	UNP P72156
I	-14	HIS	-	expression tag	UNP P72156
I	-13	HIS	-	expression tag	UNP P72156
I	-12	HIS	-	expression tag	UNP P72156
I	-11	HIS	-	expression tag	UNP P72156
I	-10	HIS	-	expression tag	UNP P72156
I	-9	SER	-	expression tag	UNP P72156
I	-8	SER	-	expression tag	UNP P72156
I	-7	GLY	-	expression tag	UNP P72156

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	expression tag	UNP P72156
I	-5	VAL	-	expression tag	UNP P72156
I	-4	PRO	-	expression tag	UNP P72156
I	-3	ARG	-	expression tag	UNP P72156
I	-2	GLY	-	expression tag	UNP P72156
I	-1	SER	-	expression tag	UNP P72156
I	0	HIS	-	expression tag	UNP P72156
J	-19	MET	-	expression tag	UNP P72156
J	-18	GLY	-	expression tag	UNP P72156
J	-17	SER	-	expression tag	UNP P72156
J	-16	SER	-	expression tag	UNP P72156
J	-15	HIS	-	expression tag	UNP P72156
J	-14	HIS	-	expression tag	UNP P72156
J	-13	HIS	-	expression tag	UNP P72156
J	-12	HIS	-	expression tag	UNP P72156
J	-11	HIS	-	expression tag	UNP P72156
J	-10	HIS	-	expression tag	UNP P72156
J	-9	SER	-	expression tag	UNP P72156
J	-8	SER	-	expression tag	UNP P72156
J	-7	GLY	-	expression tag	UNP P72156
J	-6	LEU	-	expression tag	UNP P72156
J	-5	VAL	-	expression tag	UNP P72156
J	-4	PRO	-	expression tag	UNP P72156
J	-3	ARG	-	expression tag	UNP P72156
J	-2	GLY	-	expression tag	UNP P72156
J	-1	SER	-	expression tag	UNP P72156
J	0	HIS	-	expression tag	UNP P72156
K	-19	MET	-	expression tag	UNP P72156
K	-18	GLY	-	expression tag	UNP P72156
K	-17	SER	-	expression tag	UNP P72156
K	-16	SER	-	expression tag	UNP P72156
K	-15	HIS	-	expression tag	UNP P72156
K	-14	HIS	-	expression tag	UNP P72156
K	-13	HIS	-	expression tag	UNP P72156
K	-12	HIS	-	expression tag	UNP P72156
K	-11	HIS	-	expression tag	UNP P72156
K	-10	HIS	-	expression tag	UNP P72156
K	-9	SER	-	expression tag	UNP P72156
K	-8	SER	-	expression tag	UNP P72156
K	-7	GLY	-	expression tag	UNP P72156
K	-6	LEU	-	expression tag	UNP P72156
K	-5	VAL	-	expression tag	UNP P72156

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP P72156
K	-3	ARG	-	expression tag	UNP P72156
K	-2	GLY	-	expression tag	UNP P72156
K	-1	SER	-	expression tag	UNP P72156
K	0	HIS	-	expression tag	UNP P72156
L	-19	MET	-	expression tag	UNP P72156
L	-18	GLY	-	expression tag	UNP P72156
L	-17	SER	-	expression tag	UNP P72156
L	-16	SER	-	expression tag	UNP P72156
L	-15	HIS	-	expression tag	UNP P72156
L	-14	HIS	-	expression tag	UNP P72156
L	-13	HIS	-	expression tag	UNP P72156
L	-12	HIS	-	expression tag	UNP P72156
L	-11	HIS	-	expression tag	UNP P72156
L	-10	HIS	-	expression tag	UNP P72156
L	-9	SER	-	expression tag	UNP P72156
L	-8	SER	-	expression tag	UNP P72156
L	-7	GLY	-	expression tag	UNP P72156
L	-6	LEU	-	expression tag	UNP P72156
L	-5	VAL	-	expression tag	UNP P72156
L	-4	PRO	-	expression tag	UNP P72156
L	-3	ARG	-	expression tag	UNP P72156
L	-2	GLY	-	expression tag	UNP P72156
L	-1	SER	-	expression tag	UNP P72156
L	0	HIS	-	expression tag	UNP P72156

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

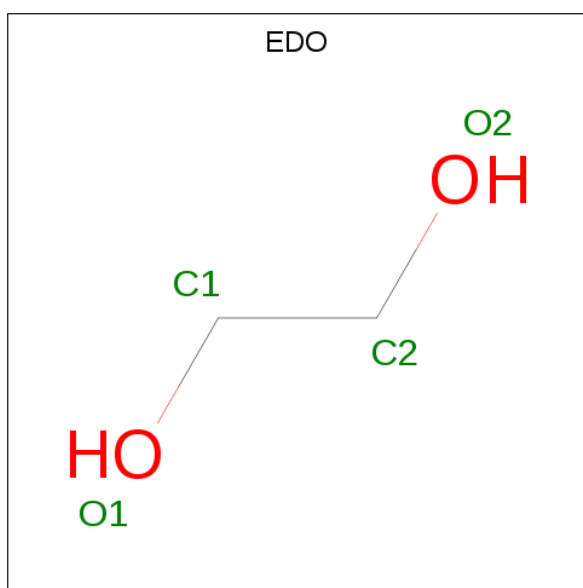
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Fe 1 1	0	0
2	J	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	L	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



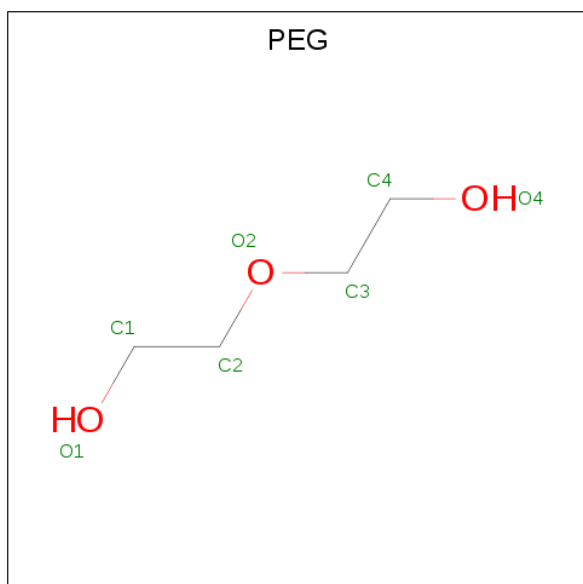
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	I	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	K	1	Total	C	O	0	0
			7	4	3		
4	L	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Cl	0	0
			1	1		

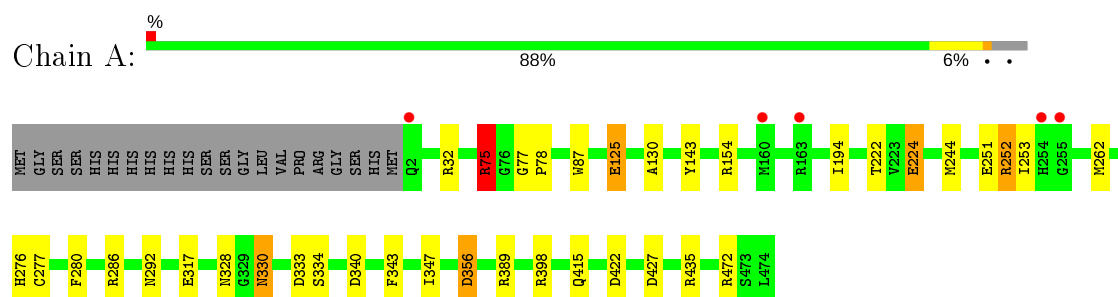
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	O	0	0
			14	14		
6	B	17	Total	O	0	0
			17	17		
6	C	11	Total	O	0	0
			11	11		
6	D	10	Total	O	0	0
			10	10		
6	E	15	Total	O	0	0
			15	15		
6	F	7	Total	O	0	0
			7	7		
6	G	11	Total	O	0	0
			11	11		
6	H	11	Total	O	0	0
			11	11		
6	I	25	Total	O	0	0
			25	25		
6	J	8	Total	O	0	0
			8	8		
6	K	20	Total	O	0	0
			20	20		
6	L	12	Total	O	0	0
			12	12		

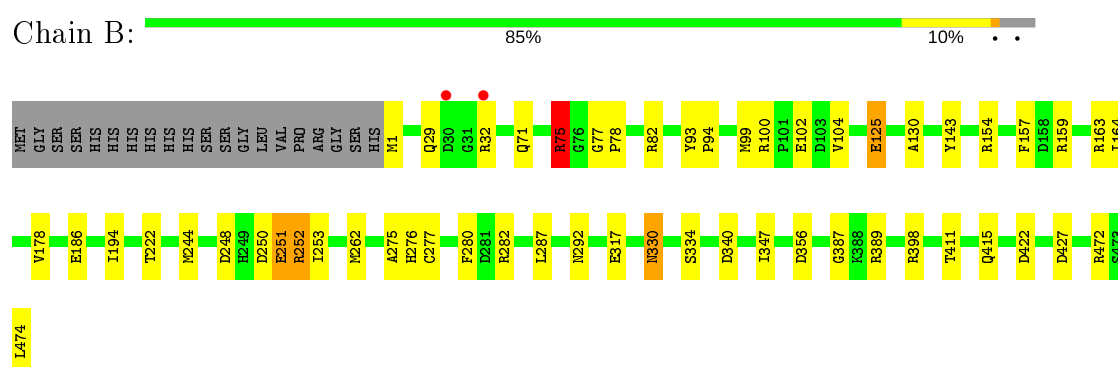
### 3 Residue-property plots [i](#)

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.

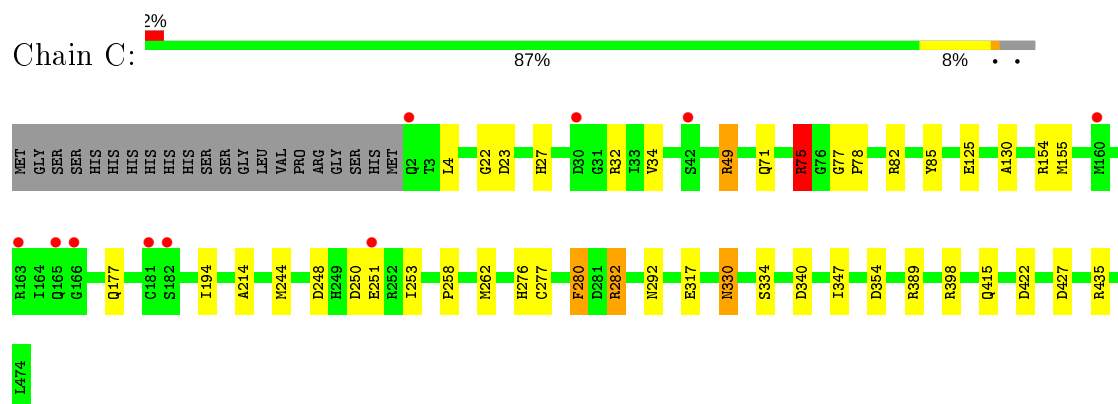
#### • Molecule 1: ATRAZINE CHLOROXYDROLASE



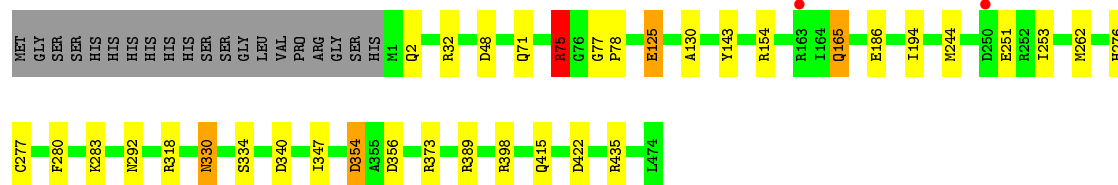

#### • Molecule 1: ATRAZINE CHLOROXYDROLASE



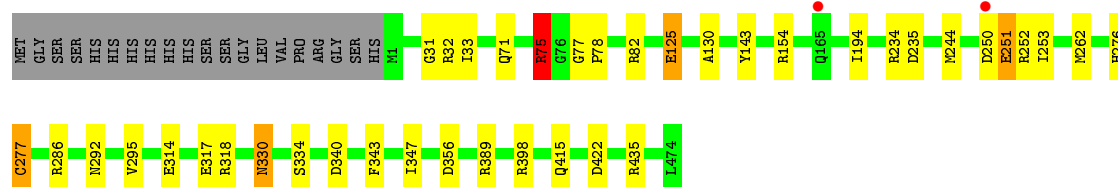

#### • Molecule 1: ATRAZINE CHLOROXYDROLASE



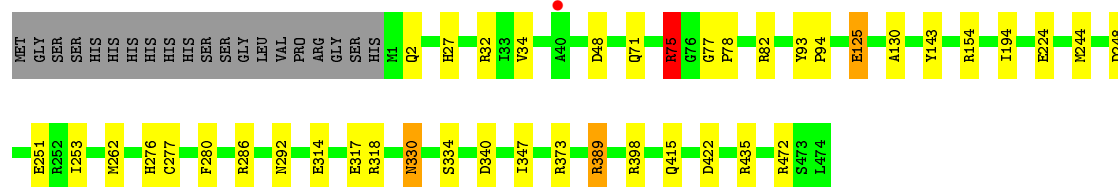
#### • Molecule 1: ATRAZINE CHLOROXYDROLASE

Chain D: 

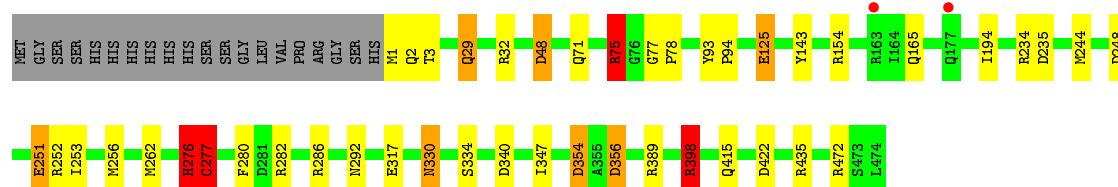

• Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain E: 

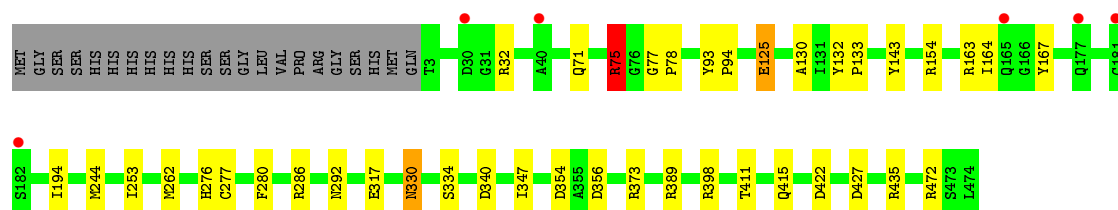

• Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain F: 

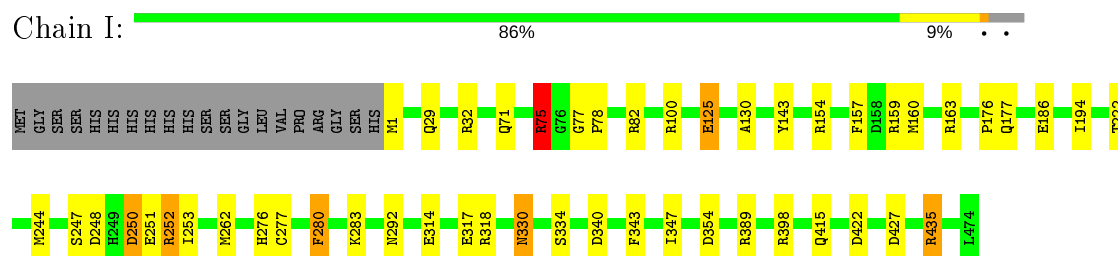
• Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain G: 

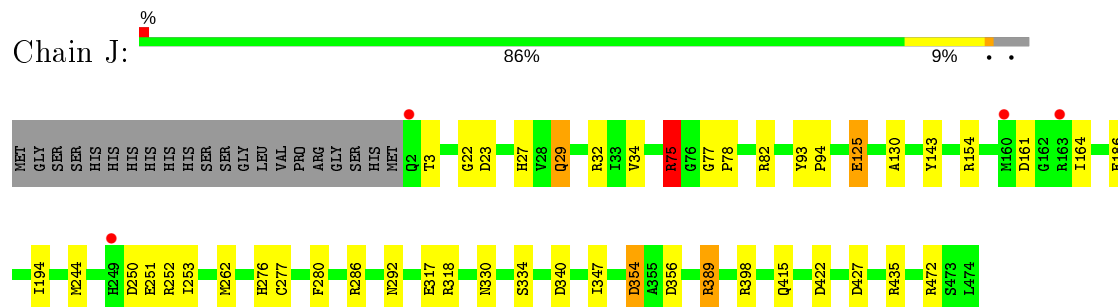
• Molecule 1: ATRAZINE CHLOROHYDROLASE

Chain H: 

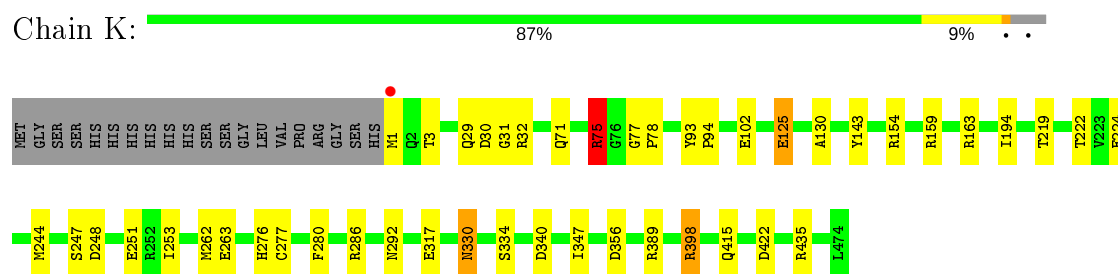
- Molecule 1: ATRAZINE CHLOROHYDROLASE



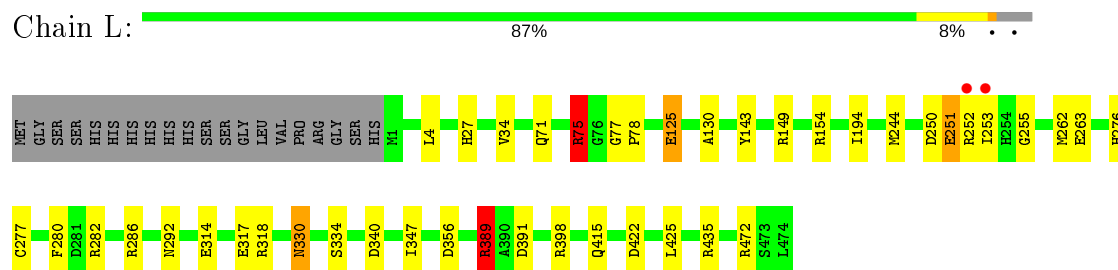
- Molecule 1: ATRAZINE CHLOROHYDROLASE



- Molecule 1: ATRAZINE CHLOROHYDROLASE



- Molecule 1: ATRAZINE CHLOROHYDROLASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.49 Å   195.56 Å   283.88 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	161.05 – 2.80 49.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (161.05-2.80) 100.0 (49.46-2.80)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.187   ,   0.218 0.191   ,   0.217	Depositor DCC
$R_{free}$ test set	7864 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 23.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	44883	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5597e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: CL, PEG, EDO, FE

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	0.71	0/3802	0.83	3/5160 (0.1%)
1	B	0.77	0/3812	0.87	3/5172 (0.1%)
1	C	0.65	0/3772	0.82	4/5121 (0.1%)
1	D	0.72	0/3781	0.84	5/5132 (0.1%)
1	E	0.73	0/3809	0.83	3/5169 (0.1%)
1	F	0.72	0/3787	0.85	4/5141 (0.1%)
1	G	0.72	1/3796 (0.0%)	0.86	9/5152 (0.2%)
1	H	0.67	0/3784	0.82	3/5136 (0.1%)
1	I	0.78	0/3789	0.86	4/5143 (0.1%)
1	J	0.72	0/3782	0.85	6/5134 (0.1%)
1	K	0.72	0/3826	0.84	4/5191 (0.1%)
1	L	0.74	0/3796	0.86	6/5153 (0.1%)
All	All	0.72	1/45536 (0.0%)	0.84	54/61804 (0.1%)

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	G	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1	MET	C-N	7.38	1.51	1.34

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	75	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	L	389	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	I	75	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	G	276	HIS	O-C-N	-8.13	109.69	122.70
1	D	435	ARG	NE-CZ-NH1	7.99	124.30	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	276	HIS	Mainchain,Peptide

## 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	3725	0	3656	38	0
1	B	3735	0	3673	53	0
1	C	3695	0	3637	27	0
1	D	3704	0	3644	30	0
1	E	3732	0	3673	30	0
1	F	3710	0	3644	30	0
1	G	3719	0	3653	39	0
1	H	3707	0	3641	26	0
1	I	3712	0	3656	41	0
1	J	3705	0	3639	29	0
1	K	3749	0	3687	29	0
1	L	3719	0	3649	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	8	0	12	0	0
3	B	4	0	6	6	0
3	C	4	0	6	2	0
3	E	4	0	6	0	0
3	F	4	0	6	0	0
3	G	4	0	6	0	0
3	H	4	0	6	0	0
3	J	8	0	12	3	0
3	L	8	0	12	3	0
4	B	7	0	10	1	0
4	C	7	0	10	0	0
4	D	7	0	10	2	0
4	F	7	0	10	0	0
4	I	7	0	10	2	0
4	K	7	0	10	1	0
4	L	7	0	10	1	0
5	H	1	0	0	0	0
6	A	14	0	0	0	0
6	B	17	0	0	4	0
6	C	11	0	0	0	0
6	D	10	0	0	0	0
6	E	15	0	0	0	0
6	F	7	0	0	0	0
6	G	11	0	0	0	0
6	H	11	0	0	1	0
6	I	25	0	0	1	0
6	J	8	0	0	0	0
6	K	20	0	0	1	0
6	L	12	0	0	0	0
All	All	44883	0	43994	340	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 4.

The worst 5 of 340 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:G:234:ARG:NH2	1:G:235:ASP:OD1	1.86	1.07
1:G:3:THR:HG22	1:G:29:GLN:HG3	1.36	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLU:HG2	1:I:222:THR:HG22	1.39	1.03
1:G:3:THR:CG2	1:G:29:GLN:HG3	1.98	0.94
1:K:277[A]:CYS:SG	1:K:280:PHE:CZ	2.62	0.93

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	476/494 (96%)	454 (95%)	22 (5%)	0	100	100
1	B	477/494 (97%)	454 (95%)	22 (5%)	1 (0%)	47	78
1	C	473/494 (96%)	454 (96%)	19 (4%)	0	100	100
1	D	474/494 (96%)	452 (95%)	22 (5%)	0	100	100
1	E	477/494 (97%)	457 (96%)	19 (4%)	1 (0%)	47	78
1	F	475/494 (96%)	456 (96%)	19 (4%)	0	100	100
1	G	476/494 (96%)	456 (96%)	19 (4%)	1 (0%)	47	78
1	H	474/494 (96%)	454 (96%)	20 (4%)	0	100	100
1	I	475/494 (96%)	456 (96%)	19 (4%)	0	100	100
1	J	474/494 (96%)	453 (96%)	20 (4%)	1 (0%)	47	78
1	K	479/494 (97%)	461 (96%)	18 (4%)	0	100	100
1	L	476/494 (96%)	457 (96%)	18 (4%)	1 (0%)	47	78
All	All	5706/5928 (96%)	5464 (96%)	237 (4%)	5 (0%)	51	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	GLU

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Mol	Chain	Res	Type
1	L	251	GLU
1	E	251	GLU
1	J	251	GLU
1	G	251	GLU

### 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	391/404 (97%)	379 (97%)	12 (3%)	40	74
1	B	392/404 (97%)	381 (97%)	11 (3%)	43	77
1	C	388/404 (96%)	375 (97%)	13 (3%)	37	71
1	D	389/404 (96%)	377 (97%)	12 (3%)	40	74
1	E	392/404 (97%)	380 (97%)	12 (3%)	40	74
1	F	389/404 (96%)	376 (97%)	13 (3%)	38	72
1	G	391/404 (97%)	375 (96%)	16 (4%)	30	64
1	H	389/404 (96%)	376 (97%)	13 (3%)	38	72
1	I	390/404 (96%)	375 (96%)	15 (4%)	33	67
1	J	389/404 (96%)	375 (96%)	14 (4%)	35	69
1	K	394/404 (98%)	381 (97%)	13 (3%)	38	72
1	L	390/404 (96%)	378 (97%)	12 (3%)	40	74
All	All	4684/4848 (97%)	4528 (97%)	156 (3%)	40	72

5 of 156 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	389	ARG
1	G	398	ARG
1	L	75	ARG
1	F	422	ASP
1	G	277[B]	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	254	HIS
1	H	276	HIS
1	L	165	GLN
1	G	276	HIS
1	G	330	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 13 are monoatomic - leaving 19 for Mogul analysis.

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	$\# Z  > 2$
3	EDO	A	1475	-	3,3,3	0.86	0	2,2,2	0.60	0
3	EDO	B	1475	-	3,3,3	0.49	0	2,2,2	0.17	0
3	EDO	G	1475	-	3,3,3	0.78	0	2,2,2	0.63	0
3	EDO	H	1475	-	3,3,3	0.68	0	2,2,2	0.16	0
3	EDO	E	1475	-	3,3,3	0.96	0	2,2,2	0.69	0
4	PEG	D	1475	-	6,6,6	0.37	0	5,5,5	0.38	0
4	PEG	F	1476	-	6,6,6	0.47	0	5,5,5	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	L	1475	-	3,3,3	0.59	0	2,2,2	0.30	0
3	EDO	J	1475	-	3,3,3	0.75	0	2,2,2	0.75	0
4	PEG	I	1475	-	6,6,6	0.93	0	5,5,5	1.21	1 (20%)
4	PEG	K	1475	-	6,6,6	0.54	0	5,5,5	0.60	0
3	EDO	J	1476	-	3,3,3	0.38	0	2,2,2	0.15	0
4	PEG	C	1476	-	6,6,6	0.33	0	5,5,5	0.32	0
3	EDO	L	1476	-	3,3,3	0.26	0	2,2,2	0.75	0
4	PEG	L	1477	-	6,6,6	0.61	0	5,5,5	0.48	0
3	EDO	A	1476	-	3,3,3	0.41	0	2,2,2	0.60	0
4	PEG	B	1476	-	6,6,6	0.52	0	5,5,5	0.80	0
3	EDO	C	1475	-	3,3,3	0.41	0	2,2,2	1.12	0
3	EDO	F	1475	-	3,3,3	0.72	0	2,2,2	0.81	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	1475	-	-	1/1/1/1	-
3	EDO	B	1475	-	-	0/1/1/1	-
3	EDO	G	1475	-	-	1/1/1/1	-
3	EDO	H	1475	-	-	1/1/1/1	-
3	EDO	E	1475	-	-	1/1/1/1	-
4	PEG	D	1475	-	-	4/4/4/4	-
4	PEG	F	1476	-	-	2/4/4/4	-
3	EDO	L	1475	-	-	1/1/1/1	-
3	EDO	J	1475	-	-	1/1/1/1	-
4	PEG	I	1475	-	-	4/4/4/4	-
4	PEG	K	1475	-	-	0/4/4/4	-
3	EDO	J	1476	-	-	1/1/1/1	-
4	PEG	C	1476	-	-	3/4/4/4	-
3	EDO	L	1476	-	-	1/1/1/1	-
4	PEG	L	1477	-	-	2/4/4/4	-
3	EDO	A	1476	-	-	0/1/1/1	-
4	PEG	B	1476	-	-	1/4/4/4	-
3	EDO	C	1475	-	-	1/1/1/1	-
3	EDO	F	1475	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	I	1475	PEG	O2-C2-C1	2.11	119.32	110.07

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1477	PEG	O2-C3-C4-O4
4	B	1476	PEG	O1-C1-C2-O2
4	C	1476	PEG	O1-C1-C2-O2
4	C	1476	PEG	O2-C3-C4-O4
3	E	1475	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1475	EDO	6	0
4	D	1475	PEG	2	0
4	I	1475	PEG	2	0
4	K	1475	PEG	1	0
3	J	1476	EDO	3	0
3	L	1476	EDO	3	0
4	L	1477	PEG	1	0
4	B	1476	PEG	1	0
3	C	1475	EDO	2	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<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	473/494 (95%)	-0.41	5 (1%) 80 75	11, 28, 53, 92	0
1	B	474/494 (95%)	-0.56	2 (0%) 92 91	10, 20, 44, 76	0
1	C	473/494 (95%)	-0.21	10 (2%) 63 54	16, 35, 64, 97	0
1	D	474/494 (95%)	-0.41	2 (0%) 92 91	14, 27, 52, 77	0
1	E	474/494 (95%)	-0.41	2 (0%) 92 91	10, 25, 54, 79	0
1	F	474/494 (95%)	-0.37	1 (0%) 95 94	13, 26, 50, 79	0
1	G	474/494 (95%)	-0.38	2 (0%) 92 91	14, 30, 59, 89	0
1	H	472/494 (95%)	-0.23	6 (1%) 77 72	18, 35, 63, 90	0
1	I	474/494 (95%)	-0.59	0 100 100	10, 19, 44, 79	0
1	J	473/494 (95%)	-0.44	4 (0%) 86 81	12, 25, 52, 85	0
1	K	474/494 (95%)	-0.38	1 (0%) 95 94	12, 25, 51, 86	0
1	L	474/494 (95%)	-0.46	2 (0%) 92 91	12, 23, 49, 77	0
All	All	5683/5928 (95%)	-0.40	37 (0%) 87 84	10, 26, 54, 97	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	ARG	5.0
1	C	181	CYS	3.9
1	K	1	MET	3.1
1	C	165	GLN	3.1
1	A	160	MET	3.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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( $\text{\AA}^2$ )	Q<0.9
2	FE	C	481	1/1	0.76	0.24	38,38,38,38	1
5	CL	H	1476	1/1	0.78	0.28	48,48,48,48	0
4	PEG	L	1477	7/7	0.82	0.23	22,24,31,31	0
4	PEG	K	1475	7/7	0.85	0.23	26,30,36,36	0
4	PEG	B	1476	7/7	0.86	0.21	20,22,26,27	0
4	PEG	D	1475	7/7	0.86	0.19	23,27,33,34	0
2	FE	E	481	1/1	0.88	0.19	33,33,33,33	1
4	PEG	I	1475	7/7	0.89	0.23	33,37,41,42	0
3	EDO	A	1475	4/4	0.89	0.20	31,33,34,35	0
2	FE	K	481	1/1	0.89	0.10	31,31,31,31	1
3	EDO	E	1475	4/4	0.89	0.17	24,26,28,28	0
2	FE	F	481	1/1	0.90	0.09	27,27,27,27	1
2	FE	G	481	1/1	0.90	0.10	31,31,31,31	1
2	FE	L	481	1/1	0.91	0.12	37,37,37,37	1
2	FE	J	481	1/1	0.92	0.24	32,32,32,32	1
3	EDO	J	1475	4/4	0.92	0.16	23,25,26,27	0
2	FE	I	481	1/1	0.92	0.09	35,35,35,35	1
3	EDO	L	1476	4/4	0.92	0.23	32,33,34,36	0
3	EDO	F	1475	4/4	0.93	0.20	23,23,24,24	0
3	EDO	J	1476	4/4	0.93	0.28	23,25,26,31	0
3	EDO	L	1475	4/4	0.93	0.20	22,23,24,25	0
4	PEG	C	1476	7/7	0.93	0.20	30,31,39,41	0
2	FE	H	481	1/1	0.93	0.18	29,29,29,29	1
3	EDO	C	1475	4/4	0.93	0.26	29,31,32,35	0
2	FE	A	481	1/1	0.94	0.22	33,33,33,33	1
3	EDO	G	1475	4/4	0.95	0.15	22,22,23,24	0
3	EDO	B	1475	4/4	0.95	0.23	29,29,30,30	0
3	EDO	H	1475	4/4	0.95	0.14	21,21,22,22	0
4	PEG	F	1476	7/7	0.95	0.20	31,34,38,39	0
2	FE	B	481	1/1	0.96	0.10	27,27,27,27	1
3	EDO	A	1476	4/4	0.96	0.25	30,32,32,35	0
2	FE	D	481	1/1	0.97	0.09	26,26,26,26	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.