



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:53 PM UTC

PDB ID : 3KIP / pdb_00003kip
Title : Crystal structure of type-II 3-dehydroquinase from *C. albicans*
Authors : Trapani, S.; Schoehn, G.; Navaza, J.; Abergel, C.
Deposited on : 2009-11-02
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

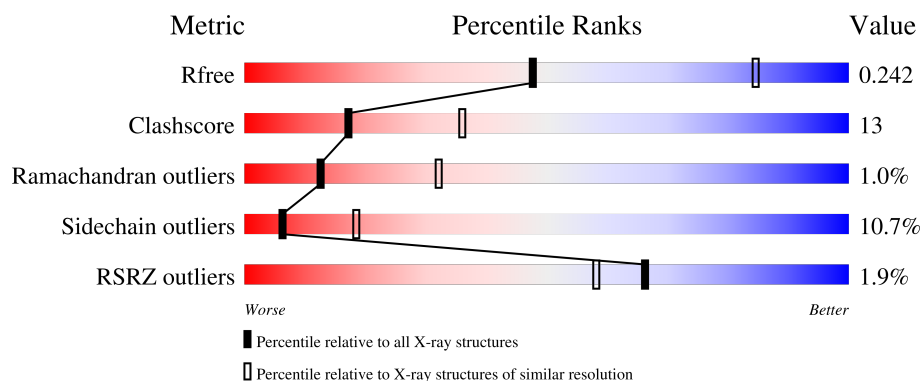
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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.



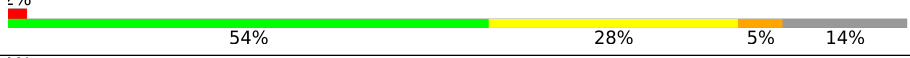
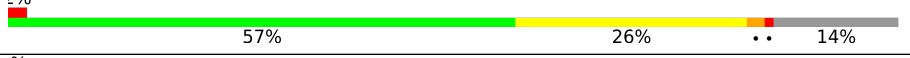
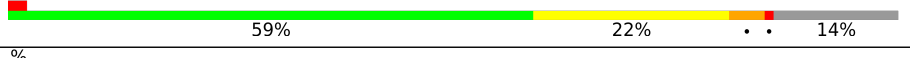
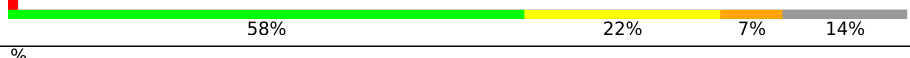
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	167	2% 50% 32% • • 14%
1	B	167	3% 49% 31% 5% • 14%
1	C	167	2% 54% 28% • 14%
1	D	167	2% 58% 23% • • 14%
1	E	167	• 56% 26% • • 13%

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Mol	Chain	Length	Quality of chain
1	F	167	
1	G	167	
1	H	167	
1	I	167	
1	J	167	
1	K	167	
1	L	167	
1	M	167	
1	N	167	
1	O	167	
1	P	167	
1	Q	167	
1	R	167	
1	S	167	
1	T	167	
1	U	167	
1	V	167	
1	W	167	
1	X	167	

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	TRS	D	156	-	X	-	-
3	TRS	P	156	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27144 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 3-dehydroquinase, type II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	B	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	C	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	D	144	Total	C	N	O	S	0	0	0
			1117	711	195	210	1			
1	E	145	Total	C	N	O	S	0	0	0
			1125	717	196	211	1			
1	F	145	Total	C	N	O	S	0	0	0
			1125	717	196	211	1			
1	G	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	H	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	I	147	Total	C	N	O	S	0	0	0
			1142	727	198	216	1			
1	J	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	K	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	L	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	M	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	N	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	O	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	P	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	R	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	S	144	Total	C	N	O	S	0	0	0
			1116	712	194	209	1			
1	T	144	Total	C	N	O	S	0	0	0
			1117	711	195	210	1			
1	U	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	V	143	Total	C	N	O	S	0	0	0
			1108	706	193	208	1			
1	W	145	Total	C	N	O	S	0	0	0
			1125	717	196	211	1			
1	X	145	Total	C	N	O	S	0	0	0
			1125	717	196	211	1			

There are 528 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	ALA	-	expression tag	UNP Q59Z17
A	-11	HIS	-	expression tag	UNP Q59Z17
A	-10	HIS	-	expression tag	UNP Q59Z17
A	-9	HIS	-	expression tag	UNP Q59Z17
A	-8	HIS	-	expression tag	UNP Q59Z17
A	-7	HIS	-	expression tag	UNP Q59Z17
A	-6	HIS	-	expression tag	UNP Q59Z17
A	-5	GLY	-	expression tag	UNP Q59Z17
A	-4	HIS	-	expression tag	UNP Q59Z17
A	-3	HIS	-	expression tag	UNP Q59Z17
A	-2	HIS	-	expression tag	UNP Q59Z17
A	-1	GLN	-	expression tag	UNP Q59Z17
A	0	LEU	-	expression tag	UNP Q59Z17
A	146	GLN	-	expression tag	UNP Q59Z17
A	147	LEU	-	expression tag	UNP Q59Z17
A	148	ASP	-	expression tag	UNP Q59Z17
A	149	GLY	-	expression tag	UNP Q59Z17
A	150	ASP	-	expression tag	UNP Q59Z17
A	151	LEU	-	expression tag	UNP Q59Z17
A	152	GLU	-	expression tag	UNP Q59Z17
A	153	ALA	-	expression tag	UNP Q59Z17
A	154	ALA	-	expression tag	UNP Q59Z17
B	-12	ALA	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP Q59Z17
B	-10	HIS	-	expression tag	UNP Q59Z17
B	-9	HIS	-	expression tag	UNP Q59Z17
B	-8	HIS	-	expression tag	UNP Q59Z17
B	-7	HIS	-	expression tag	UNP Q59Z17
B	-6	HIS	-	expression tag	UNP Q59Z17
B	-5	GLY	-	expression tag	UNP Q59Z17
B	-4	HIS	-	expression tag	UNP Q59Z17
B	-3	HIS	-	expression tag	UNP Q59Z17
B	-2	HIS	-	expression tag	UNP Q59Z17
B	-1	GLN	-	expression tag	UNP Q59Z17
B	0	LEU	-	expression tag	UNP Q59Z17
B	146	GLN	-	expression tag	UNP Q59Z17
B	147	LEU	-	expression tag	UNP Q59Z17
B	148	ASP	-	expression tag	UNP Q59Z17
B	149	GLY	-	expression tag	UNP Q59Z17
B	150	ASP	-	expression tag	UNP Q59Z17
B	151	LEU	-	expression tag	UNP Q59Z17
B	152	GLU	-	expression tag	UNP Q59Z17
B	153	ALA	-	expression tag	UNP Q59Z17
B	154	ALA	-	expression tag	UNP Q59Z17
C	-12	ALA	-	expression tag	UNP Q59Z17
C	-11	HIS	-	expression tag	UNP Q59Z17
C	-10	HIS	-	expression tag	UNP Q59Z17
C	-9	HIS	-	expression tag	UNP Q59Z17
C	-8	HIS	-	expression tag	UNP Q59Z17
C	-7	HIS	-	expression tag	UNP Q59Z17
C	-6	HIS	-	expression tag	UNP Q59Z17
C	-5	GLY	-	expression tag	UNP Q59Z17
C	-4	HIS	-	expression tag	UNP Q59Z17
C	-3	HIS	-	expression tag	UNP Q59Z17
C	-2	HIS	-	expression tag	UNP Q59Z17
C	-1	GLN	-	expression tag	UNP Q59Z17
C	0	LEU	-	expression tag	UNP Q59Z17
C	146	GLN	-	expression tag	UNP Q59Z17
C	147	LEU	-	expression tag	UNP Q59Z17
C	148	ASP	-	expression tag	UNP Q59Z17
C	149	GLY	-	expression tag	UNP Q59Z17
C	150	ASP	-	expression tag	UNP Q59Z17
C	151	LEU	-	expression tag	UNP Q59Z17
C	152	GLU	-	expression tag	UNP Q59Z17
C	153	ALA	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
C	154	ALA	-	expression tag	UNP Q59Z17
D	-12	ALA	-	expression tag	UNP Q59Z17
D	-11	HIS	-	expression tag	UNP Q59Z17
D	-10	HIS	-	expression tag	UNP Q59Z17
D	-9	HIS	-	expression tag	UNP Q59Z17
D	-8	HIS	-	expression tag	UNP Q59Z17
D	-7	HIS	-	expression tag	UNP Q59Z17
D	-6	HIS	-	expression tag	UNP Q59Z17
D	-5	GLY	-	expression tag	UNP Q59Z17
D	-4	HIS	-	expression tag	UNP Q59Z17
D	-3	HIS	-	expression tag	UNP Q59Z17
D	-2	HIS	-	expression tag	UNP Q59Z17
D	-1	GLN	-	expression tag	UNP Q59Z17
D	0	LEU	-	expression tag	UNP Q59Z17
D	146	GLN	-	expression tag	UNP Q59Z17
D	147	LEU	-	expression tag	UNP Q59Z17
D	148	ASP	-	expression tag	UNP Q59Z17
D	149	GLY	-	expression tag	UNP Q59Z17
D	150	ASP	-	expression tag	UNP Q59Z17
D	151	LEU	-	expression tag	UNP Q59Z17
D	152	GLU	-	expression tag	UNP Q59Z17
D	153	ALA	-	expression tag	UNP Q59Z17
D	154	ALA	-	expression tag	UNP Q59Z17
E	-12	ALA	-	expression tag	UNP Q59Z17
E	-11	HIS	-	expression tag	UNP Q59Z17
E	-10	HIS	-	expression tag	UNP Q59Z17
E	-9	HIS	-	expression tag	UNP Q59Z17
E	-8	HIS	-	expression tag	UNP Q59Z17
E	-7	HIS	-	expression tag	UNP Q59Z17
E	-6	HIS	-	expression tag	UNP Q59Z17
E	-5	GLY	-	expression tag	UNP Q59Z17
E	-4	HIS	-	expression tag	UNP Q59Z17
E	-3	HIS	-	expression tag	UNP Q59Z17
E	-2	HIS	-	expression tag	UNP Q59Z17
E	-1	GLN	-	expression tag	UNP Q59Z17
E	0	LEU	-	expression tag	UNP Q59Z17
E	146	GLN	-	expression tag	UNP Q59Z17
E	147	LEU	-	expression tag	UNP Q59Z17
E	148	ASP	-	expression tag	UNP Q59Z17
E	149	GLY	-	expression tag	UNP Q59Z17
E	150	ASP	-	expression tag	UNP Q59Z17
E	151	LEU	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
E	152	GLU	-	expression tag	UNP Q59Z17
E	153	ALA	-	expression tag	UNP Q59Z17
E	154	ALA	-	expression tag	UNP Q59Z17
F	-12	ALA	-	expression tag	UNP Q59Z17
F	-11	HIS	-	expression tag	UNP Q59Z17
F	-10	HIS	-	expression tag	UNP Q59Z17
F	-9	HIS	-	expression tag	UNP Q59Z17
F	-8	HIS	-	expression tag	UNP Q59Z17
F	-7	HIS	-	expression tag	UNP Q59Z17
F	-6	HIS	-	expression tag	UNP Q59Z17
F	-5	GLY	-	expression tag	UNP Q59Z17
F	-4	HIS	-	expression tag	UNP Q59Z17
F	-3	HIS	-	expression tag	UNP Q59Z17
F	-2	HIS	-	expression tag	UNP Q59Z17
F	-1	GLN	-	expression tag	UNP Q59Z17
F	0	LEU	-	expression tag	UNP Q59Z17
F	146	GLN	-	expression tag	UNP Q59Z17
F	147	LEU	-	expression tag	UNP Q59Z17
F	148	ASP	-	expression tag	UNP Q59Z17
F	149	GLY	-	expression tag	UNP Q59Z17
F	150	ASP	-	expression tag	UNP Q59Z17
F	151	LEU	-	expression tag	UNP Q59Z17
F	152	GLU	-	expression tag	UNP Q59Z17
F	153	ALA	-	expression tag	UNP Q59Z17
F	154	ALA	-	expression tag	UNP Q59Z17
G	-12	ALA	-	expression tag	UNP Q59Z17
G	-11	HIS	-	expression tag	UNP Q59Z17
G	-10	HIS	-	expression tag	UNP Q59Z17
G	-9	HIS	-	expression tag	UNP Q59Z17
G	-8	HIS	-	expression tag	UNP Q59Z17
G	-7	HIS	-	expression tag	UNP Q59Z17
G	-6	HIS	-	expression tag	UNP Q59Z17
G	-5	GLY	-	expression tag	UNP Q59Z17
G	-4	HIS	-	expression tag	UNP Q59Z17
G	-3	HIS	-	expression tag	UNP Q59Z17
G	-2	HIS	-	expression tag	UNP Q59Z17
G	-1	GLN	-	expression tag	UNP Q59Z17
G	0	LEU	-	expression tag	UNP Q59Z17
G	146	GLN	-	expression tag	UNP Q59Z17
G	147	LEU	-	expression tag	UNP Q59Z17
G	148	ASP	-	expression tag	UNP Q59Z17
G	149	GLY	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
G	150	ASP	-	expression tag	UNP Q59Z17
G	151	LEU	-	expression tag	UNP Q59Z17
G	152	GLU	-	expression tag	UNP Q59Z17
G	153	ALA	-	expression tag	UNP Q59Z17
G	154	ALA	-	expression tag	UNP Q59Z17
H	-12	ALA	-	expression tag	UNP Q59Z17
H	-11	HIS	-	expression tag	UNP Q59Z17
H	-10	HIS	-	expression tag	UNP Q59Z17
H	-9	HIS	-	expression tag	UNP Q59Z17
H	-8	HIS	-	expression tag	UNP Q59Z17
H	-7	HIS	-	expression tag	UNP Q59Z17
H	-6	HIS	-	expression tag	UNP Q59Z17
H	-5	GLY	-	expression tag	UNP Q59Z17
H	-4	HIS	-	expression tag	UNP Q59Z17
H	-3	HIS	-	expression tag	UNP Q59Z17
H	-2	HIS	-	expression tag	UNP Q59Z17
H	-1	GLN	-	expression tag	UNP Q59Z17
H	0	LEU	-	expression tag	UNP Q59Z17
H	146	GLN	-	expression tag	UNP Q59Z17
H	147	LEU	-	expression tag	UNP Q59Z17
H	148	ASP	-	expression tag	UNP Q59Z17
H	149	GLY	-	expression tag	UNP Q59Z17
H	150	ASP	-	expression tag	UNP Q59Z17
H	151	LEU	-	expression tag	UNP Q59Z17
H	152	GLU	-	expression tag	UNP Q59Z17
H	153	ALA	-	expression tag	UNP Q59Z17
H	154	ALA	-	expression tag	UNP Q59Z17
I	-12	ALA	-	expression tag	UNP Q59Z17
I	-11	HIS	-	expression tag	UNP Q59Z17
I	-10	HIS	-	expression tag	UNP Q59Z17
I	-9	HIS	-	expression tag	UNP Q59Z17
I	-8	HIS	-	expression tag	UNP Q59Z17
I	-7	HIS	-	expression tag	UNP Q59Z17
I	-6	HIS	-	expression tag	UNP Q59Z17
I	-5	GLY	-	expression tag	UNP Q59Z17
I	-4	HIS	-	expression tag	UNP Q59Z17
I	-3	HIS	-	expression tag	UNP Q59Z17
I	-2	HIS	-	expression tag	UNP Q59Z17
I	-1	GLN	-	expression tag	UNP Q59Z17
I	0	LEU	-	expression tag	UNP Q59Z17
I	146	GLN	-	expression tag	UNP Q59Z17
I	147	LEU	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
I	148	ASP	-	expression tag	UNP Q59Z17
I	149	GLY	-	expression tag	UNP Q59Z17
I	150	ASP	-	expression tag	UNP Q59Z17
I	151	LEU	-	expression tag	UNP Q59Z17
I	152	GLU	-	expression tag	UNP Q59Z17
I	153	ALA	-	expression tag	UNP Q59Z17
I	154	ALA	-	expression tag	UNP Q59Z17
J	-12	ALA	-	expression tag	UNP Q59Z17
J	-11	HIS	-	expression tag	UNP Q59Z17
J	-10	HIS	-	expression tag	UNP Q59Z17
J	-9	HIS	-	expression tag	UNP Q59Z17
J	-8	HIS	-	expression tag	UNP Q59Z17
J	-7	HIS	-	expression tag	UNP Q59Z17
J	-6	HIS	-	expression tag	UNP Q59Z17
J	-5	GLY	-	expression tag	UNP Q59Z17
J	-4	HIS	-	expression tag	UNP Q59Z17
J	-3	HIS	-	expression tag	UNP Q59Z17
J	-2	HIS	-	expression tag	UNP Q59Z17
J	-1	GLN	-	expression tag	UNP Q59Z17
J	0	LEU	-	expression tag	UNP Q59Z17
J	146	GLN	-	expression tag	UNP Q59Z17
J	147	LEU	-	expression tag	UNP Q59Z17
J	148	ASP	-	expression tag	UNP Q59Z17
J	149	GLY	-	expression tag	UNP Q59Z17
J	150	ASP	-	expression tag	UNP Q59Z17
J	151	LEU	-	expression tag	UNP Q59Z17
J	152	GLU	-	expression tag	UNP Q59Z17
J	153	ALA	-	expression tag	UNP Q59Z17
J	154	ALA	-	expression tag	UNP Q59Z17
K	-12	ALA	-	expression tag	UNP Q59Z17
K	-11	HIS	-	expression tag	UNP Q59Z17
K	-10	HIS	-	expression tag	UNP Q59Z17
K	-9	HIS	-	expression tag	UNP Q59Z17
K	-8	HIS	-	expression tag	UNP Q59Z17
K	-7	HIS	-	expression tag	UNP Q59Z17
K	-6	HIS	-	expression tag	UNP Q59Z17
K	-5	GLY	-	expression tag	UNP Q59Z17
K	-4	HIS	-	expression tag	UNP Q59Z17
K	-3	HIS	-	expression tag	UNP Q59Z17
K	-2	HIS	-	expression tag	UNP Q59Z17
K	-1	GLN	-	expression tag	UNP Q59Z17
K	0	LEU	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
K	146	GLN	-	expression tag	UNP Q59Z17
K	147	LEU	-	expression tag	UNP Q59Z17
K	148	ASP	-	expression tag	UNP Q59Z17
K	149	GLY	-	expression tag	UNP Q59Z17
K	150	ASP	-	expression tag	UNP Q59Z17
K	151	LEU	-	expression tag	UNP Q59Z17
K	152	GLU	-	expression tag	UNP Q59Z17
K	153	ALA	-	expression tag	UNP Q59Z17
K	154	ALA	-	expression tag	UNP Q59Z17
L	-12	ALA	-	expression tag	UNP Q59Z17
L	-11	HIS	-	expression tag	UNP Q59Z17
L	-10	HIS	-	expression tag	UNP Q59Z17
L	-9	HIS	-	expression tag	UNP Q59Z17
L	-8	HIS	-	expression tag	UNP Q59Z17
L	-7	HIS	-	expression tag	UNP Q59Z17
L	-6	HIS	-	expression tag	UNP Q59Z17
L	-5	GLY	-	expression tag	UNP Q59Z17
L	-4	HIS	-	expression tag	UNP Q59Z17
L	-3	HIS	-	expression tag	UNP Q59Z17
L	-2	HIS	-	expression tag	UNP Q59Z17
L	-1	GLN	-	expression tag	UNP Q59Z17
L	0	LEU	-	expression tag	UNP Q59Z17
L	146	GLN	-	expression tag	UNP Q59Z17
L	147	LEU	-	expression tag	UNP Q59Z17
L	148	ASP	-	expression tag	UNP Q59Z17
L	149	GLY	-	expression tag	UNP Q59Z17
L	150	ASP	-	expression tag	UNP Q59Z17
L	151	LEU	-	expression tag	UNP Q59Z17
L	152	GLU	-	expression tag	UNP Q59Z17
L	153	ALA	-	expression tag	UNP Q59Z17
L	154	ALA	-	expression tag	UNP Q59Z17
M	-12	ALA	-	expression tag	UNP Q59Z17
M	-11	HIS	-	expression tag	UNP Q59Z17
M	-10	HIS	-	expression tag	UNP Q59Z17
M	-9	HIS	-	expression tag	UNP Q59Z17
M	-8	HIS	-	expression tag	UNP Q59Z17
M	-7	HIS	-	expression tag	UNP Q59Z17
M	-6	HIS	-	expression tag	UNP Q59Z17
M	-5	GLY	-	expression tag	UNP Q59Z17
M	-4	HIS	-	expression tag	UNP Q59Z17
M	-3	HIS	-	expression tag	UNP Q59Z17
M	-2	HIS	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	GLN	-	expression tag	UNP Q59Z17
M	0	LEU	-	expression tag	UNP Q59Z17
M	146	GLN	-	expression tag	UNP Q59Z17
M	147	LEU	-	expression tag	UNP Q59Z17
M	148	ASP	-	expression tag	UNP Q59Z17
M	149	GLY	-	expression tag	UNP Q59Z17
M	150	ASP	-	expression tag	UNP Q59Z17
M	151	LEU	-	expression tag	UNP Q59Z17
M	152	GLU	-	expression tag	UNP Q59Z17
M	153	ALA	-	expression tag	UNP Q59Z17
M	154	ALA	-	expression tag	UNP Q59Z17
N	-12	ALA	-	expression tag	UNP Q59Z17
N	-11	HIS	-	expression tag	UNP Q59Z17
N	-10	HIS	-	expression tag	UNP Q59Z17
N	-9	HIS	-	expression tag	UNP Q59Z17
N	-8	HIS	-	expression tag	UNP Q59Z17
N	-7	HIS	-	expression tag	UNP Q59Z17
N	-6	HIS	-	expression tag	UNP Q59Z17
N	-5	GLY	-	expression tag	UNP Q59Z17
N	-4	HIS	-	expression tag	UNP Q59Z17
N	-3	HIS	-	expression tag	UNP Q59Z17
N	-2	HIS	-	expression tag	UNP Q59Z17
N	-1	GLN	-	expression tag	UNP Q59Z17
N	0	LEU	-	expression tag	UNP Q59Z17
N	146	GLN	-	expression tag	UNP Q59Z17
N	147	LEU	-	expression tag	UNP Q59Z17
N	148	ASP	-	expression tag	UNP Q59Z17
N	149	GLY	-	expression tag	UNP Q59Z17
N	150	ASP	-	expression tag	UNP Q59Z17
N	151	LEU	-	expression tag	UNP Q59Z17
N	152	GLU	-	expression tag	UNP Q59Z17
N	153	ALA	-	expression tag	UNP Q59Z17
N	154	ALA	-	expression tag	UNP Q59Z17
O	-12	ALA	-	expression tag	UNP Q59Z17
O	-11	HIS	-	expression tag	UNP Q59Z17
O	-10	HIS	-	expression tag	UNP Q59Z17
O	-9	HIS	-	expression tag	UNP Q59Z17
O	-8	HIS	-	expression tag	UNP Q59Z17
O	-7	HIS	-	expression tag	UNP Q59Z17
O	-6	HIS	-	expression tag	UNP Q59Z17
O	-5	GLY	-	expression tag	UNP Q59Z17
O	-4	HIS	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-3	HIS	-	expression tag	UNP Q59Z17
O	-2	HIS	-	expression tag	UNP Q59Z17
O	-1	GLN	-	expression tag	UNP Q59Z17
O	0	LEU	-	expression tag	UNP Q59Z17
O	146	GLN	-	expression tag	UNP Q59Z17
O	147	LEU	-	expression tag	UNP Q59Z17
O	148	ASP	-	expression tag	UNP Q59Z17
O	149	GLY	-	expression tag	UNP Q59Z17
O	150	ASP	-	expression tag	UNP Q59Z17
O	151	LEU	-	expression tag	UNP Q59Z17
O	152	GLU	-	expression tag	UNP Q59Z17
O	153	ALA	-	expression tag	UNP Q59Z17
O	154	ALA	-	expression tag	UNP Q59Z17
P	-12	ALA	-	expression tag	UNP Q59Z17
P	-11	HIS	-	expression tag	UNP Q59Z17
P	-10	HIS	-	expression tag	UNP Q59Z17
P	-9	HIS	-	expression tag	UNP Q59Z17
P	-8	HIS	-	expression tag	UNP Q59Z17
P	-7	HIS	-	expression tag	UNP Q59Z17
P	-6	HIS	-	expression tag	UNP Q59Z17
P	-5	GLY	-	expression tag	UNP Q59Z17
P	-4	HIS	-	expression tag	UNP Q59Z17
P	-3	HIS	-	expression tag	UNP Q59Z17
P	-2	HIS	-	expression tag	UNP Q59Z17
P	-1	GLN	-	expression tag	UNP Q59Z17
P	0	LEU	-	expression tag	UNP Q59Z17
P	146	GLN	-	expression tag	UNP Q59Z17
P	147	LEU	-	expression tag	UNP Q59Z17
P	148	ASP	-	expression tag	UNP Q59Z17
P	149	GLY	-	expression tag	UNP Q59Z17
P	150	ASP	-	expression tag	UNP Q59Z17
P	151	LEU	-	expression tag	UNP Q59Z17
P	152	GLU	-	expression tag	UNP Q59Z17
P	153	ALA	-	expression tag	UNP Q59Z17
P	154	ALA	-	expression tag	UNP Q59Z17
Q	-12	ALA	-	expression tag	UNP Q59Z17
Q	-11	HIS	-	expression tag	UNP Q59Z17
Q	-10	HIS	-	expression tag	UNP Q59Z17
Q	-9	HIS	-	expression tag	UNP Q59Z17
Q	-8	HIS	-	expression tag	UNP Q59Z17
Q	-7	HIS	-	expression tag	UNP Q59Z17
Q	-6	HIS	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-5	GLY	-	expression tag	UNP Q59Z17
Q	-4	HIS	-	expression tag	UNP Q59Z17
Q	-3	HIS	-	expression tag	UNP Q59Z17
Q	-2	HIS	-	expression tag	UNP Q59Z17
Q	-1	GLN	-	expression tag	UNP Q59Z17
Q	0	LEU	-	expression tag	UNP Q59Z17
Q	146	GLN	-	expression tag	UNP Q59Z17
Q	147	LEU	-	expression tag	UNP Q59Z17
Q	148	ASP	-	expression tag	UNP Q59Z17
Q	149	GLY	-	expression tag	UNP Q59Z17
Q	150	ASP	-	expression tag	UNP Q59Z17
Q	151	LEU	-	expression tag	UNP Q59Z17
Q	152	GLU	-	expression tag	UNP Q59Z17
Q	153	ALA	-	expression tag	UNP Q59Z17
Q	154	ALA	-	expression tag	UNP Q59Z17
R	-12	ALA	-	expression tag	UNP Q59Z17
R	-11	HIS	-	expression tag	UNP Q59Z17
R	-10	HIS	-	expression tag	UNP Q59Z17
R	-9	HIS	-	expression tag	UNP Q59Z17
R	-8	HIS	-	expression tag	UNP Q59Z17
R	-7	HIS	-	expression tag	UNP Q59Z17
R	-6	HIS	-	expression tag	UNP Q59Z17
R	-5	GLY	-	expression tag	UNP Q59Z17
R	-4	HIS	-	expression tag	UNP Q59Z17
R	-3	HIS	-	expression tag	UNP Q59Z17
R	-2	HIS	-	expression tag	UNP Q59Z17
R	-1	GLN	-	expression tag	UNP Q59Z17
R	0	LEU	-	expression tag	UNP Q59Z17
R	146	GLN	-	expression tag	UNP Q59Z17
R	147	LEU	-	expression tag	UNP Q59Z17
R	148	ASP	-	expression tag	UNP Q59Z17
R	149	GLY	-	expression tag	UNP Q59Z17
R	150	ASP	-	expression tag	UNP Q59Z17
R	151	LEU	-	expression tag	UNP Q59Z17
R	152	GLU	-	expression tag	UNP Q59Z17
R	153	ALA	-	expression tag	UNP Q59Z17
R	154	ALA	-	expression tag	UNP Q59Z17
S	-12	ALA	-	expression tag	UNP Q59Z17
S	-11	HIS	-	expression tag	UNP Q59Z17
S	-10	HIS	-	expression tag	UNP Q59Z17
S	-9	HIS	-	expression tag	UNP Q59Z17
S	-8	HIS	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-7	HIS	-	expression tag	UNP Q59Z17
S	-6	HIS	-	expression tag	UNP Q59Z17
S	-5	GLY	-	expression tag	UNP Q59Z17
S	-4	HIS	-	expression tag	UNP Q59Z17
S	-3	HIS	-	expression tag	UNP Q59Z17
S	-2	HIS	-	expression tag	UNP Q59Z17
S	-1	GLN	-	expression tag	UNP Q59Z17
S	0	LEU	-	expression tag	UNP Q59Z17
S	146	GLN	-	expression tag	UNP Q59Z17
S	147	LEU	-	expression tag	UNP Q59Z17
S	148	ASP	-	expression tag	UNP Q59Z17
S	149	GLY	-	expression tag	UNP Q59Z17
S	150	ASP	-	expression tag	UNP Q59Z17
S	151	LEU	-	expression tag	UNP Q59Z17
S	152	GLU	-	expression tag	UNP Q59Z17
S	153	ALA	-	expression tag	UNP Q59Z17
S	154	ALA	-	expression tag	UNP Q59Z17
T	-12	ALA	-	expression tag	UNP Q59Z17
T	-11	HIS	-	expression tag	UNP Q59Z17
T	-10	HIS	-	expression tag	UNP Q59Z17
T	-9	HIS	-	expression tag	UNP Q59Z17
T	-8	HIS	-	expression tag	UNP Q59Z17
T	-7	HIS	-	expression tag	UNP Q59Z17
T	-6	HIS	-	expression tag	UNP Q59Z17
T	-5	GLY	-	expression tag	UNP Q59Z17
T	-4	HIS	-	expression tag	UNP Q59Z17
T	-3	HIS	-	expression tag	UNP Q59Z17
T	-2	HIS	-	expression tag	UNP Q59Z17
T	-1	GLN	-	expression tag	UNP Q59Z17
T	0	LEU	-	expression tag	UNP Q59Z17
T	146	GLN	-	expression tag	UNP Q59Z17
T	147	LEU	-	expression tag	UNP Q59Z17
T	148	ASP	-	expression tag	UNP Q59Z17
T	149	GLY	-	expression tag	UNP Q59Z17
T	150	ASP	-	expression tag	UNP Q59Z17
T	151	LEU	-	expression tag	UNP Q59Z17
T	152	GLU	-	expression tag	UNP Q59Z17
T	153	ALA	-	expression tag	UNP Q59Z17
T	154	ALA	-	expression tag	UNP Q59Z17
U	-12	ALA	-	expression tag	UNP Q59Z17
U	-11	HIS	-	expression tag	UNP Q59Z17
U	-10	HIS	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-9	HIS	-	expression tag	UNP Q59Z17
U	-8	HIS	-	expression tag	UNP Q59Z17
U	-7	HIS	-	expression tag	UNP Q59Z17
U	-6	HIS	-	expression tag	UNP Q59Z17
U	-5	GLY	-	expression tag	UNP Q59Z17
U	-4	HIS	-	expression tag	UNP Q59Z17
U	-3	HIS	-	expression tag	UNP Q59Z17
U	-2	HIS	-	expression tag	UNP Q59Z17
U	-1	GLN	-	expression tag	UNP Q59Z17
U	0	LEU	-	expression tag	UNP Q59Z17
U	146	GLN	-	expression tag	UNP Q59Z17
U	147	LEU	-	expression tag	UNP Q59Z17
U	148	ASP	-	expression tag	UNP Q59Z17
U	149	GLY	-	expression tag	UNP Q59Z17
U	150	ASP	-	expression tag	UNP Q59Z17
U	151	LEU	-	expression tag	UNP Q59Z17
U	152	GLU	-	expression tag	UNP Q59Z17
U	153	ALA	-	expression tag	UNP Q59Z17
U	154	ALA	-	expression tag	UNP Q59Z17
V	-12	ALA	-	expression tag	UNP Q59Z17
V	-11	HIS	-	expression tag	UNP Q59Z17
V	-10	HIS	-	expression tag	UNP Q59Z17
V	-9	HIS	-	expression tag	UNP Q59Z17
V	-8	HIS	-	expression tag	UNP Q59Z17
V	-7	HIS	-	expression tag	UNP Q59Z17
V	-6	HIS	-	expression tag	UNP Q59Z17
V	-5	GLY	-	expression tag	UNP Q59Z17
V	-4	HIS	-	expression tag	UNP Q59Z17
V	-3	HIS	-	expression tag	UNP Q59Z17
V	-2	HIS	-	expression tag	UNP Q59Z17
V	-1	GLN	-	expression tag	UNP Q59Z17
V	0	LEU	-	expression tag	UNP Q59Z17
V	146	GLN	-	expression tag	UNP Q59Z17
V	147	LEU	-	expression tag	UNP Q59Z17
V	148	ASP	-	expression tag	UNP Q59Z17
V	149	GLY	-	expression tag	UNP Q59Z17
V	150	ASP	-	expression tag	UNP Q59Z17
V	151	LEU	-	expression tag	UNP Q59Z17
V	152	GLU	-	expression tag	UNP Q59Z17
V	153	ALA	-	expression tag	UNP Q59Z17
V	154	ALA	-	expression tag	UNP Q59Z17
W	-12	ALA	-	expression tag	UNP Q59Z17

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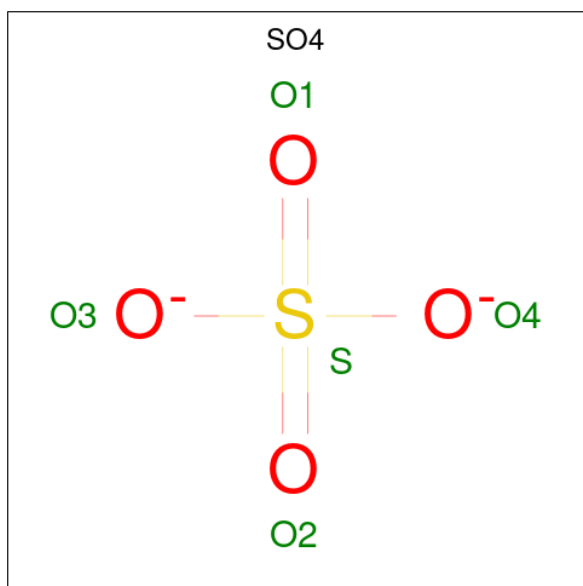
Chain	Residue	Modelled	Actual	Comment	Reference
W	-11	HIS	-	expression tag	UNP Q59Z17
W	-10	HIS	-	expression tag	UNP Q59Z17
W	-9	HIS	-	expression tag	UNP Q59Z17
W	-8	HIS	-	expression tag	UNP Q59Z17
W	-7	HIS	-	expression tag	UNP Q59Z17
W	-6	HIS	-	expression tag	UNP Q59Z17
W	-5	GLY	-	expression tag	UNP Q59Z17
W	-4	HIS	-	expression tag	UNP Q59Z17
W	-3	HIS	-	expression tag	UNP Q59Z17
W	-2	HIS	-	expression tag	UNP Q59Z17
W	-1	GLN	-	expression tag	UNP Q59Z17
W	0	LEU	-	expression tag	UNP Q59Z17
W	146	GLN	-	expression tag	UNP Q59Z17
W	147	LEU	-	expression tag	UNP Q59Z17
W	148	ASP	-	expression tag	UNP Q59Z17
W	149	GLY	-	expression tag	UNP Q59Z17
W	150	ASP	-	expression tag	UNP Q59Z17
W	151	LEU	-	expression tag	UNP Q59Z17
W	152	GLU	-	expression tag	UNP Q59Z17
W	153	ALA	-	expression tag	UNP Q59Z17
W	154	ALA	-	expression tag	UNP Q59Z17
X	-12	ALA	-	expression tag	UNP Q59Z17
X	-11	HIS	-	expression tag	UNP Q59Z17
X	-10	HIS	-	expression tag	UNP Q59Z17
X	-9	HIS	-	expression tag	UNP Q59Z17
X	-8	HIS	-	expression tag	UNP Q59Z17
X	-7	HIS	-	expression tag	UNP Q59Z17
X	-6	HIS	-	expression tag	UNP Q59Z17
X	-5	GLY	-	expression tag	UNP Q59Z17
X	-4	HIS	-	expression tag	UNP Q59Z17
X	-3	HIS	-	expression tag	UNP Q59Z17
X	-2	HIS	-	expression tag	UNP Q59Z17
X	-1	GLN	-	expression tag	UNP Q59Z17
X	0	LEU	-	expression tag	UNP Q59Z17
X	146	GLN	-	expression tag	UNP Q59Z17
X	147	LEU	-	expression tag	UNP Q59Z17
X	148	ASP	-	expression tag	UNP Q59Z17
X	149	GLY	-	expression tag	UNP Q59Z17
X	150	ASP	-	expression tag	UNP Q59Z17
X	151	LEU	-	expression tag	UNP Q59Z17
X	152	GLU	-	expression tag	UNP Q59Z17
X	153	ALA	-	expression tag	UNP Q59Z17

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Chain	Residue	Modelled	Actual	Comment	Reference
X	154	ALA	-	expression tag	UNP Q59Z17

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



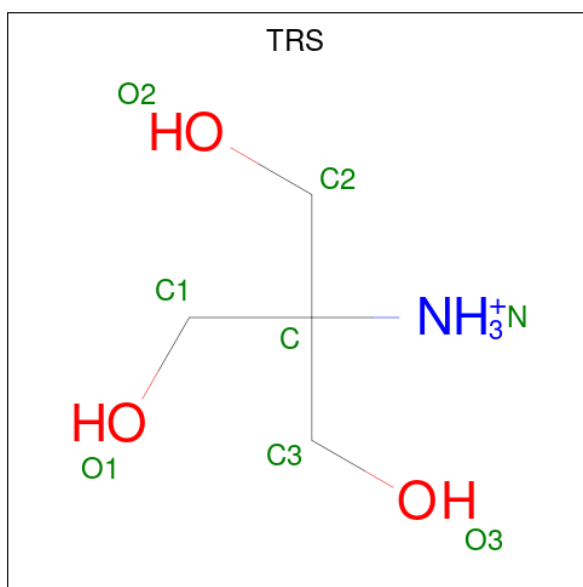
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	K	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	U	1	Total	O	S	0	0
			5	4	1		
2	V	1	Total	O	S	0	0
			5	4	1		
2	W	1	Total	O	S	0	0
			5	4	1		
2	X	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		
3	G	1	Total	C	N	O	0	0
			8	4	1	3		
3	J	1	Total	C	N	O	0	0
			8	4	1	3		
3	N	1	Total	C	N	O	0	0
			8	4	1	3		
3	P	1	Total	C	N	O	0	0
			8	4	1	3		
3	T	1	Total	C	N	O	0	0
			8	4	1	3		
3	W	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is water.

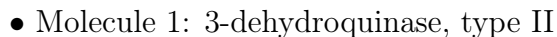
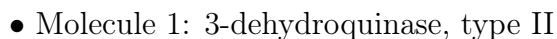
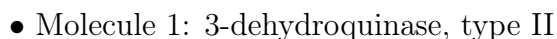
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	13	Total	O	0	0
			13	13		
4	C	7	Total	O	0	0
			7	7		
4	D	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	17	Total 17	O 17	0	0
4	F	10	Total 10	O 10	0	0
4	G	9	Total 9	O 9	0	0
4	H	4	Total 4	O 4	0	0
4	I	11	Total 11	O 11	0	0
4	J	4	Total 4	O 4	0	0
4	K	5	Total 5	O 5	0	0
4	L	4	Total 4	O 4	0	0
4	M	4	Total 4	O 4	0	0
4	N	11	Total 11	O 11	0	0
4	O	2	Total 2	O 2	0	0
4	P	8	Total 8	O 8	0	0
4	Q	7	Total 7	O 7	0	0
4	R	13	Total 13	O 13	0	0
4	S	4	Total 4	O 4	0	0
4	T	3	Total 3	O 3	0	0
4	U	5	Total 5	O 5	0	0
4	V	5	Total 5	O 5	0	0
4	W	5	Total 5	O 5	0	0
4	X	2	Total 2	O 2	0	0

- Molecule 1: 3-dehydroquinase, type II

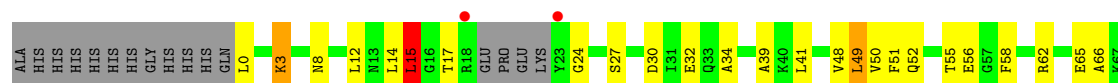


Chain I: 58% 27% 12%

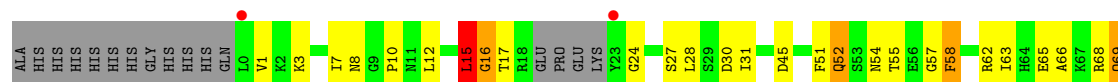




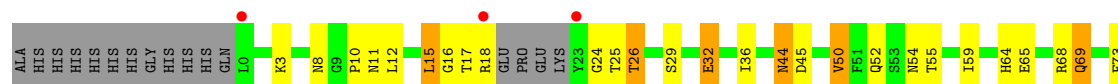
- Molecule 1: 3-dehydroquinase, type II



- Molecule 1: 3-dehydroquinase, type II



- Molecule 1: 3-dehydroquinase, type II

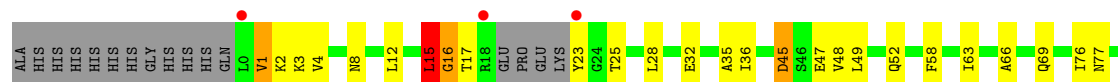


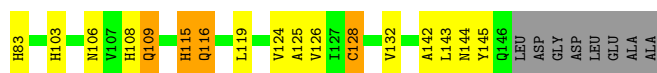
- Molecule 1: 3-dehydroquinase, type II



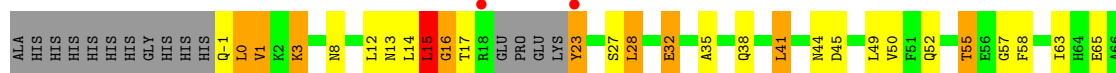
- Molecule 1: 3-dehydroquinase, type II







- Molecule 1: 3-dehydroquinase, type II



- Molecule 1: 3-dehydroquinase, type II



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.10Å 308.11Å 97.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.68 – 2.95 70.68 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.68-2.95) 99.9 (70.68-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.96Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.245 (Not available) , 0.242	Depositor DCC
R_{free} test set	5090 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27144	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, TRS

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	1.47	6/1126 (0.5%)	1.50	16/1527 (1.0%)
1	B	1.54	8/1126 (0.7%)	1.46	12/1527 (0.8%)
1	C	1.43	3/1126 (0.3%)	1.38	8/1527 (0.5%)
1	D	1.40	5/1135 (0.4%)	1.49	13/1539 (0.8%)
1	E	1.43	4/1143 (0.3%)	1.47	10/1550 (0.6%)
1	F	1.57	10/1143 (0.9%)	1.44	7/1550 (0.5%)
1	G	1.41	5/1126 (0.4%)	1.44	11/1527 (0.7%)
1	H	1.40	6/1134 (0.5%)	1.42	3/1538 (0.2%)
1	I	1.45	4/1162 (0.3%)	1.42	7/1577 (0.4%)
1	J	1.27	3/1126 (0.3%)	1.39	4/1527 (0.3%)
1	K	1.33	6/1134 (0.5%)	1.44	11/1538 (0.7%)
1	L	1.32	3/1134 (0.3%)	1.37	9/1538 (0.6%)
1	M	1.44	7/1134 (0.6%)	1.51	14/1538 (0.9%)
1	N	1.40	4/1134 (0.4%)	1.39	4/1538 (0.3%)
1	O	1.34	3/1134 (0.3%)	1.40	11/1538 (0.7%)
1	P	1.34	4/1134 (0.4%)	1.38	7/1538 (0.5%)
1	Q	1.42	4/1134 (0.4%)	1.47	9/1538 (0.6%)
1	R	1.42	2/1134 (0.2%)	1.40	12/1538 (0.8%)
1	S	1.37	2/1134 (0.2%)	1.45	8/1538 (0.5%)
1	T	1.35	5/1135 (0.4%)	1.40	10/1539 (0.6%)
1	U	1.40	9/1126 (0.8%)	1.39	8/1527 (0.5%)
1	V	1.22	1/1126 (0.1%)	1.32	3/1527 (0.2%)
1	W	1.33	6/1143 (0.5%)	1.40	11/1550 (0.7%)
1	X	1.28	2/1143 (0.2%)	1.42	3/1550 (0.2%)
All	All	1.39	112/27226 (0.4%)	1.42	211/36924 (0.6%)

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	1
1	M	0	1
1	V	0	1
All	All	0	3

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	25	THR	CA-CB	9.28	1.69	1.53
1	W	63	ILE	CA-CB	-8.42	1.44	1.54
1	F	55	THR	CA-CB	-8.22	1.42	1.53
1	X	25	THR	CA-CB	7.92	1.66	1.53
1	F	96	ALA	CA-CB	-7.47	1.42	1.53

The worst 5 of 211 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	97	ILE	CA-C-N	-10.01	110.60	120.21
1	D	97	ILE	C-N-CA	-10.01	110.60	120.21
1	S	111	GLU	CA-C-N	9.48	131.69	119.84
1	S	111	GLU	C-N-CA	9.48	131.69	119.84
1	N	34	ALA	N-CA-C	-8.79	100.23	112.45

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	45	ASP	Peptide
1	M	145	TYR	Peptide
1	V	145	TYR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1108	0	1117	27	0
1	B	1108	0	1117	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1108	0	1117	30	0
1	D	1117	0	1125	24	0
1	E	1125	0	1136	31	0
1	F	1125	0	1136	32	0
1	G	1108	0	1117	23	0
1	H	1116	0	1128	23	0
1	I	1142	0	1150	30	0
1	J	1108	0	1117	30	0
1	K	1116	0	1128	25	0
1	L	1116	0	1128	30	0
1	M	1116	0	1128	36	0
1	N	1116	0	1128	30	0
1	O	1116	0	1128	25	0
1	P	1116	0	1128	28	0
1	Q	1116	0	1128	32	0
1	R	1116	0	1128	27	0
1	S	1116	0	1128	35	0
1	T	1117	0	1125	42	0
1	U	1108	0	1117	34	0
1	V	1108	0	1117	29	0
1	W	1125	0	1136	38	0
1	X	1125	0	1136	29	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	5	0	0	0	0
2	Q	5	0	0	0	0
2	R	5	0	0	0	0
2	S	5	0	0	0	0
2	T	5	0	0	0	0
2	U	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	5	0	0	0	0
2	W	5	0	0	0	0
2	X	5	0	0	0	0
3	A	8	0	12	0	0
3	D	8	0	12	1	0
3	G	8	0	12	0	0
3	J	8	0	12	0	0
3	N	8	0	12	1	0
3	P	8	0	12	1	0
3	T	8	0	12	0	0
3	W	8	0	12	1	0
4	A	8	0	0	0	0
4	B	13	0	0	2	0
4	C	7	0	0	1	0
4	D	7	0	0	1	0
4	E	17	0	0	1	0
4	F	10	0	0	0	0
4	G	9	0	0	0	0
4	H	4	0	0	0	0
4	I	11	0	0	1	0
4	J	4	0	0	0	0
4	K	5	0	0	0	0
4	L	4	0	0	0	0
4	M	4	0	0	0	0
4	N	11	0	0	0	0
4	O	2	0	0	0	0
4	P	8	0	0	0	0
4	Q	7	0	0	0	0
4	R	13	0	0	0	0
4	S	4	0	0	1	0
4	T	3	0	0	0	0
4	U	5	0	0	0	0
4	V	5	0	0	1	0
4	W	5	0	0	0	0
4	X	2	0	0	0	0
All	All	27144	0	27139	681	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 13.

The worst 5 of 681 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:J:12:LEU:O	1:J:15:LEU:HD22	1.54	1.07
1:N:146:GLN:HE21	1:N:146:GLN:HA	0.94	1.06
1:T:103:HIS:HB2	1:T:128:CYS:HB2	1.44	0.99
1:N:146:GLN:HA	1:N:146:GLN:NE2	1.68	0.98
1:W:103:HIS:HB2	1:W:128:CYS:HB2	1.46	0.98

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	139/167 (83%)	131 (94%)	6 (4%)	2 (1%)	9	24
1	B	139/167 (83%)	131 (94%)	8 (6%)	0	100	100
1	C	139/167 (83%)	132 (95%)	6 (4%)	1 (1%)	18	40
1	D	140/167 (84%)	132 (94%)	7 (5%)	1 (1%)	18	40
1	E	141/167 (84%)	127 (90%)	13 (9%)	1 (1%)	18	40
1	F	141/167 (84%)	133 (94%)	7 (5%)	1 (1%)	18	40
1	G	139/167 (83%)	132 (95%)	6 (4%)	1 (1%)	18	40
1	H	140/167 (84%)	133 (95%)	6 (4%)	1 (1%)	18	40
1	I	145/167 (87%)	136 (94%)	8 (6%)	1 (1%)	18	40
1	J	139/167 (83%)	127 (91%)	10 (7%)	2 (1%)	9	24
1	K	140/167 (84%)	130 (93%)	9 (6%)	1 (1%)	18	40
1	L	140/167 (84%)	128 (91%)	11 (8%)	1 (1%)	18	40
1	M	140/167 (84%)	127 (91%)	10 (7%)	3 (2%)	5	16
1	N	140/167 (84%)	131 (94%)	8 (6%)	1 (1%)	18	40
1	O	140/167 (84%)	129 (92%)	11 (8%)	0	100	100
1	P	140/167 (84%)	131 (94%)	8 (6%)	1 (1%)	18	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	140/167 (84%)	126 (90%)	13 (9%)	1 (1%)	18	40
1	R	140/167 (84%)	133 (95%)	7 (5%)	0	100	100
1	S	140/167 (84%)	124 (89%)	13 (9%)	3 (2%)	5	16
1	T	140/167 (84%)	129 (92%)	7 (5%)	4 (3%)	3	10
1	U	139/167 (83%)	132 (95%)	6 (4%)	1 (1%)	18	40
1	V	139/167 (83%)	121 (87%)	16 (12%)	2 (1%)	9	24
1	W	141/167 (84%)	131 (93%)	8 (6%)	2 (1%)	9	24
1	X	141/167 (84%)	127 (90%)	13 (9%)	1 (1%)	18	40
All	All	3362/4008 (84%)	3113 (93%)	217 (6%)	32 (1%)	12	32

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	25	THR
1	G	25	THR
1	Q	25	THR
1	S	146	GLN
1	U	25	THR

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	118/137 (86%)	105 (89%)	13 (11%)	6	17
1	B	118/137 (86%)	105 (89%)	13 (11%)	6	17
1	C	118/137 (86%)	103 (87%)	15 (13%)	4	13
1	D	119/137 (87%)	106 (89%)	13 (11%)	6	18
1	E	120/137 (88%)	109 (91%)	11 (9%)	8	23
1	F	120/137 (88%)	110 (92%)	10 (8%)	10	27
1	G	118/137 (86%)	106 (90%)	12 (10%)	7	20
1	H	119/137 (87%)	109 (92%)	10 (8%)	10	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	122/137 (89%)	112 (92%)	10 (8%)	10	27
1	J	118/137 (86%)	104 (88%)	14 (12%)	5	15
1	K	119/137 (87%)	104 (87%)	15 (13%)	4	13
1	L	119/137 (87%)	111 (93%)	8 (7%)	15	36
1	M	119/137 (87%)	109 (92%)	10 (8%)	10	26
1	N	119/137 (87%)	107 (90%)	12 (10%)	7	20
1	O	119/137 (87%)	108 (91%)	11 (9%)	8	23
1	P	119/137 (87%)	104 (87%)	15 (13%)	4	13
1	Q	119/137 (87%)	107 (90%)	12 (10%)	7	20
1	R	119/137 (87%)	110 (92%)	9 (8%)	12	31
1	S	119/137 (87%)	101 (85%)	18 (15%)	3	8
1	T	119/137 (87%)	104 (87%)	15 (13%)	4	13
1	U	118/137 (86%)	104 (88%)	14 (12%)	5	15
1	V	118/137 (86%)	106 (90%)	12 (10%)	7	20
1	W	120/137 (88%)	106 (88%)	14 (12%)	5	16
1	X	120/137 (88%)	100 (83%)	20 (17%)	2	6
All	All	2856/3288 (87%)	2550 (89%)	306 (11%)	6	18

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	-1	GLN
1	X	-1	GLN
1	T	29	SER
1	V	1	VAL
1	X	117	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
1	V	8	ASN
1	W	8	ASN
1	I	144	ASN
1	I	109	GLN
1	W	106	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	U	155	-	4,4,4	0.37	0	6,6,6	1.44	1 (16%)
2	SO4	G	155	-	4,4,4	0.63	0	6,6,6	1.13	1 (16%)
2	SO4	P	155	-	4,4,4	0.37	0	6,6,6	0.84	0
2	SO4	X	155	-	4,4,4	0.50	0	6,6,6	0.79	0
2	SO4	A	156	-	4,4,4	0.58	0	6,6,6	0.77	0
2	SO4	E	155	-	4,4,4	0.32	0	6,6,6	0.97	0
2	SO4	T	155	-	4,4,4	0.40	0	6,6,6	0.88	0
2	SO4	I	155	-	4,4,4	0.49	0	6,6,6	1.42	1 (16%)
2	SO4	R	155	-	4,4,4	0.28	0	6,6,6	1.19	1 (16%)
2	SO4	V	155	-	4,4,4	0.32	0	6,6,6	0.42	0
2	SO4	O	155	-	4,4,4	0.44	0	6,6,6	0.98	0
3	TRS	D	156	-	7,7,7	0.66	0	9,9,9	1.79	3 (33%)
2	SO4	S	155	-	4,4,4	0.51	0	6,6,6	1.01	0
2	SO4	H	155	-	4,4,4	0.54	0	6,6,6	0.83	0
3	TRS	W	156	-	7,7,7	0.78	0	9,9,9	1.18	1 (11%)
2	SO4	W	155	-	4,4,4	0.41	0	6,6,6	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	155	-	4,4,4	0.54	0	6,6,6	1.41	0
2	SO4	M	155	-	4,4,4	0.59	0	6,6,6	0.95	0
3	TRS	N	156	-	7,7,7	0.39	0	9,9,9	0.63	0
2	SO4	F	155	-	4,4,4	0.53	0	6,6,6	1.54	1 (16%)
3	TRS	J	156	-	7,7,7	0.69	0	9,9,9	0.79	0
2	SO4	K	155	-	4,4,4	0.26	0	6,6,6	0.60	0
2	SO4	D	155	-	4,4,4	0.56	0	6,6,6	0.71	0
2	SO4	A	155	-	4,4,4	0.56	0	6,6,6	1.07	1 (16%)
2	SO4	C	155	-	4,4,4	0.48	0	6,6,6	0.84	0
3	TRS	G	156	-	7,7,7	0.81	0	9,9,9	1.44	1 (11%)
3	TRS	T	156	-	7,7,7	0.55	0	9,9,9	1.08	0
3	TRS	P	156	-	7,7,7	0.63	0	9,9,9	1.93	5 (55%)
2	SO4	Q	155	-	4,4,4	0.62	0	6,6,6	1.12	1 (16%)
2	SO4	N	155	-	4,4,4	0.27	0	6,6,6	1.02	0
2	SO4	J	155	-	4,4,4	0.54	0	6,6,6	0.80	0
3	TRS	A	157	-	7,7,7	0.75	0	9,9,9	1.33	1 (11%)

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	TRS	W	156	-	-	5/9/9/9	-
3	TRS	T	156	-	-	2/9/9/9	-
3	TRS	G	156	-	-	2/9/9/9	-
3	TRS	P	156	-	-	5/9/9/9	-
3	TRS	N	156	-	-	3/9/9/9	-
3	TRS	D	156	-	-	9/9/9/9	-
3	TRS	A	157	-	-	2/9/9/9	-
3	TRS	J	156	-	-	0/9/9/9	-

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	156	TRS	C3-C-N	3.18	116.29	108.17
2	F	155	SO4	O3-S-O1	3.06	125.55	109.56
3	A	157	TRS	O1-C1-C	-2.99	102.55	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	156	TRS	C3-C-C2	-2.83	103.13	110.66
3	D	156	TRS	C2-C-N	2.75	115.20	108.17

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	156	TRS	C1-C-C2-O2
3	D	156	TRS	C3-C-C2-O2
3	D	156	TRS	C1-C-C3-O3
3	N	156	TRS	C3-C-C2-O2
3	N	156	TRS	N-C-C2-O2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	156	TRS	1	0
3	W	156	TRS	1	0
3	N	156	TRS	1	0
3	P	156	TRS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	143/167 (85%)	-0.29	4 (2%)	55	47	35, 49, 85, 114	0
1	B	143/167 (85%)	-0.25	5 (3%)	47	40	34, 47, 73, 93	0
1	C	143/167 (85%)	-0.25	3 (2%)	63	55	37, 54, 93, 112	0
1	D	144/167 (86%)	-0.25	3 (2%)	63	55	36, 51, 90, 120	0
1	E	145/167 (86%)	-0.42	2 (1%)	73	67	33, 46, 85, 113	0
1	F	145/167 (86%)	-0.40	1 (0%)	84	80	34, 45, 75, 105	0
1	G	143/167 (85%)	-0.21	3 (2%)	63	55	37, 52, 96, 113	0
1	H	144/167 (86%)	-0.19	4 (2%)	55	47	37, 54, 93, 110	0
1	I	147/167 (88%)	-0.30	1 (0%)	84	80	36, 45, 78, 102	0
1	J	143/167 (85%)	-0.13	3 (2%)	63	55	44, 57, 96, 120	0
1	K	144/167 (86%)	-0.10	3 (2%)	63	55	44, 57, 100, 111	0
1	L	144/167 (86%)	-0.02	3 (2%)	63	55	46, 59, 104, 118	0
1	M	144/167 (86%)	-0.33	2 (1%)	73	67	40, 51, 95, 112	0
1	N	144/167 (86%)	-0.18	2 (1%)	73	67	39, 49, 81, 96	0
1	O	144/167 (86%)	-0.36	2 (1%)	73	67	40, 54, 95, 106	0
1	P	144/167 (86%)	-0.40	3 (2%)	63	55	39, 53, 97, 113	0
1	Q	144/167 (86%)	-0.41	2 (1%)	73	67	37, 50, 92, 112	0
1	R	144/167 (86%)	-0.30	2 (1%)	73	67	34, 48, 89, 108	0
1	S	144/167 (86%)	-0.22	3 (2%)	63	55	41, 56, 101, 113	0
1	T	144/167 (86%)	-0.07	2 (1%)	73	67	43, 60, 109, 127	0
1	U	143/167 (85%)	-0.24	2 (1%)	73	67	41, 53, 93, 119	0
1	V	143/167 (85%)	-0.25	3 (2%)	63	55	48, 60, 102, 124	0
1	W	145/167 (86%)	-0.04	3 (2%)	63	55	49, 60, 110, 121	0
1	X	145/167 (86%)	-0.19	3 (2%)	63	55	47, 59, 108, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3456/4008 (86%)	-0.24	64 (1%) 66 58	33, 54, 97, 127	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	23	TYR	4.7
1	V	23	TYR	4.6
1	K	23	TYR	4.3
1	B	23	TYR	4.2
1	D	23	TYR	4.2

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	X	155	5/5	0.74	0.15	107,109,111,113	0
2	SO4	J	155	5/5	0.78	0.17	116,118,119,119	0
2	SO4	M	155	5/5	0.80	0.19	106,108,111,112	0
2	SO4	P	155	5/5	0.80	0.17	106,107,108,110	0
2	SO4	E	155	5/5	0.80	0.15	108,110,111,113	0
2	SO4	U	155	5/5	0.81	0.17	101,103,104,105	0
2	SO4	C	155	5/5	0.81	0.13	111,112,114,117	0
2	SO4	T	155	5/5	0.82	0.13	113,115,116,117	0
2	SO4	K	155	5/5	0.84	0.17	116,117,118,118	0
2	SO4	D	155	5/5	0.85	0.12	95,95,97,100	0
2	SO4	O	155	5/5	0.85	0.12	111,114,115,116	0
2	SO4	H	155	5/5	0.85	0.17	101,103,105,108	0
2	SO4	Q	155	5/5	0.86	0.16	94,97,99,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	G	155	5/5	0.87	0.13	86,90,93,95	0
2	SO4	A	155	5/5	0.87	0.14	100,102,105,107	0
2	SO4	W	155	5/5	0.87	0.14	110,113,114,115	0
2	SO4	R	155	5/5	0.87	0.13	96,98,99,100	0
2	SO4	F	155	5/5	0.88	0.15	88,91,96,97	0
2	SO4	S	155	5/5	0.88	0.20	100,102,105,106	0
2	SO4	B	155	5/5	0.89	0.14	84,84,90,91	0
2	SO4	V	155	5/5	0.89	0.09	110,111,112,112	0
2	SO4	A	156	5/5	0.90	0.15	88,89,91,91	0
2	SO4	I	155	5/5	0.91	0.15	67,67,71,72	0
3	TRS	J	156	8/8	0.93	0.09	45,49,50,50	0
3	TRS	W	156	8/8	0.94	0.10	52,55,56,56	0
3	TRS	G	156	8/8	0.95	0.10	41,43,44,44	0
2	SO4	N	155	5/5	0.95	0.10	85,88,88,91	0
3	TRS	A	157	8/8	0.95	0.08	38,44,45,45	0
3	TRS	N	156	8/8	0.96	0.07	35,38,39,39	0
3	TRS	P	156	8/8	0.97	0.07	35,38,38,41	0
3	TRS	T	156	8/8	0.97	0.07	50,52,52,53	0
3	TRS	D	156	8/8	0.97	0.08	40,40,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.