



# wwPDB X-ray Structure Validation Summary Report

Aug 29, 2023 – 11:18 AM EDT

PDB ID : 3N8K  
Title : Type II dehydroquinase from Mycobacterium tuberculosis complexed with citrazinic acid  
Authors : Snee, W.C.; Palaninathan, S.K.; Sacchettini, J.C.; Dias, M.V.B.; Bromfield, K.M.; Payne, R.; Ciulli, A.; Howard, N.I.; Abell, C.; Blundell, T.L.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2010-05-28  
Resolution : 2.25 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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

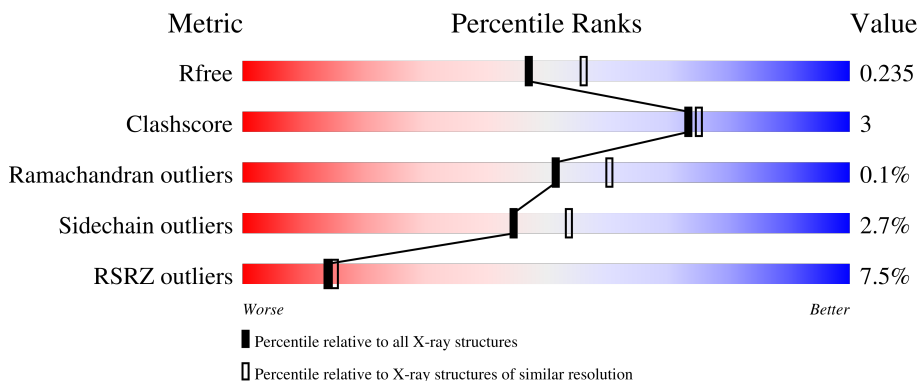
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	172	
1	B	172	
1	C	172	
1	D	172	

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Mol	Chain	Length	Quality of chain
1	E	172	% 77% 6% • 17%
1	F	172	73% 6% • 18%
1	G	172	% 76% 6% • 17%
1	H	172	77% • • 18%
1	I	172	73% 8% • 18%
1	J	172	73% 8% • 18%
1	K	172	% 75% 5% • 18%
1	L	172	2% 77% • • 18%
1	M	172	% 80% 6% • 12%
1	N	172	8% 73% 9% • 18%
1	O	172	23% 72% 9% • 18%
1	P	172	% 71% 9% • 18%
1	Q	172	13% 69% 9% • 21%
1	R	172	% 73% 9% • 18%
1	S	172	2% 74% 7% • 18%
1	T	172	28% 72% 10% • 18%
1	U	172	% 73% 9% • 18%
1	V	172	37% 74% 6% • 18%
1	W	172	8% 77% 5% • 18%
1	X	172	20% 71% 6% • 22%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27184 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-dehydroquinate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	142	1075	678	197	199	1	0	0	0
1	B	142	1073	674	197	201	1	0	0	0
1	C	142	1070	674	194	201	1	0	0	0
1	D	143	1079	680	198	200	1	0	0	0
1	E	143	1074	674	198	201	1	0	0	1
1	F	141	1067	673	193	200	1	0	0	0
1	G	143	1078	682	192	203	1	0	2	0
1	H	141	1061	670	190	200	1	0	0	0
1	I	141	1063	672	192	198	1	0	1	0
1	J	141	1072	677	194	200	1	0	1	0
1	K	141	1055	663	193	198	1	0	0	0
1	L	141	1062	669	192	200	1	0	1	0
1	M	151	1140	715	208	216	1	0	0	0
1	N	141	1068	671	196	200	1	0	0	0
1	O	141	1068	671	196	200	1	0	0	0
1	P	141	1071	674	196	200	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	136	Total	C	N	O	S	0	0	0
			1021	640	188	192	1			
1	R	141	Total	C	N	O	S	0	0	0
			1068	671	196	200	1			
1	S	141	Total	C	N	O	S	0	0	0
			1068	671	196	200	1			
1	T	141	Total	C	N	O	S	0	0	0
			1064	669	196	198	1			
1	U	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	V	141	Total	C	N	O	S	0	0	0
			1068	671	196	200	1			
1	W	141	Total	C	N	O	S	0	0	0
			1064	668	195	200	1			
1	X	134	Total	C	N	O	S	0	0	0
			1009	634	186	188	1			

There are 600 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	expression tag	UNP P0A4Z6
A	-24	GLY	-	expression tag	UNP P0A4Z6
A	-23	SER	-	expression tag	UNP P0A4Z6
A	-22	SER	-	expression tag	UNP P0A4Z6
A	-21	HIS	-	expression tag	UNP P0A4Z6
A	-20	HIS	-	expression tag	UNP P0A4Z6
A	-19	HIS	-	expression tag	UNP P0A4Z6
A	-18	HIS	-	expression tag	UNP P0A4Z6
A	-17	HIS	-	expression tag	UNP P0A4Z6
A	-16	HIS	-	expression tag	UNP P0A4Z6
A	-15	SER	-	expression tag	UNP P0A4Z6
A	-14	SER	-	expression tag	UNP P0A4Z6
A	-13	GLY	-	expression tag	UNP P0A4Z6
A	-12	LEU	-	expression tag	UNP P0A4Z6
A	-11	GLN	-	expression tag	UNP P0A4Z6
A	-10	GLY	-	expression tag	UNP P0A4Z6
A	-9	THR	-	expression tag	UNP P0A4Z6
A	-8	GLU	-	expression tag	UNP P0A4Z6
A	-7	ASN	-	expression tag	UNP P0A4Z6
A	-6	LEU	-	expression tag	UNP P0A4Z6
A	-5	TYR	-	expression tag	UNP P0A4Z6
A	-4	PHE	-	expression tag	UNP P0A4Z6
A	-3	GLN	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P0A4Z6
A	-1	HIS	-	expression tag	UNP P0A4Z6
B	-25	MET	-	expression tag	UNP P0A4Z6
B	-24	GLY	-	expression tag	UNP P0A4Z6
B	-23	SER	-	expression tag	UNP P0A4Z6
B	-22	SER	-	expression tag	UNP P0A4Z6
B	-21	HIS	-	expression tag	UNP P0A4Z6
B	-20	HIS	-	expression tag	UNP P0A4Z6
B	-19	HIS	-	expression tag	UNP P0A4Z6
B	-18	HIS	-	expression tag	UNP P0A4Z6
B	-17	HIS	-	expression tag	UNP P0A4Z6
B	-16	HIS	-	expression tag	UNP P0A4Z6
B	-15	SER	-	expression tag	UNP P0A4Z6
B	-14	SER	-	expression tag	UNP P0A4Z6
B	-13	GLY	-	expression tag	UNP P0A4Z6
B	-12	LEU	-	expression tag	UNP P0A4Z6
B	-11	GLN	-	expression tag	UNP P0A4Z6
B	-10	GLY	-	expression tag	UNP P0A4Z6
B	-9	THR	-	expression tag	UNP P0A4Z6
B	-8	GLU	-	expression tag	UNP P0A4Z6
B	-7	ASN	-	expression tag	UNP P0A4Z6
B	-6	LEU	-	expression tag	UNP P0A4Z6
B	-5	TYR	-	expression tag	UNP P0A4Z6
B	-4	PHE	-	expression tag	UNP P0A4Z6
B	-3	GLN	-	expression tag	UNP P0A4Z6
B	-2	SER	-	expression tag	UNP P0A4Z6
B	-1	HIS	-	expression tag	UNP P0A4Z6
C	-25	MET	-	expression tag	UNP P0A4Z6
C	-24	GLY	-	expression tag	UNP P0A4Z6
C	-23	SER	-	expression tag	UNP P0A4Z6
C	-22	SER	-	expression tag	UNP P0A4Z6
C	-21	HIS	-	expression tag	UNP P0A4Z6
C	-20	HIS	-	expression tag	UNP P0A4Z6
C	-19	HIS	-	expression tag	UNP P0A4Z6
C	-18	HIS	-	expression tag	UNP P0A4Z6
C	-17	HIS	-	expression tag	UNP P0A4Z6
C	-16	HIS	-	expression tag	UNP P0A4Z6
C	-15	SER	-	expression tag	UNP P0A4Z6
C	-14	SER	-	expression tag	UNP P0A4Z6
C	-13	GLY	-	expression tag	UNP P0A4Z6
C	-12	LEU	-	expression tag	UNP P0A4Z6
C	-11	GLN	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLY	-	expression tag	UNP P0A4Z6
C	-9	THR	-	expression tag	UNP P0A4Z6
C	-8	GLU	-	expression tag	UNP P0A4Z6
C	-7	ASN	-	expression tag	UNP P0A4Z6
C	-6	LEU	-	expression tag	UNP P0A4Z6
C	-5	TYR	-	expression tag	UNP P0A4Z6
C	-4	PHE	-	expression tag	UNP P0A4Z6
C	-3	GLN	-	expression tag	UNP P0A4Z6
C	-2	SER	-	expression tag	UNP P0A4Z6
C	-1	HIS	-	expression tag	UNP P0A4Z6
D	-25	MET	-	expression tag	UNP P0A4Z6
D	-24	GLY	-	expression tag	UNP P0A4Z6
D	-23	SER	-	expression tag	UNP P0A4Z6
D	-22	SER	-	expression tag	UNP P0A4Z6
D	-21	HIS	-	expression tag	UNP P0A4Z6
D	-20	HIS	-	expression tag	UNP P0A4Z6
D	-19	HIS	-	expression tag	UNP P0A4Z6
D	-18	HIS	-	expression tag	UNP P0A4Z6
D	-17	HIS	-	expression tag	UNP P0A4Z6
D	-16	HIS	-	expression tag	UNP P0A4Z6
D	-15	SER	-	expression tag	UNP P0A4Z6
D	-14	SER	-	expression tag	UNP P0A4Z6
D	-13	GLY	-	expression tag	UNP P0A4Z6
D	-12	LEU	-	expression tag	UNP P0A4Z6
D	-11	GLN	-	expression tag	UNP P0A4Z6
D	-10	GLY	-	expression tag	UNP P0A4Z6
D	-9	THR	-	expression tag	UNP P0A4Z6
D	-8	GLU	-	expression tag	UNP P0A4Z6
D	-7	ASN	-	expression tag	UNP P0A4Z6
D	-6	LEU	-	expression tag	UNP P0A4Z6
D	-5	TYR	-	expression tag	UNP P0A4Z6
D	-4	PHE	-	expression tag	UNP P0A4Z6
D	-3	GLN	-	expression tag	UNP P0A4Z6
D	-2	SER	-	expression tag	UNP P0A4Z6
D	-1	HIS	-	expression tag	UNP P0A4Z6
E	-25	MET	-	expression tag	UNP P0A4Z6
E	-24	GLY	-	expression tag	UNP P0A4Z6
E	-23	SER	-	expression tag	UNP P0A4Z6
E	-22	SER	-	expression tag	UNP P0A4Z6
E	-21	HIS	-	expression tag	UNP P0A4Z6
E	-20	HIS	-	expression tag	UNP P0A4Z6
E	-19	HIS	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-18	HIS	-	expression tag	UNP P0A4Z6
E	-17	HIS	-	expression tag	UNP P0A4Z6
E	-16	HIS	-	expression tag	UNP P0A4Z6
E	-15	SER	-	expression tag	UNP P0A4Z6
E	-14	SER	-	expression tag	UNP P0A4Z6
E	-13	GLY	-	expression tag	UNP P0A4Z6
E	-12	LEU	-	expression tag	UNP P0A4Z6
E	-11	GLN	-	expression tag	UNP P0A4Z6
E	-10	GLY	-	expression tag	UNP P0A4Z6
E	-9	THR	-	expression tag	UNP P0A4Z6
E	-8	GLU	-	expression tag	UNP P0A4Z6
E	-7	ASN	-	expression tag	UNP P0A4Z6
E	-6	LEU	-	expression tag	UNP P0A4Z6
E	-5	TYR	-	expression tag	UNP P0A4Z6
E	-4	PHE	-	expression tag	UNP P0A4Z6
E	-3	GLN	-	expression tag	UNP P0A4Z6
E	-2	SER	-	expression tag	UNP P0A4Z6
E	-1	HIS	-	expression tag	UNP P0A4Z6
F	-25	MET	-	expression tag	UNP P0A4Z6
F	-24	GLY	-	expression tag	UNP P0A4Z6
F	-23	SER	-	expression tag	UNP P0A4Z6
F	-22	SER	-	expression tag	UNP P0A4Z6
F	-21	HIS	-	expression tag	UNP P0A4Z6
F	-20	HIS	-	expression tag	UNP P0A4Z6
F	-19	HIS	-	expression tag	UNP P0A4Z6
F	-18	HIS	-	expression tag	UNP P0A4Z6
F	-17	HIS	-	expression tag	UNP P0A4Z6
F	-16	HIS	-	expression tag	UNP P0A4Z6
F	-15	SER	-	expression tag	UNP P0A4Z6
F	-14	SER	-	expression tag	UNP P0A4Z6
F	-13	GLY	-	expression tag	UNP P0A4Z6
F	-12	LEU	-	expression tag	UNP P0A4Z6
F	-11	GLN	-	expression tag	UNP P0A4Z6
F	-10	GLY	-	expression tag	UNP P0A4Z6
F	-9	THR	-	expression tag	UNP P0A4Z6
F	-8	GLU	-	expression tag	UNP P0A4Z6
F	-7	ASN	-	expression tag	UNP P0A4Z6
F	-6	LEU	-	expression tag	UNP P0A4Z6
F	-5	TYR	-	expression tag	UNP P0A4Z6
F	-4	PHE	-	expression tag	UNP P0A4Z6
F	-3	GLN	-	expression tag	UNP P0A4Z6
F	-2	SER	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	HIS	-	expression tag	UNP P0A4Z6
G	-25	MET	-	expression tag	UNP P0A4Z6
G	-24	GLY	-	expression tag	UNP P0A4Z6
G	-23	SER	-	expression tag	UNP P0A4Z6
G	-22	SER	-	expression tag	UNP P0A4Z6
G	-21	HIS	-	expression tag	UNP P0A4Z6
G	-20	HIS	-	expression tag	UNP P0A4Z6
G	-19	HIS	-	expression tag	UNP P0A4Z6
G	-18	HIS	-	expression tag	UNP P0A4Z6
G	-17	HIS	-	expression tag	UNP P0A4Z6
G	-16	HIS	-	expression tag	UNP P0A4Z6
G	-15	SER	-	expression tag	UNP P0A4Z6
G	-14	SER	-	expression tag	UNP P0A4Z6
G	-13	GLY	-	expression tag	UNP P0A4Z6
G	-12	LEU	-	expression tag	UNP P0A4Z6
G	-11	GLN	-	expression tag	UNP P0A4Z6
G	-10	GLY	-	expression tag	UNP P0A4Z6
G	-9	THR	-	expression tag	UNP P0A4Z6
G	-8	GLU	-	expression tag	UNP P0A4Z6
G	-7	ASN	-	expression tag	UNP P0A4Z6
G	-6	LEU	-	expression tag	UNP P0A4Z6
G	-5	TYR	-	expression tag	UNP P0A4Z6
G	-4	PHE	-	expression tag	UNP P0A4Z6
G	-3	GLN	-	expression tag	UNP P0A4Z6
G	-2	SER	-	expression tag	UNP P0A4Z6
G	-1	HIS	-	expression tag	UNP P0A4Z6
H	-25	MET	-	expression tag	UNP P0A4Z6
H	-24	GLY	-	expression tag	UNP P0A4Z6
H	-23	SER	-	expression tag	UNP P0A4Z6
H	-22	SER	-	expression tag	UNP P0A4Z6
H	-21	HIS	-	expression tag	UNP P0A4Z6
H	-20	HIS	-	expression tag	UNP P0A4Z6
H	-19	HIS	-	expression tag	UNP P0A4Z6
H	-18	HIS	-	expression tag	UNP P0A4Z6
H	-17	HIS	-	expression tag	UNP P0A4Z6
H	-16	HIS	-	expression tag	UNP P0A4Z6
H	-15	SER	-	expression tag	UNP P0A4Z6
H	-14	SER	-	expression tag	UNP P0A4Z6
H	-13	GLY	-	expression tag	UNP P0A4Z6
H	-12	LEU	-	expression tag	UNP P0A4Z6
H	-11	GLN	-	expression tag	UNP P0A4Z6
H	-10	GLY	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	THR	-	expression tag	UNP P0A4Z6
H	-8	GLU	-	expression tag	UNP P0A4Z6
H	-7	ASN	-	expression tag	UNP P0A4Z6
H	-6	LEU	-	expression tag	UNP P0A4Z6
H	-5	TYR	-	expression tag	UNP P0A4Z6
H	-4	PHE	-	expression tag	UNP P0A4Z6
H	-3	GLN	-	expression tag	UNP P0A4Z6
H	-2	SER	-	expression tag	UNP P0A4Z6
H	-1	HIS	-	expression tag	UNP P0A4Z6
I	-25	MET	-	expression tag	UNP P0A4Z6
I	-24	GLY	-	expression tag	UNP P0A4Z6
I	-23	SER	-	expression tag	UNP P0A4Z6
I	-22	SER	-	expression tag	UNP P0A4Z6
I	-21	HIS	-	expression tag	UNP P0A4Z6
I	-20	HIS	-	expression tag	UNP P0A4Z6
I	-19	HIS	-	expression tag	UNP P0A4Z6
I	-18	HIS	-	expression tag	UNP P0A4Z6
I	-17	HIS	-	expression tag	UNP P0A4Z6
I	-16	HIS	-	expression tag	UNP P0A4Z6
I	-15	SER	-	expression tag	UNP P0A4Z6
I	-14	SER	-	expression tag	UNP P0A4Z6
I	-13	GLY	-	expression tag	UNP P0A4Z6
I	-12	LEU	-	expression tag	UNP P0A4Z6
I	-11	GLN	-	expression tag	UNP P0A4Z6
I	-10	GLY	-	expression tag	UNP P0A4Z6
I	-9	THR	-	expression tag	UNP P0A4Z6
I	-8	GLU	-	expression tag	UNP P0A4Z6
I	-7	ASN	-	expression tag	UNP P0A4Z6
I	-6	LEU	-	expression tag	UNP P0A4Z6
I	-5	TYR	-	expression tag	UNP P0A4Z6
I	-4	PHE	-	expression tag	UNP P0A4Z6
I	-3	GLN	-	expression tag	UNP P0A4Z6
I	-2	SER	-	expression tag	UNP P0A4Z6
I	-1	HIS	-	expression tag	UNP P0A4Z6
J	-25	MET	-	expression tag	UNP P0A4Z6
J	-24	GLY	-	expression tag	UNP P0A4Z6
J	-23	SER	-	expression tag	UNP P0A4Z6
J	-22	SER	-	expression tag	UNP P0A4Z6
J	-21	HIS	-	expression tag	UNP P0A4Z6
J	-20	HIS	-	expression tag	UNP P0A4Z6
J	-19	HIS	-	expression tag	UNP P0A4Z6
J	-18	HIS	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-17	HIS	-	expression tag	UNP P0A4Z6
J	-16	HIS	-	expression tag	UNP P0A4Z6
J	-15	SER	-	expression tag	UNP P0A4Z6
J	-14	SER	-	expression tag	UNP P0A4Z6
J	-13	GLY	-	expression tag	UNP P0A4Z6
J	-12	LEU	-	expression tag	UNP P0A4Z6
J	-11	GLN	-	expression tag	UNP P0A4Z6
J	-10	GLY	-	expression tag	UNP P0A4Z6
J	-9	THR	-	expression tag	UNP P0A4Z6
J	-8	GLU	-	expression tag	UNP P0A4Z6
J	-7	ASN	-	expression tag	UNP P0A4Z6
J	-6	LEU	-	expression tag	UNP P0A4Z6
J	-5	TYR	-	expression tag	UNP P0A4Z6
J	-4	PHE	-	expression tag	UNP P0A4Z6
J	-3	GLN	-	expression tag	UNP P0A4Z6
J	-2	SER	-	expression tag	UNP P0A4Z6
J	-1	HIS	-	expression tag	UNP P0A4Z6
K	-25	MET	-	expression tag	UNP P0A4Z6
K	-24	GLY	-	expression tag	UNP P0A4Z6
K	-23	SER	-	expression tag	UNP P0A4Z6
K	-22	SER	-	expression tag	UNP P0A4Z6
K	-21	HIS	-	expression tag	UNP P0A4Z6
K	-20	HIS	-	expression tag	UNP P0A4Z6
K	-19	HIS	-	expression tag	UNP P0A4Z6
K	-18	HIS	-	expression tag	UNP P0A4Z6
K	-17	HIS	-	expression tag	UNP P0A4Z6
K	-16	HIS	-	expression tag	UNP P0A4Z6
K	-15	SER	-	expression tag	UNP P0A4Z6
K	-14	SER	-	expression tag	UNP P0A4Z6
K	-13	GLY	-	expression tag	UNP P0A4Z6
K	-12	LEU	-	expression tag	UNP P0A4Z6
K	-11	GLN	-	expression tag	UNP P0A4Z6
K	-10	GLY	-	expression tag	UNP P0A4Z6
K	-9	THR	-	expression tag	UNP P0A4Z6
K	-8	GLU	-	expression tag	UNP P0A4Z6
K	-7	ASN	-	expression tag	UNP P0A4Z6
K	-6	LEU	-	expression tag	UNP P0A4Z6
K	-5	TYR	-	expression tag	UNP P0A4Z6
K	-4	PHE	-	expression tag	UNP P0A4Z6
K	-3	GLN	-	expression tag	UNP P0A4Z6
K	-2	SER	-	expression tag	UNP P0A4Z6
K	-1	HIS	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-25	MET	-	expression tag	UNP P0A4Z6
L	-24	GLY	-	expression tag	UNP P0A4Z6
L	-23	SER	-	expression tag	UNP P0A4Z6
L	-22	SER	-	expression tag	UNP P0A4Z6
L	-21	HIS	-	expression tag	UNP P0A4Z6
L	-20	HIS	-	expression tag	UNP P0A4Z6
L	-19	HIS	-	expression tag	UNP P0A4Z6
L	-18	HIS	-	expression tag	UNP P0A4Z6
L	-17	HIS	-	expression tag	UNP P0A4Z6
L	-16	HIS	-	expression tag	UNP P0A4Z6
L	-15	SER	-	expression tag	UNP P0A4Z6
L	-14	SER	-	expression tag	UNP P0A4Z6
L	-13	GLY	-	expression tag	UNP P0A4Z6
L	-12	LEU	-	expression tag	UNP P0A4Z6
L	-11	GLN	-	expression tag	UNP P0A4Z6
L	-10	GLY	-	expression tag	UNP P0A4Z6
L	-9	THR	-	expression tag	UNP P0A4Z6
L	-8	GLU	-	expression tag	UNP P0A4Z6
L	-7	ASN	-	expression tag	UNP P0A4Z6
L	-6	LEU	-	expression tag	UNP P0A4Z6
L	-5	TYR	-	expression tag	UNP P0A4Z6
L	-4	PHE	-	expression tag	UNP P0A4Z6
L	-3	GLN	-	expression tag	UNP P0A4Z6
L	-2	SER	-	expression tag	UNP P0A4Z6
L	-1	HIS	-	expression tag	UNP P0A4Z6
M	-25	MET	-	expression tag	UNP P0A4Z6
M	-24	GLY	-	expression tag	UNP P0A4Z6
M	-23	SER	-	expression tag	UNP P0A4Z6
M	-22	SER	-	expression tag	UNP P0A4Z6
M	-21	HIS	-	expression tag	UNP P0A4Z6
M	-20	HIS	-	expression tag	UNP P0A4Z6
M	-19	HIS	-	expression tag	UNP P0A4Z6
M	-18	HIS	-	expression tag	UNP P0A4Z6
M	-17	HIS	-	expression tag	UNP P0A4Z6
M	-16	HIS	-	expression tag	UNP P0A4Z6
M	-15	SER	-	expression tag	UNP P0A4Z6
M	-14	SER	-	expression tag	UNP P0A4Z6
M	-13	GLY	-	expression tag	UNP P0A4Z6
M	-12	LEU	-	expression tag	UNP P0A4Z6
M	-11	GLN	-	expression tag	UNP P0A4Z6
M	-10	GLY	-	expression tag	UNP P0A4Z6
M	-9	THR	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-8	GLU	-	expression tag	UNP P0A4Z6
M	-7	ASN	-	expression tag	UNP P0A4Z6
M	-6	LEU	-	expression tag	UNP P0A4Z6
M	-5	TYR	-	expression tag	UNP P0A4Z6
M	-4	PHE	-	expression tag	UNP P0A4Z6
M	-3	GLN	-	expression tag	UNP P0A4Z6
M	-2	SER	-	expression tag	UNP P0A4Z6
M	-1	HIS	-	expression tag	UNP P0A4Z6
N	-25	MET	-	expression tag	UNP P0A4Z6
N	-24	GLY	-	expression tag	UNP P0A4Z6
N	-23	SER	-	expression tag	UNP P0A4Z6
N	-22	SER	-	expression tag	UNP P0A4Z6
N	-21	HIS	-	expression tag	UNP P0A4Z6
N	-20	HIS	-	expression tag	UNP P0A4Z6
N	-19	HIS	-	expression tag	UNP P0A4Z6
N	-18	HIS	-	expression tag	UNP P0A4Z6
N	-17	HIS	-	expression tag	UNP P0A4Z6
N	-16	HIS	-	expression tag	UNP P0A4Z6
N	-15	SER	-	expression tag	UNP P0A4Z6
N	-14	SER	-	expression tag	UNP P0A4Z6
N	-13	GLY	-	expression tag	UNP P0A4Z6
N	-12	LEU	-	expression tag	UNP P0A4Z6
N	-11	GLN	-	expression tag	UNP P0A4Z6
N	-10	GLY	-	expression tag	UNP P0A4Z6
N	-9	THR	-	expression tag	UNP P0A4Z6
N	-8	GLU	-	expression tag	UNP P0A4Z6
N	-7	ASN	-	expression tag	UNP P0A4Z6
N	-6	LEU	-	expression tag	UNP P0A4Z6
N	-5	TYR	-	expression tag	UNP P0A4Z6
N	-4	PHE	-	expression tag	UNP P0A4Z6
N	-3	GLN	-	expression tag	UNP P0A4Z6
N	-2	SER	-	expression tag	UNP P0A4Z6
N	-1	HIS	-	expression tag	UNP P0A4Z6
O	-25	MET	-	expression tag	UNP P0A4Z6
O	-24	GLY	-	expression tag	UNP P0A4Z6
O	-23	SER	-	expression tag	UNP P0A4Z6
O	-22	SER	-	expression tag	UNP P0A4Z6
O	-21	HIS	-	expression tag	UNP P0A4Z6
O	-20	HIS	-	expression tag	UNP P0A4Z6
O	-19	HIS	-	expression tag	UNP P0A4Z6
O	-18	HIS	-	expression tag	UNP P0A4Z6
O	-17	HIS	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-16	HIS	-	expression tag	UNP P0A4Z6
O	-15	SER	-	expression tag	UNP P0A4Z6
O	-14	SER	-	expression tag	UNP P0A4Z6
O	-13	GLY	-	expression tag	UNP P0A4Z6
O	-12	LEU	-	expression tag	UNP P0A4Z6
O	-11	GLN	-	expression tag	UNP P0A4Z6
O	-10	GLY	-	expression tag	UNP P0A4Z6
O	-9	THR	-	expression tag	UNP P0A4Z6
O	-8	GLU	-	expression tag	UNP P0A4Z6
O	-7	ASN	-	expression tag	UNP P0A4Z6
O	-6	LEU	-	expression tag	UNP P0A4Z6
O	-5	TYR	-	expression tag	UNP P0A4Z6
O	-4	PHE	-	expression tag	UNP P0A4Z6
O	-3	GLN	-	expression tag	UNP P0A4Z6
O	-2	SER	-	expression tag	UNP P0A4Z6
O	-1	HIS	-	expression tag	UNP P0A4Z6
P	-25	MET	-	expression tag	UNP P0A4Z6
P	-24	GLY	-	expression tag	UNP P0A4Z6
P	-23	SER	-	expression tag	UNP P0A4Z6
P	-22	SER	-	expression tag	UNP P0A4Z6
P	-21	HIS	-	expression tag	UNP P0A4Z6
P	-20	HIS	-	expression tag	UNP P0A4Z6
P	-19	HIS	-	expression tag	UNP P0A4Z6
P	-18	HIS	-	expression tag	UNP P0A4Z6
P	-17	HIS	-	expression tag	UNP P0A4Z6
P	-16	HIS	-	expression tag	UNP P0A4Z6
P	-15	SER	-	expression tag	UNP P0A4Z6
P	-14	SER	-	expression tag	UNP P0A4Z6
P	-13	GLY	-	expression tag	UNP P0A4Z6
P	-12	LEU	-	expression tag	UNP P0A4Z6
P	-11	GLN	-	expression tag	UNP P0A4Z6
P	-10	GLY	-	expression tag	UNP P0A4Z6
P	-9	THR	-	expression tag	UNP P0A4Z6
P	-8	GLU	-	expression tag	UNP P0A4Z6
P	-7	ASN	-	expression tag	UNP P0A4Z6
P	-6	LEU	-	expression tag	UNP P0A4Z6
P	-5	TYR	-	expression tag	UNP P0A4Z6
P	-4	PHE	-	expression tag	UNP P0A4Z6
P	-3	GLN	-	expression tag	UNP P0A4Z6
P	-2	SER	-	expression tag	UNP P0A4Z6
P	-1	HIS	-	expression tag	UNP P0A4Z6
Q	-25	MET	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-24	GLY	-	expression tag	UNP P0A4Z6
Q	-23	SER	-	expression tag	UNP P0A4Z6
Q	-22	SER	-	expression tag	UNP P0A4Z6
Q	-21	HIS	-	expression tag	UNP P0A4Z6
Q	-20	HIS	-	expression tag	UNP P0A4Z6
Q	-19	HIS	-	expression tag	UNP P0A4Z6
Q	-18	HIS	-	expression tag	UNP P0A4Z6
Q	-17	HIS	-	expression tag	UNP P0A4Z6
Q	-16	HIS	-	expression tag	UNP P0A4Z6
Q	-15	SER	-	expression tag	UNP P0A4Z6
Q	-14	SER	-	expression tag	UNP P0A4Z6
Q	-13	GLY	-	expression tag	UNP P0A4Z6
Q	-12	LEU	-	expression tag	UNP P0A4Z6
Q	-11	GLN	-	expression tag	UNP P0A4Z6
Q	-10	GLY	-	expression tag	UNP P0A4Z6
Q	-9	THR	-	expression tag	UNP P0A4Z6
Q	-8	GLU	-	expression tag	UNP P0A4Z6
Q	-7	ASN	-	expression tag	UNP P0A4Z6
Q	-6	LEU	-	expression tag	UNP P0A4Z6
Q	-5	TYR	-	expression tag	UNP P0A4Z6
Q	-4	PHE	-	expression tag	UNP P0A4Z6
Q	-3	GLN	-	expression tag	UNP P0A4Z6
Q	-2	SER	-	expression tag	UNP P0A4Z6
Q	-1	HIS	-	expression tag	UNP P0A4Z6
R	-25	MET	-	expression tag	UNP P0A4Z6
R	-24	GLY	-	expression tag	UNP P0A4Z6
R	-23	SER	-	expression tag	UNP P0A4Z6
R	-22	SER	-	expression tag	UNP P0A4Z6
R	-21	HIS	-	expression tag	UNP P0A4Z6
R	-20	HIS	-	expression tag	UNP P0A4Z6
R	-19	HIS	-	expression tag	UNP P0A4Z6
R	-18	HIS	-	expression tag	UNP P0A4Z6
R	-17	HIS	-	expression tag	UNP P0A4Z6
R	-16	HIS	-	expression tag	UNP P0A4Z6
R	-15	SER	-	expression tag	UNP P0A4Z6
R	-14	SER	-	expression tag	UNP P0A4Z6
R	-13	GLY	-	expression tag	UNP P0A4Z6
R	-12	LEU	-	expression tag	UNP P0A4Z6
R	-11	GLN	-	expression tag	UNP P0A4Z6
R	-10	GLY	-	expression tag	UNP P0A4Z6
R	-9	THR	-	expression tag	UNP P0A4Z6
R	-8	GLU	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-7	ASN	-	expression tag	UNP P0A4Z6
R	-6	LEU	-	expression tag	UNP P0A4Z6
R	-5	TYR	-	expression tag	UNP P0A4Z6
R	-4	PHE	-	expression tag	UNP P0A4Z6
R	-3	GLN	-	expression tag	UNP P0A4Z6
R	-2	SER	-	expression tag	UNP P0A4Z6
R	-1	HIS	-	expression tag	UNP P0A4Z6
S	-25	MET	-	expression tag	UNP P0A4Z6
S	-24	GLY	-	expression tag	UNP P0A4Z6
S	-23	SER	-	expression tag	UNP P0A4Z6
S	-22	SER	-	expression tag	UNP P0A4Z6
S	-21	HIS	-	expression tag	UNP P0A4Z6
S	-20	HIS	-	expression tag	UNP P0A4Z6
S	-19	HIS	-	expression tag	UNP P0A4Z6
S	-18	HIS	-	expression tag	UNP P0A4Z6
S	-17	HIS	-	expression tag	UNP P0A4Z6
S	-16	HIS	-	expression tag	UNP P0A4Z6
S	-15	SER	-	expression tag	UNP P0A4Z6
S	-14	SER	-	expression tag	UNP P0A4Z6
S	-13	GLY	-	expression tag	UNP P0A4Z6
S	-12	LEU	-	expression tag	UNP P0A4Z6
S	-11	GLN	-	expression tag	UNP P0A4Z6
S	-10	GLY	-	expression tag	UNP P0A4Z6
S	-9	THR	-	expression tag	UNP P0A4Z6
S	-8	GLU	-	expression tag	UNP P0A4Z6
S	-7	ASN	-	expression tag	UNP P0A4Z6
S	-6	LEU	-	expression tag	UNP P0A4Z6
S	-5	TYR	-	expression tag	UNP P0A4Z6
S	-4	PHE	-	expression tag	UNP P0A4Z6
S	-3	GLN	-	expression tag	UNP P0A4Z6
S	-2	SER	-	expression tag	UNP P0A4Z6
S	-1	HIS	-	expression tag	UNP P0A4Z6
T	-25	MET	-	expression tag	UNP P0A4Z6
T	-24	GLY	-	expression tag	UNP P0A4Z6
T	-23	SER	-	expression tag	UNP P0A4Z6
T	-22	SER	-	expression tag	UNP P0A4Z6
T	-21	HIS	-	expression tag	UNP P0A4Z6
T	-20	HIS	-	expression tag	UNP P0A4Z6
T	-19	HIS	-	expression tag	UNP P0A4Z6
T	-18	HIS	-	expression tag	UNP P0A4Z6
T	-17	HIS	-	expression tag	UNP P0A4Z6
T	-16	HIS	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-15	SER	-	expression tag	UNP P0A4Z6
T	-14	SER	-	expression tag	UNP P0A4Z6
T	-13	GLY	-	expression tag	UNP P0A4Z6
T	-12	LEU	-	expression tag	UNP P0A4Z6
T	-11	GLN	-	expression tag	UNP P0A4Z6
T	-10	GLY	-	expression tag	UNP P0A4Z6
T	-9	THR	-	expression tag	UNP P0A4Z6
T	-8	GLU	-	expression tag	UNP P0A4Z6
T	-7	ASN	-	expression tag	UNP P0A4Z6
T	-6	LEU	-	expression tag	UNP P0A4Z6
T	-5	TYR	-	expression tag	UNP P0A4Z6
T	-4	PHE	-	expression tag	UNP P0A4Z6
T	-3	GLN	-	expression tag	UNP P0A4Z6
T	-2	SER	-	expression tag	UNP P0A4Z6
T	-1	HIS	-	expression tag	UNP P0A4Z6
U	-25	MET	-	expression tag	UNP P0A4Z6
U	-24	GLY	-	expression tag	UNP P0A4Z6
U	-23	SER	-	expression tag	UNP P0A4Z6
U	-22	SER	-	expression tag	UNP P0A4Z6
U	-21	HIS	-	expression tag	UNP P0A4Z6
U	-20	HIS	-	expression tag	UNP P0A4Z6
U	-19	HIS	-	expression tag	UNP P0A4Z6
U	-18	HIS	-	expression tag	UNP P0A4Z6
U	-17	HIS	-	expression tag	UNP P0A4Z6
U	-16	HIS	-	expression tag	UNP P0A4Z6
U	-15	SER	-	expression tag	UNP P0A4Z6
U	-14	SER	-	expression tag	UNP P0A4Z6
U	-13	GLY	-	expression tag	UNP P0A4Z6
U	-12	LEU	-	expression tag	UNP P0A4Z6
U	-11	GLN	-	expression tag	UNP P0A4Z6
U	-10	GLY	-	expression tag	UNP P0A4Z6
U	-9	THR	-	expression tag	UNP P0A4Z6
U	-8	GLU	-	expression tag	UNP P0A4Z6
U	-7	ASN	-	expression tag	UNP P0A4Z6
U	-6	LEU	-	expression tag	UNP P0A4Z6
U	-5	TYR	-	expression tag	UNP P0A4Z6
U	-4	PHE	-	expression tag	UNP P0A4Z6
U	-3	GLN	-	expression tag	UNP P0A4Z6
U	-2	SER	-	expression tag	UNP P0A4Z6
U	-1	HIS	-	expression tag	UNP P0A4Z6
V	-25	MET	-	expression tag	UNP P0A4Z6
V	-24	GLY	-	expression tag	UNP P0A4Z6

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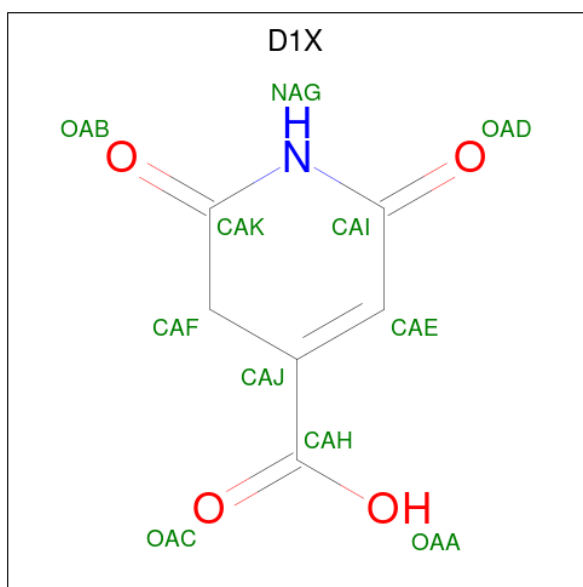
Chain	Residue	Modelled	Actual	Comment	Reference
V	-23	SER	-	expression tag	UNP P0A4Z6
V	-22	SER	-	expression tag	UNP P0A4Z6
V	-21	HIS	-	expression tag	UNP P0A4Z6
V	-20	HIS	-	expression tag	UNP P0A4Z6
V	-19	HIS	-	expression tag	UNP P0A4Z6
V	-18	HIS	-	expression tag	UNP P0A4Z6
V	-17	HIS	-	expression tag	UNP P0A4Z6
V	-16	HIS	-	expression tag	UNP P0A4Z6
V	-15	SER	-	expression tag	UNP P0A4Z6
V	-14	SER	-	expression tag	UNP P0A4Z6
V	-13	GLY	-	expression tag	UNP P0A4Z6
V	-12	LEU	-	expression tag	UNP P0A4Z6
V	-11	GLN	-	expression tag	UNP P0A4Z6
V	-10	GLY	-	expression tag	UNP P0A4Z6
V	-9	THR	-	expression tag	UNP P0A4Z6
V	-8	GLU	-	expression tag	UNP P0A4Z6
V	-7	ASN	-	expression tag	UNP P0A4Z6
V	-6	LEU	-	expression tag	UNP P0A4Z6
V	-5	TYR	-	expression tag	UNP P0A4Z6
V	-4	PHE	-	expression tag	UNP P0A4Z6
V	-3	GLN	-	expression tag	UNP P0A4Z6
V	-2	SER	-	expression tag	UNP P0A4Z6
V	-1	HIS	-	expression tag	UNP P0A4Z6
W	-25	MET	-	expression tag	UNP P0A4Z6
W	-24	GLY	-	expression tag	UNP P0A4Z6
W	-23	SER	-	expression tag	UNP P0A4Z6
W	-22	SER	-	expression tag	UNP P0A4Z6
W	-21	HIS	-	expression tag	UNP P0A4Z6
W	-20	HIS	-	expression tag	UNP P0A4Z6
W	-19	HIS	-	expression tag	UNP P0A4Z6
W	-18	HIS	-	expression tag	UNP P0A4Z6
W	-17	HIS	-	expression tag	UNP P0A4Z6
W	-16	HIS	-	expression tag	UNP P0A4Z6
W	-15	SER	-	expression tag	UNP P0A4Z6
W	-14	SER	-	expression tag	UNP P0A4Z6
W	-13	GLY	-	expression tag	UNP P0A4Z6
W	-12	LEU	-	expression tag	UNP P0A4Z6
W	-11	GLN	-	expression tag	UNP P0A4Z6
W	-10	GLY	-	expression tag	UNP P0A4Z6
W	-9	THR	-	expression tag	UNP P0A4Z6
W	-8	GLU	-	expression tag	UNP P0A4Z6
W	-7	ASN	-	expression tag	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
W	-6	LEU	-	expression tag	UNP P0A4Z6
W	-5	TYR	-	expression tag	UNP P0A4Z6
W	-4	PHE	-	expression tag	UNP P0A4Z6
W	-3	GLN	-	expression tag	UNP P0A4Z6
W	-2	SER	-	expression tag	UNP P0A4Z6
W	-1	HIS	-	expression tag	UNP P0A4Z6
X	-25	MET	-	expression tag	UNP P0A4Z6
X	-24	GLY	-	expression tag	UNP P0A4Z6
X	-23	SER	-	expression tag	UNP P0A4Z6
X	-22	SER	-	expression tag	UNP P0A4Z6
X	-21	HIS	-	expression tag	UNP P0A4Z6
X	-20	HIS	-	expression tag	UNP P0A4Z6
X	-19	HIS	-	expression tag	UNP P0A4Z6
X	-18	HIS	-	expression tag	UNP P0A4Z6
X	-17	HIS	-	expression tag	UNP P0A4Z6
X	-16	HIS	-	expression tag	UNP P0A4Z6
X	-15	SER	-	expression tag	UNP P0A4Z6
X	-14	SER	-	expression tag	UNP P0A4Z6
X	-13	GLY	-	expression tag	UNP P0A4Z6
X	-12	LEU	-	expression tag	UNP P0A4Z6
X	-11	GLN	-	expression tag	UNP P0A4Z6
X	-10	GLY	-	expression tag	UNP P0A4Z6
X	-9	THR	-	expression tag	UNP P0A4Z6
X	-8	GLU	-	expression tag	UNP P0A4Z6
X	-7	ASN	-	expression tag	UNP P0A4Z6
X	-6	LEU	-	expression tag	UNP P0A4Z6
X	-5	TYR	-	expression tag	UNP P0A4Z6
X	-4	PHE	-	expression tag	UNP P0A4Z6
X	-3	GLN	-	expression tag	UNP P0A4Z6
X	-2	SER	-	expression tag	UNP P0A4Z6
X	-1	HIS	-	expression tag	UNP P0A4Z6

- Molecule 2 is 2,6-dioxo-1,2,3,6-tetrahydropyridine-4-carboxylic acid (three-letter code: D1X) (formula: C<sub>6</sub>H<sub>5</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	11	6	1	4	0	0
2	B	1	11	6	1	4	0	0
2	C	1	11	6	1	4	0	0
2	D	1	11	6	1	4	0	0
2	E	1	11	6	1	4	0	0
2	F	1	11	6	1	4	0	0
2	G	1	11	6	1	4	0	0
2	H	1	11	6	1	4	0	0
2	I	1	11	6	1	4	0	0
2	J	1	11	6	1	4	0	0
2	K	1	11	6	1	4	0	0
2	L	1	11	6	1	4	0	0
2	M	1	11	6	1	4	0	0
2	N	1	11	6	1	4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	N	O	0	0
			11	6	1	4		
2	P	1	Total	C	N	O	0	0
			11	6	1	4		
2	R	1	Total	C	N	O	0	0
			11	6	1	4		
2	S	1	Total	C	N	O	0	0
			11	6	1	4		
2	T	1	Total	C	N	O	0	0
			11	6	1	4		
2	U	1	Total	C	N	O	0	0
			11	6	1	4		
2	V	1	Total	C	N	O	0	0
			11	6	1	4		
2	W	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	3	Total	Cl	0	0
			3	3		
3	D	3	Total	Cl	0	0
			3	3		
3	E	2	Total	Cl	0	0
			2	2		
3	F	1	Total	Cl	0	0
			1	1		
3	H	1	Total	Cl	0	0
			1	1		
3	I	1	Total	Cl	0	0
			1	1		
3	J	2	Total	Cl	0	0
			2	2		
3	K	2	Total	Cl	0	0
			2	2		
3	L	2	Total	Cl	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total Cl 1 1	0	0
3	N	1	Total Cl 1 1	0	0
3	O	1	Total Cl 1 1	0	0
3	P	1	Total Cl 1 1	0	0
3	Q	1	Total Cl 1 1	0	0
3	S	1	Total Cl 1 1	0	0
3	V	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	81	Total O 81 81	0	0
4	B	73	Total O 73 73	0	0
4	C	77	Total O 77 77	0	0
4	D	92	Total O 92 92	0	0
4	E	81	Total O 81 81	0	0
4	F	97	Total O 97 97	0	0
4	G	85	Total O 85 85	0	0
4	H	60	Total O 60 60	0	0
4	I	69	Total O 69 69	0	0
4	J	77	Total O 77 77	0	0
4	K	63	Total O 63 63	0	0
4	L	60	Total O 60 60	0	0

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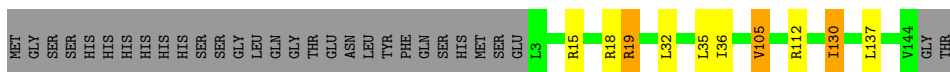
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	45	Total 45	O 45	0	0
4	N	23	Total 23	O 23	0	0
4	O	8	Total 8	O 8	0	0
4	P	87	Total 87	O 87	0	0
4	Q	12	Total 12	O 12	0	0
4	R	52	Total 52	O 52	0	0
4	S	70	Total 70	O 70	0	0
4	T	15	Total 15	O 15	0	0
4	U	51	Total 51	O 51	0	0
4	V	4	Total 4	O 4	0	0
4	W	13	Total 13	O 13	0	0
4	X	12	Total 12	O 12	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.

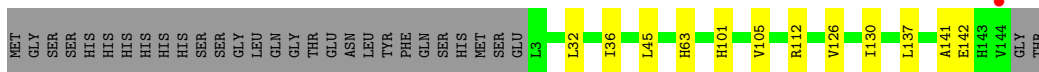
- Molecule 1: 3-dehydroquinatase dehydratase

Chain A:  77% . . 17%




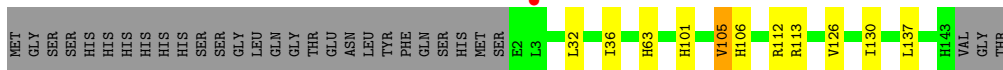
- Molecule 1: 3-dehydroquinatase dehydratase

Chain B:  76% 7% 17%




- Molecule 1: 3-dehydroquinatase dehydratase

Chain C:  76% 6% . 17%




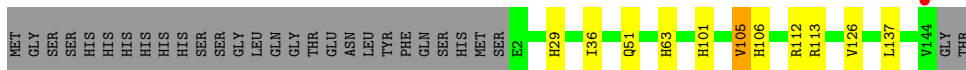
- Molecule 1: 3-dehydroquinatase dehydratase

Chain D:  74% 8% . 17%



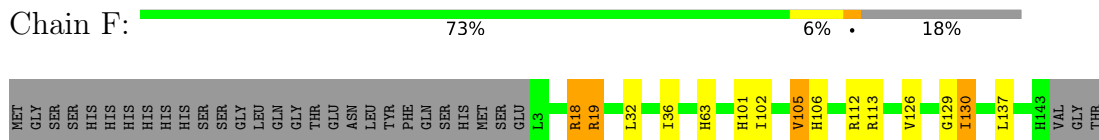
- Molecule 1: 3-dehydroquinatase dehydratase

Chain E:  77% 6% . 17%

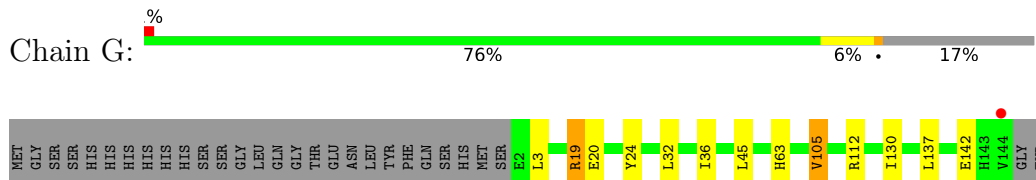


- Molecule 1: 3-dehydroquinatase dehydratase

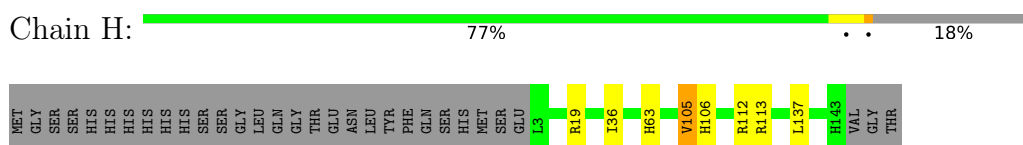




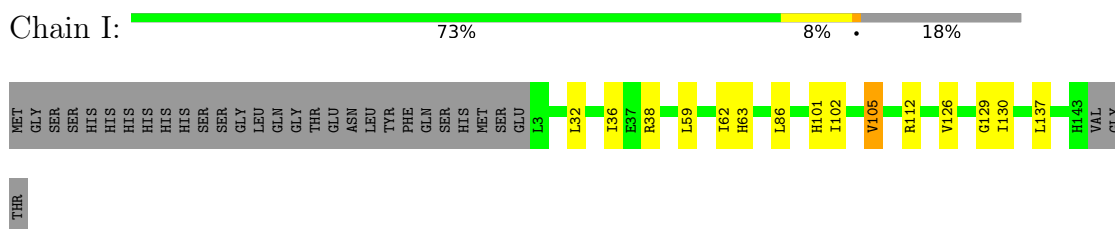
- Molecule 1: 3-dehydroquinatase dehydratase



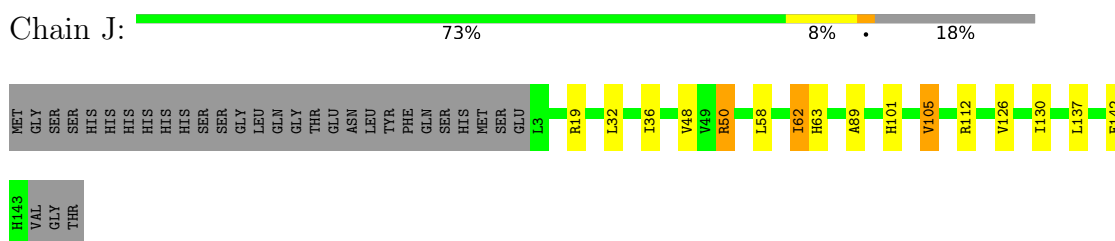
- Molecule 1: 3-dehydroquinatase dehydratase



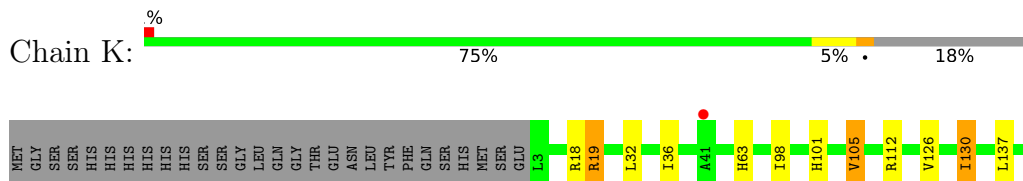
- Molecule 1: 3-dehydroquinatase dehydratase



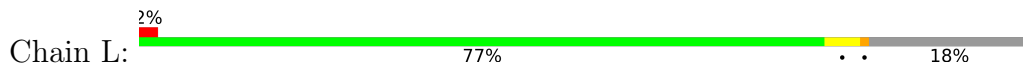
- Molecule 1: 3-dehydroquinatase dehydratase

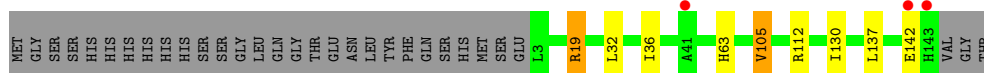


- Molecule 1: 3-dehydroquinatase dehydratase

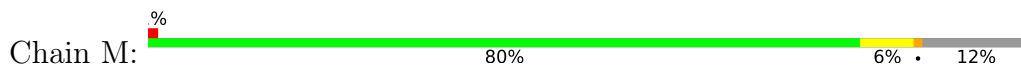


- Molecule 1: 3-dehydroquinatase dehydratase

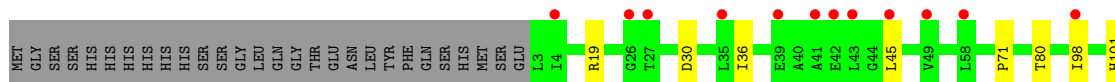




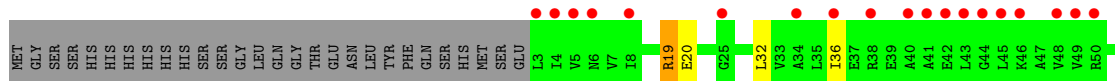
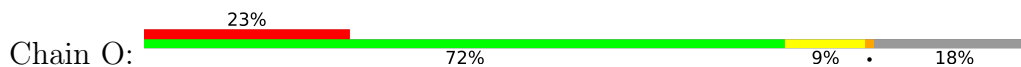
• Molecule 1: 3-dehydroquinate dehydratase



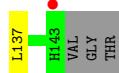
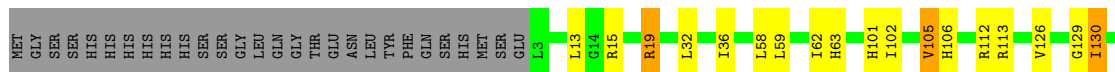
• Molecule 1: 3-dehydroquinate dehydratase



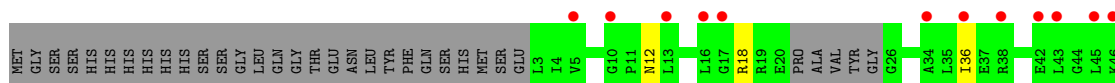
• Molecule 1: 3-dehydroquinate dehydratase



• Molecule 1: 3-dehydroquinate dehydratase

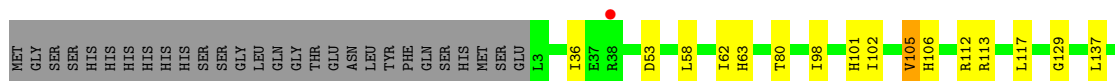


• Molecule 1: 3-dehydroquinate dehydratase

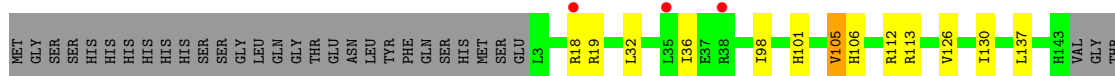
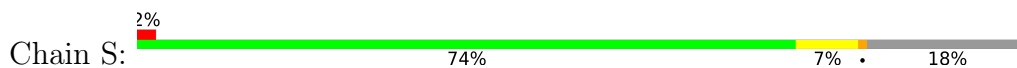




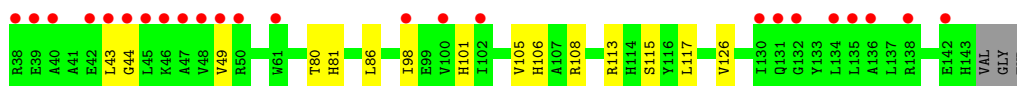
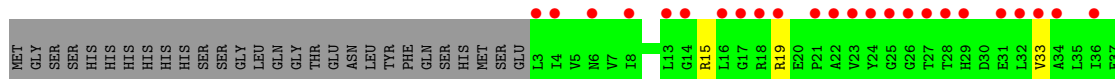
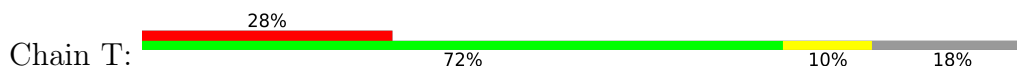
- Molecule 1: 3-dehydroquinatase dehydratase



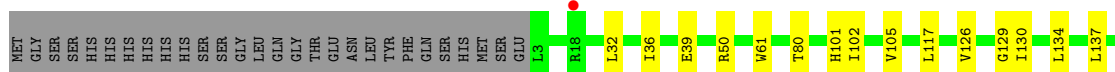
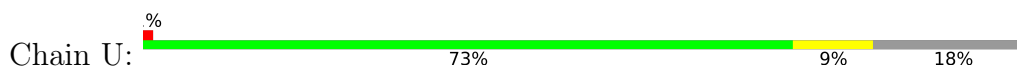
- Molecule 1: 3-dehydroquinatase dehydratase



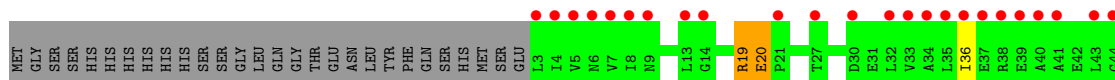
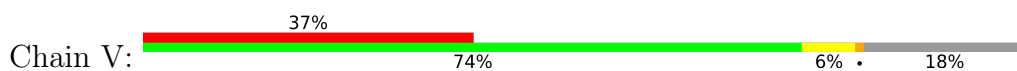
- Molecule 1: 3-dehydroquinatase dehydratase

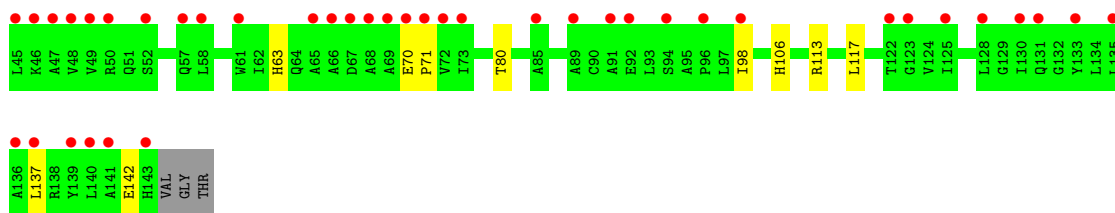


- Molecule 1: 3-dehydroquinatase dehydratase

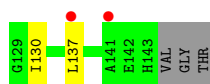
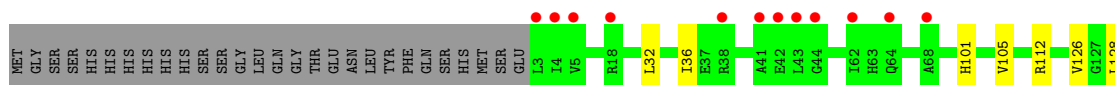
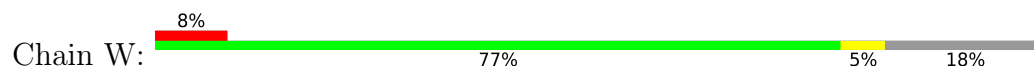


- Molecule 1: 3-dehydroquinatase dehydratase

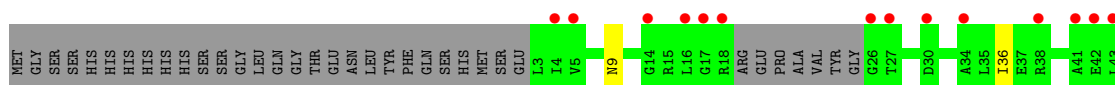




- Molecule 1: 3-dehydroquinate dehydratase



- Molecule 1: 3-dehydroquinate dehydratase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.32Å 137.21Å 146.71Å 90.00° 96.59° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 49.95 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-2.25) 98.4 (49.95-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.25Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.205 , 0.236 0.204 , 0.235	Depositor DCC
$R_{free}$ test set	8851 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	27184	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D1X, CL

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	0.30	0/1093	0.48	0/1489
1	B	0.30	0/1091	0.48	0/1486
1	C	0.29	0/1088	0.47	0/1483
1	D	0.30	0/1097	0.49	0/1494
1	E	0.30	0/1092	0.47	0/1487
1	F	0.31	0/1085	0.48	0/1478
1	G	0.30	0/1102	0.48	0/1504
1	H	0.29	0/1079	0.47	0/1471
1	I	0.30	0/1084	0.48	0/1479
1	J	0.30	0/1093	0.49	0/1489
1	K	0.29	0/1073	0.48	0/1462
1	L	0.28	0/1083	0.47	0/1477
1	M	0.29	0/1161	0.45	0/1581
1	N	0.29	0/1086	0.47	0/1479
1	O	0.30	0/1086	0.47	0/1479
1	P	0.30	0/1089	0.49	0/1483
1	Q	0.28	0/1036	0.46	0/1408
1	R	0.29	0/1086	0.47	0/1479
1	S	0.29	0/1086	0.47	0/1479
1	T	0.30	0/1082	0.46	0/1474
1	U	0.29	0/1089	0.48	0/1483
1	V	0.28	0/1086	0.45	0/1479
1	W	0.28	0/1082	0.45	0/1475
1	X	0.29	0/1024	0.47	0/1393
All	All	0.29	0/26053	0.47	0/35491

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1075	0	1086	6	0
1	B	1073	0	1072	6	0
1	C	1070	0	1070	7	0
1	D	1079	0	1087	10	0
1	E	1074	0	1072	6	0
1	F	1067	0	1072	9	0
1	G	1078	0	1073	8	0
1	H	1061	0	1061	4	0
1	I	1063	0	1066	7	0
1	J	1072	0	1083	10	0
1	K	1055	0	1043	7	0
1	L	1062	0	1054	5	0
1	M	1140	0	1115	6	0
1	N	1068	0	1070	6	0
1	O	1068	0	1070	10	0
1	P	1071	0	1079	11	0
1	Q	1021	0	1019	10	0
1	R	1068	0	1070	9	0
1	S	1068	0	1070	7	0
1	T	1064	0	1066	8	0
1	U	1071	0	1079	7	0
1	V	1068	0	1070	6	0
1	W	1064	0	1059	5	0
1	X	1009	0	1013	5	0
2	A	11	0	4	0	0
2	B	11	0	4	0	0
2	C	11	0	4	0	0
2	D	11	0	4	0	0
2	E	11	0	4	0	0
2	F	11	0	4	0	0
2	G	11	0	4	1	0
2	H	11	0	4	0	0
2	I	11	0	4	0	0
2	J	11	0	4	0	0
2	K	11	0	4	0	0
2	L	11	0	4	0	0
2	M	11	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	11	0	4	0	0
2	O	11	0	4	0	0
2	P	11	0	4	0	0
2	R	11	0	4	0	0
2	S	11	0	4	0	0
2	T	11	0	4	0	0
2	U	11	0	4	0	0
2	V	11	0	4	0	0
2	W	11	0	4	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	S	1	0	0	0	0
3	V	1	0	0	0	0
4	A	81	0	0	1	0
4	B	73	0	0	1	0
4	C	77	0	0	1	0
4	D	92	0	0	3	0
4	E	81	0	0	1	0
4	F	97	0	0	2	0
4	G	85	0	0	1	0
4	H	60	0	0	1	0
4	I	69	0	0	1	0
4	J	77	0	0	1	0
4	K	63	0	0	2	0
4	L	60	0	0	2	0
4	M	45	0	0	0	0
4	N	23	0	0	0	0
4	O	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	87	0	0	1	0
4	Q	12	0	0	0	0
4	R	52	0	0	1	0
4	S	70	0	0	1	0
4	T	15	0	0	1	0
4	U	51	0	0	0	0
4	V	4	0	0	0	0
4	W	13	0	0	0	0
4	X	12	0	0	0	0
All	All	27184	0	25707	171	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 3.

The worst 5 of 171 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:P:32:LEU:HD13	1:P:130:ILE:HG13	1.57	0.85
1:C:105:VAL:HG22	1:C:112:ARG:HB3	1.59	0.83
1:K:105:VAL:HG22	1:K:112:ARG:HB3	1.61	0.82
1:R:105:VAL:HG22	1:R:112:ARG:HB3	1.61	0.81
1:A:32:LEU:HD13	1:A:130:ILE:HG13	1.63	0.81

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	140/172 (81%)	135 (96%)	5 (4%)	0	100 100
1	B	140/172 (81%)	136 (97%)	4 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	140/172 (81%)	135 (96%)	5 (4%)	0	100	100
1	D	141/172 (82%)	136 (96%)	5 (4%)	0	100	100
1	E	141/172 (82%)	135 (96%)	6 (4%)	0	100	100
1	F	139/172 (81%)	135 (97%)	4 (3%)	0	100	100
1	G	143/172 (83%)	140 (98%)	3 (2%)	0	100	100
1	H	139/172 (81%)	134 (96%)	5 (4%)	0	100	100
1	I	140/172 (81%)	137 (98%)	3 (2%)	0	100	100
1	J	140/172 (81%)	135 (96%)	5 (4%)	0	100	100
1	K	139/172 (81%)	134 (96%)	5 (4%)	0	100	100
1	L	140/172 (81%)	135 (96%)	5 (4%)	0	100	100
1	M	149/172 (87%)	144 (97%)	5 (3%)	0	100	100
1	N	139/172 (81%)	132 (95%)	7 (5%)	0	100	100
1	O	139/172 (81%)	134 (96%)	5 (4%)	0	100	100
1	P	139/172 (81%)	136 (98%)	3 (2%)	0	100	100
1	Q	132/172 (77%)	129 (98%)	3 (2%)	0	100	100
1	R	139/172 (81%)	135 (97%)	4 (3%)	0	100	100
1	S	139/172 (81%)	135 (97%)	4 (3%)	0	100	100
1	T	139/172 (81%)	131 (94%)	6 (4%)	2 (1%)	11	7
1	U	139/172 (81%)	134 (96%)	5 (4%)	0	100	100
1	V	139/172 (81%)	134 (96%)	4 (3%)	1 (1%)	22	21
1	W	139/172 (81%)	133 (96%)	6 (4%)	0	100	100
1	X	130/172 (76%)	127 (98%)	3 (2%)	0	100	100
All	All	3344/4128 (81%)	3231 (97%)	110 (3%)	3 (0%)	51	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	44	GLY
1	T	108	ARG
1	V	20	GLU

### 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	110/137 (80%)	106 (96%)	4 (4%)	35	42
1	B	109/137 (80%)	108 (99%)	1 (1%)	78	86
1	C	109/137 (80%)	108 (99%)	1 (1%)	78	86
1	D	110/137 (80%)	106 (96%)	4 (4%)	35	42
1	E	109/137 (80%)	108 (99%)	1 (1%)	78	86
1	F	109/137 (80%)	105 (96%)	4 (4%)	34	40
1	G	109/137 (80%)	106 (97%)	3 (3%)	43	52
1	H	108/137 (79%)	106 (98%)	2 (2%)	57	66
1	I	108/137 (79%)	104 (96%)	4 (4%)	34	40
1	J	110/137 (80%)	105 (96%)	5 (4%)	27	31
1	K	105/137 (77%)	100 (95%)	5 (5%)	25	28
1	L	107/137 (78%)	104 (97%)	3 (3%)	43	52
1	M	115/137 (84%)	112 (97%)	3 (3%)	46	55
1	N	109/137 (80%)	104 (95%)	5 (5%)	27	30
1	O	109/137 (80%)	106 (97%)	3 (3%)	43	52
1	P	110/137 (80%)	106 (96%)	4 (4%)	35	42
1	Q	104/137 (76%)	102 (98%)	2 (2%)	57	66
1	R	109/137 (80%)	107 (98%)	2 (2%)	59	68
1	S	109/137 (80%)	106 (97%)	3 (3%)	43	52
1	T	108/137 (79%)	104 (96%)	4 (4%)	34	40
1	U	110/137 (80%)	108 (98%)	2 (2%)	59	68
1	V	109/137 (80%)	106 (97%)	3 (3%)	43	52
1	W	108/137 (79%)	108 (100%)	0	100	100
1	X	103/137 (75%)	100 (97%)	3 (3%)	42	51
All	All	2606/3288 (79%)	2535 (97%)	71 (3%)	44	54

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	98	ILE
1	T	19	ARG
1	V	19	ARG
1	J	19	ARG
1	I	105	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	131	GLN
1	X	131	GLN
1	Q	12	ASN
1	V	131	GLN
1	P	64	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 26 are monoatomic - leaving 22 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
2	D1X	B	147	-	11,11,11	3.05	4 (36%)	11,15,15	2.97	5 (45%)
2	D1X	M	150	-	11,11,11	3.07	4 (36%)	11,15,15	2.91	5 (45%)
2	D1X	F	147	-	11,11,11	3.03	5 (45%)	11,15,15	2.99	4 (36%)
2	D1X	H	147	-	11,11,11	3.05	4 (36%)	11,15,15	2.86	5 (45%)
2	D1X	E	147	-	11,11,11	3.07	4 (36%)	11,15,15	2.99	5 (45%)
2	D1X	L	147	-	11,11,11	3.01	4 (36%)	11,15,15	2.98	5 (45%)
2	D1X	V	147	-	11,11,11	3.07	5 (45%)	11,15,15	2.98	5 (45%)
2	D1X	D	147	-	11,11,11	3.06	4 (36%)	11,15,15	2.88	4 (36%)
2	D1X	P	147	-	11,11,11	3.10	5 (45%)	11,15,15	2.97	5 (45%)
2	D1X	S	147	-	11,11,11	3.06	4 (36%)	11,15,15	2.96	5 (45%)
2	D1X	C	147	-	11,11,11	3.05	5 (45%)	11,15,15	2.90	4 (36%)
2	D1X	A	147	-	11,11,11	3.03	4 (36%)	11,15,15	2.97	4 (36%)
2	D1X	T	147	-	11,11,11	3.08	4 (36%)	11,15,15	3.00	5 (45%)
2	D1X	R	147	-	11,11,11	3.07	4 (36%)	11,15,15	2.89	4 (36%)
2	D1X	K	147	-	11,11,11	3.02	4 (36%)	11,15,15	2.89	5 (45%)
2	D1X	G	147	-	11,11,11	3.06	4 (36%)	11,15,15	2.92	4 (36%)
2	D1X	I	147	-	11,11,11	3.04	5 (45%)	11,15,15	2.98	5 (45%)
2	D1X	N	147	-	11,11,11	3.06	4 (36%)	11,15,15	3.01	5 (45%)
2	D1X	W	147	-	11,11,11	3.09	5 (45%)	11,15,15	2.94	5 (45%)
2	D1X	U	147	-	11,11,11	3.03	4 (36%)	11,15,15	2.92	4 (36%)
2	D1X	O	147	-	11,11,11	3.06	4 (36%)	11,15,15	3.02	5 (45%)
2	D1X	J	147	-	11,11,11	3.06	5 (45%)	11,15,15	2.98	5 (45%)

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	D1X	B	147	-	-	4/4/16/16	0/1/1/1
2	D1X	M	150	-	-	4/4/16/16	0/1/1/1
2	D1X	F	147	-	-	2/4/16/16	0/1/1/1
2	D1X	H	147	-	-	4/4/16/16	0/1/1/1
2	D1X	E	147	-	-	4/4/16/16	0/1/1/1
2	D1X	L	147	-	-	4/4/16/16	0/1/1/1
2	D1X	V	147	-	-	4/4/16/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D1X	D	147	-	-	2/4/16/16	0/1/1/1
2	D1X	P	147	-	-	4/4/16/16	0/1/1/1
2	D1X	S	147	-	-	4/4/16/16	0/1/1/1
2	D1X	C	147	-	-	3/4/16/16	0/1/1/1
2	D1X	A	147	-	-	2/4/16/16	0/1/1/1
2	D1X	T	147	-	-	4/4/16/16	0/1/1/1
2	D1X	R	147	-	-	4/4/16/16	0/1/1/1
2	D1X	K	147	-	-	4/4/16/16	0/1/1/1
2	D1X	G	147	-	-	3/4/16/16	0/1/1/1
2	D1X	I	147	-	-	4/4/16/16	0/1/1/1
2	D1X	N	147	-	-	4/4/16/16	0/1/1/1
2	D1X	W	147	-	-	2/4/16/16	0/1/1/1
2	D1X	U	147	-	-	4/4/16/16	0/1/1/1
2	D1X	O	147	-	-	4/4/16/16	0/1/1/1
2	D1X	J	147	-	-	4/4/16/16	0/1/1/1

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	150	D1X	CAF-CAJ	-6.48	1.39	1.50
2	V	147	D1X	CAF-CAJ	-6.48	1.39	1.50
2	S	147	D1X	CAF-CAJ	-6.42	1.40	1.50
2	E	147	D1X	CAF-CAJ	-6.41	1.40	1.50
2	R	147	D1X	CAF-CAJ	-6.41	1.40	1.50

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	147	D1X	CAK-NAG-CAI	-6.94	119.63	127.22
2	O	147	D1X	CAK-NAG-CAI	-6.89	119.69	127.22
2	E	147	D1X	CAK-NAG-CAI	-6.81	119.77	127.22
2	N	147	D1X	CAK-NAG-CAI	-6.79	119.79	127.22
2	A	147	D1X	CAK-NAG-CAI	-6.79	119.80	127.22

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	147	D1X	OAA-CAH-CAJ-CAF
2	A	147	D1X	OAC-CAH-CAJ-CAF
2	B	147	D1X	OAA-CAH-CAJ-CAF
2	B	147	D1X	OAC-CAH-CAJ-CAF
2	C	147	D1X	OAA-CAH-CAJ-CAF

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	147	D1X	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	142/172 (82%)	-0.11	0 100 100	15, 22, 33, 42	0
1	B	142/172 (82%)	-0.42	1 (0%) 87 88	17, 24, 38, 45	0
1	C	142/172 (82%)	-0.35	1 (0%) 87 88	18, 26, 44, 52	0
1	D	143/172 (83%)	-0.33	1 (0%) 87 88	13, 20, 34, 40	0
1	E	143/172 (83%)	-0.40	1 (0%) 87 88	17, 24, 37, 43	0
1	F	141/172 (81%)	-0.38	0 100 100	14, 19, 30, 38	0
1	G	143/172 (83%)	-0.42	1 (0%) 87 88	13, 20, 36, 44	0
1	H	141/172 (81%)	-0.25	0 100 100	21, 28, 44, 52	0
1	I	141/172 (81%)	-0.32	0 100 100	16, 25, 37, 45	0
1	J	141/172 (81%)	-0.30	0 100 100	22, 29, 47, 54	0
1	K	141/172 (81%)	-0.20	1 (0%) 87 88	19, 28, 47, 56	0
1	L	141/172 (81%)	-0.18	3 (2%) 63 66	19, 27, 47, 58	0
1	M	151/172 (87%)	-0.18	1 (0%) 87 88	25, 37, 59, 69	0
1	N	141/172 (81%)	0.67	14 (9%) 7 7	39, 61, 84, 94	0
1	O	141/172 (81%)	1.56	39 (27%) 0 0	56, 82, 116, 127	0
1	P	141/172 (81%)	-0.22	1 (0%) 87 88	17, 24, 34, 39	0
1	Q	136/172 (79%)	1.02	23 (16%) 1 1	49, 73, 108, 116	0
1	R	141/172 (81%)	-0.06	2 (1%) 75 77	22, 37, 61, 76	0
1	S	141/172 (81%)	-0.23	3 (2%) 63 66	21, 30, 50, 61	0
1	T	141/172 (81%)	1.62	48 (34%) 0 0	50, 81, 121, 130	0
1	U	141/172 (81%)	-0.12	1 (0%) 87 88	23, 41, 63, 69	0
1	V	141/172 (81%)	1.96	64 (45%) 0 0	70, 114, 169, 185	0
1	W	141/172 (81%)	0.72	14 (9%) 7 7	47, 63, 89, 95	0
1	X	134/172 (77%)	1.28	35 (26%) 0 0	45, 77, 122, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3391/4128 (82%)	0.18	254 (7%) 14 15	13, 33, 105, 185	0

The worst 5 of 254 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	45	LEU	7.1
1	V	4	ILE	7.0
1	V	27	THR	6.8
1	O	143	HIS	6.4
1	T	26	GLY	6.3

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

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

## 6.3 Carbohydrates [i](#)

There are no 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	D1X	W	147	11/11	0.77	0.20	44,45,45,45	0
2	D1X	V	147	11/11	0.81	0.24	54,54,55,55	0
2	D1X	T	147	11/11	0.82	0.22	44,45,45,45	0
2	D1X	O	147	11/11	0.84	0.15	46,47,47,47	0
3	CL	L	149	1/1	0.85	0.15	53,53,53,53	0
2	D1X	N	147	11/11	0.86	0.17	44,44,44,44	0
3	CL	E	149	1/1	0.87	0.09	60,60,60,60	0
3	CL	K	149	1/1	0.88	0.07	56,56,56,56	0
2	D1X	U	147	11/11	0.89	0.17	36,37,37,37	0
3	CL	H	148	1/1	0.90	0.13	60,60,60,60	0
3	CL	O	148	1/1	0.90	0.13	58,58,58,58	0
3	CL	L	148	1/1	0.91	0.10	63,63,63,63	0
2	D1X	M	150	11/11	0.92	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CL	C	149	1/1	0.93	0.07	60,60,60,60	0
3	CL	Q	147	1/1	0.93	0.12	51,51,51,51	0
2	D1X	H	147	11/11	0.94	0.10	28,28,29,29	0
3	CL	F	148	1/1	0.94	0.10	50,50,50,50	0
2	D1X	K	147	11/11	0.94	0.11	23,23,24,24	0
3	CL	D	150	1/1	0.94	0.10	55,55,55,55	0
2	D1X	C	147	11/11	0.95	0.11	25,25,26,26	0
3	CL	N	148	1/1	0.95	0.09	41,41,41,41	0
3	CL	V	148	1/1	0.95	0.11	52,52,52,52	0
2	D1X	B	147	11/11	0.96	0.10	26,27,27,27	0
2	D1X	P	147	11/11	0.96	0.11	24,25,26,26	0
2	D1X	S	147	11/11	0.96	0.10	25,26,27,27	0
2	D1X	D	147	11/11	0.96	0.11	20,21,21,22	0
3	CL	I	148	1/1	0.96	0.07	44,44,44,44	0
3	CL	P	148	1/1	0.96	0.06	29,29,29,29	0
3	CL	J	149	1/1	0.96	0.04	49,49,49,49	0
3	CL	K	148	1/1	0.96	0.12	44,44,44,44	0
3	CL	D	149	1/1	0.97	0.06	42,42,42,42	0
2	D1X	R	147	11/11	0.97	0.12	26,27,27,28	0
2	D1X	F	147	11/11	0.97	0.11	21,22,22,22	0
2	D1X	L	147	11/11	0.97	0.10	26,26,27,27	0
2	D1X	G	147	11/11	0.97	0.12	20,21,21,21	0
2	D1X	E	147	11/11	0.97	0.09	26,26,26,26	0
2	D1X	I	147	11/11	0.97	0.12	24,25,25,25	0
2	D1X	J	147	11/11	0.97	0.08	26,26,27,27	0
3	CL	C	148	1/1	0.98	0.09	26,26,26,26	0
3	CL	S	148	1/1	0.98	0.08	39,39,39,39	0
2	D1X	A	147	11/11	0.98	0.10	23,23,23,23	0
3	CL	M	147	1/1	0.99	0.09	29,29,29,29	0
3	CL	J	148	1/1	0.99	0.07	28,28,28,28	0
3	CL	E	148	1/1	0.99	0.11	27,27,27,27	0
3	CL	C	150	1/1	0.99	0.11	33,33,33,33	0
3	CL	D	148	1/1	0.99	0.11	22,22,22,22	0
3	CL	A	148	1/1	0.99	0.11	23,23,23,23	0
3	CL	B	148	1/1	0.99	0.08	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.