wwPDB X-ray Structure Validation Summary Report (i)

Aug 28, 2023 – 09:54 PM EDT

PDB ID	:	3N59
Title	:	Type II dehydroquinase from Mycobacterium Tuberculosis complexed with 3-dehydroshikimate
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	:	2010-05-24
Resolution	:	2.52 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

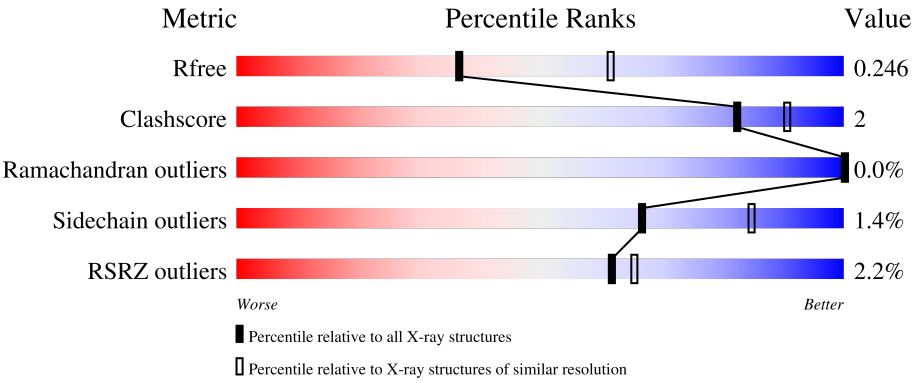
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	172	77% • • 19%
1	B	172	% 70% 7% • 21%
1	C	172	76% 6% • 17%
1	D	172	2% 74% 5% • 20%

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Mol	Chain	Length	Quality of chain
1	E	172	74% 5% 21%
1	F	172	73% 5% 22%
1	G	172	76% 6% 17%
1	H	172	74% 22%
1	I	172	73% 5% 22%
1	J	172	73% 22%
1	K	172	74% 5% 20%
1	L	172	75% 5% 20%
1	M	172	78% 6% 15%
1	N	172	74% 5% 21%
1	O	172	76% 22%
1	P	172	73% 5% 22%
1	Q	172	77% 20%
1	R	172	72% 6% 22%
1	S	172	75% 21%
1	T	172	74% 22%
1	U	172	74% 5% 22%
1	V	172	74% 5% 22%
1	W	172	73% 6% 22%
1	X	172	72% 8% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26321 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
1	A	139	Total	C	N	O	S	0	1	0
			1045	656	191	197	1			
1	B	136	Total	C	N	O	S	0	0	0
			1022	641	188	192	1			
1	C	142	Total	C	N	O	S	0	0	0
			1071	674	197	199	1			
1	D	138	Total	C	N	O	S	0	1	0
			1033	650	190	192	1			
1	E	136	Total	C	N	O	S	0	0	1
			1019	639	188	191	1			
1	F	135	Total	C	N	O	S	0	0	0
			1010	635	183	191	1			
1	G	142	Total	C	N	O	S	0	2	0
			1077	678	195	203	1			
1	H	135	Total	C	N	O	S	0	0	0
			1008	636	180	191	1			
1	I	135	Total	C	N	O	S	0	1	0
			1013	639	184	189	1			
1	J	135	Total	C	N	O	S	0	0	0
			1012	638	184	189	1			
1	K	137	Total	C	N	O	S	0	0	0
			1017	637	186	193	1			
1	L	138	Total	C	N	O	S	0	0	0
			1020	642	183	194	1			
1	M	146	Total	C	N	O	S	0	0	0
			1103	692	201	209	1			
1	N	136	Total	C	N	O	S	0	0	0
			1022	641	188	192	1			
1	O	135	Total	C	N	O	S	0	0	0
			1017	638	187	191	1			
1	P	135	Total	C	N	O	S	0	1	0
			1020	640	190	189	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	138	Total	C	N	O	S	0	0	0
			1023	641	187	194	1			
1	R	135	Total	C	N	O	S	0	1	0
			1019	641	184	193	1			
1	S	136	Total	C	N	O	S	0	0	0
			1023	644	188	190	1			
1	T	135	Total	C	N	O	S	0	0	0
			1017	638	187	191	1			
1	U	135	Total	C	N	O	S	0	1	0
			1021	645	186	189	1			
1	V	135	Total	C	N	O	S	0	0	0
			1017	638	187	191	1			
1	W	135	Total	C	N	O	S	0	0	0
			1013	635	186	191	1			
1	X	137	Total	C	N	O	S	0	0	0
			1027	644	189	193	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	2	Total Cl 2 2	0	0
2	C	1	Total Cl 1 1	0	0
2	D	2	Total Cl 2 2	0	0

Continued on next page...

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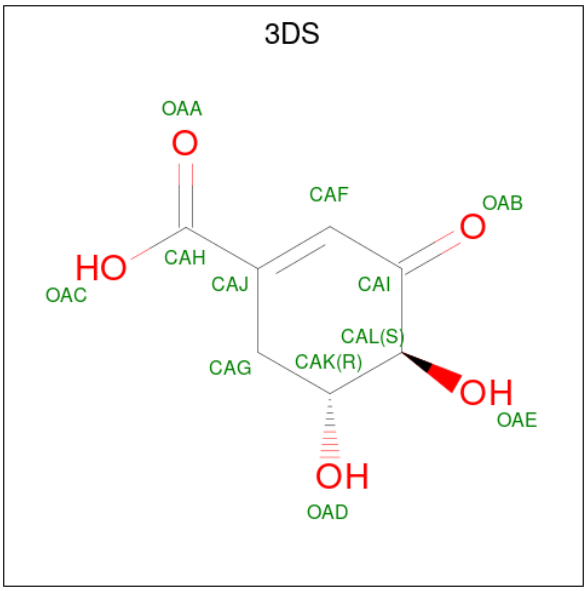
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	2	Total Cl 2 2	0	0
2	G	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	J	2	Total Cl 2 2	0	0
2	M	1	Total Cl 1 1	0	0
2	N	1	Total Cl 1 1	0	0
2	O	1	Total Cl 1 1	0	0
2	P	1	Total Cl 1 1	0	0
2	Q	1	Total Cl 1 1	0	0
2	R	1	Total Cl 1 1	0	0
2	S	1	Total Cl 1 1	0	0
2	T	1	Total Cl 1 1	0	0
2	U	1	Total Cl 1 1	0	0
2	V	2	Total Cl 2 2	0	0
2	W	1	Total Cl 1 1	0	0

- Molecule 3 is (4S,5R)-4,5-dihydroxy-3-oxocyclohex-1-ene-1-carboxylic acid (three-letter code: 3DS) (formula: $C_7H_8O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 12 7 5	0	0
3	G	1	Total C O 12 7 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	84	Total O 84 84	0	0
4	B	88	Total O 88 88	0	0
4	C	69	Total O 69 69	0	0
4	D	88	Total O 88 88	0	0
4	E	69	Total O 69 69	0	0
4	F	79	Total O 79 79	0	0
4	G	82	Total O 82 82	0	0
4	H	62	Total O 62 62	0	0
4	I	66	Total O 66 66	0	0
4	J	63	Total O 63 63	0	0

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Continued from previous page...

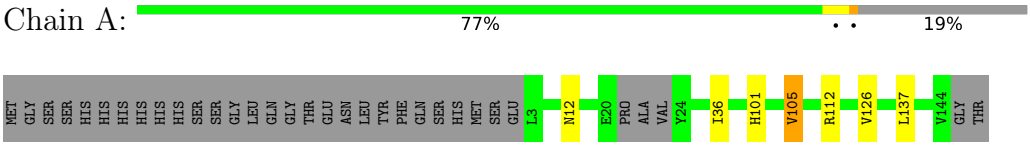
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	77	Total O 77 77	0	0
4	L	74	Total O 74 74	0	0
4	M	63	Total O 63 63	0	0
4	N	74	Total O 74 74	0	0
4	O	48	Total O 48 48	0	0
4	P	83	Total O 83 83	0	0
4	Q	46	Total O 46 46	0	0
4	R	79	Total O 79 79	0	0
4	S	63	Total O 63 63	0	0
4	T	52	Total O 52 52	0	0
4	U	67	Total O 67 67	0	0
4	V	47	Total O 47 47	0	0
4	W	47	Total O 47 47	0	0
4	X	34	Total O 34 34	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.

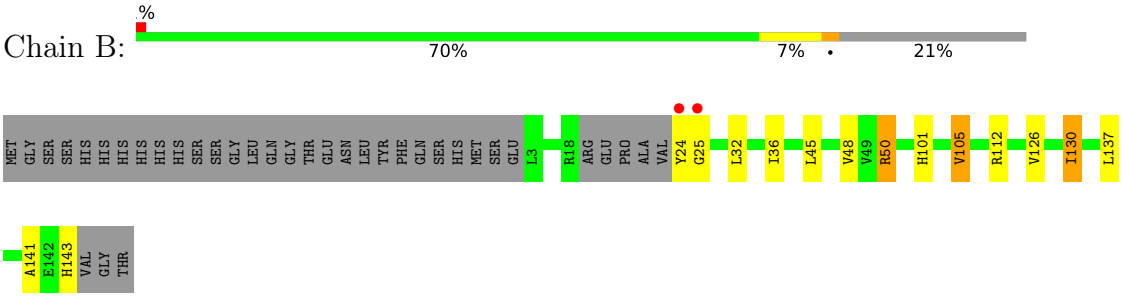
• Molecule 1: 3-dehydroquinate dehydratase

Chain A:



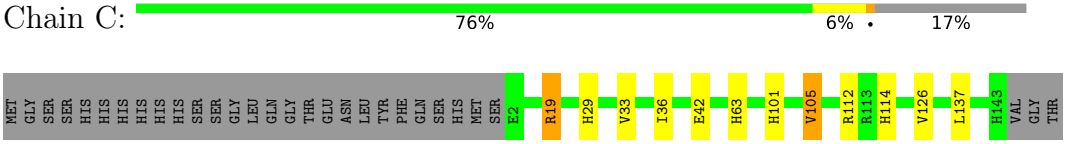
• Molecule 1: 3-dehydroquinate dehydratase

Chain B:



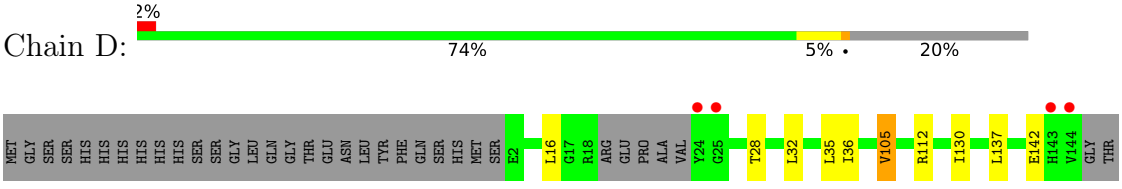
• Molecule 1: 3-dehydroquinate dehydratase

Chain C:



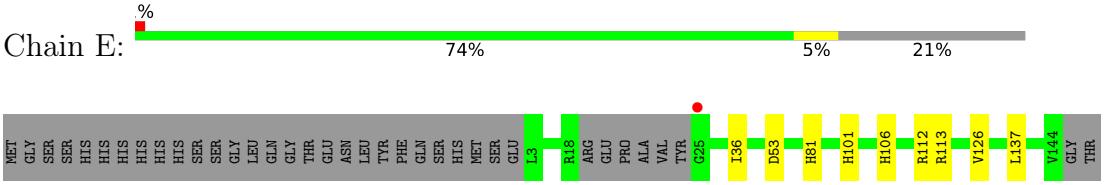
• Molecule 1: 3-dehydroquinate dehydratase

Chain D:



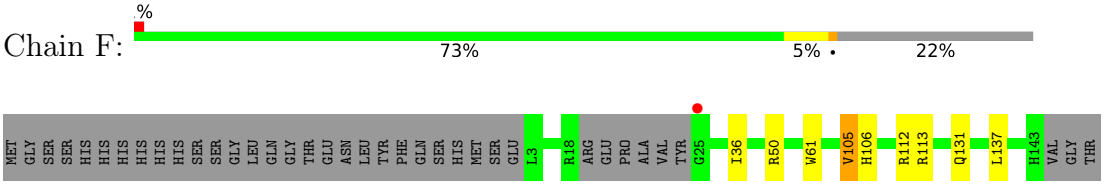
• Molecule 1: 3-dehydroquinate dehydratase

Chain E:



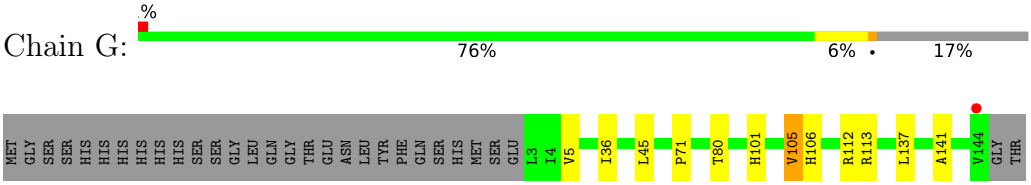
• Molecule 1: 3-dehydroquinate dehydratase

Chain F:



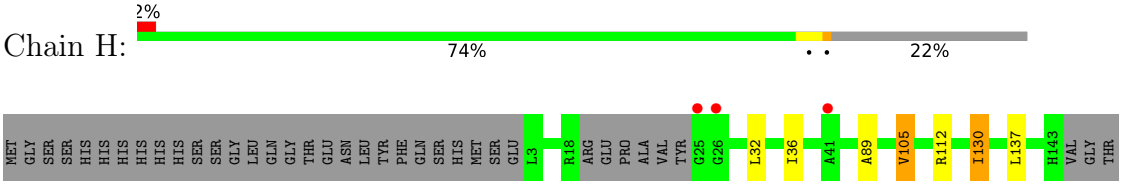
• Molecule 1: 3-dehydroquinate dehydratase

Chain G:



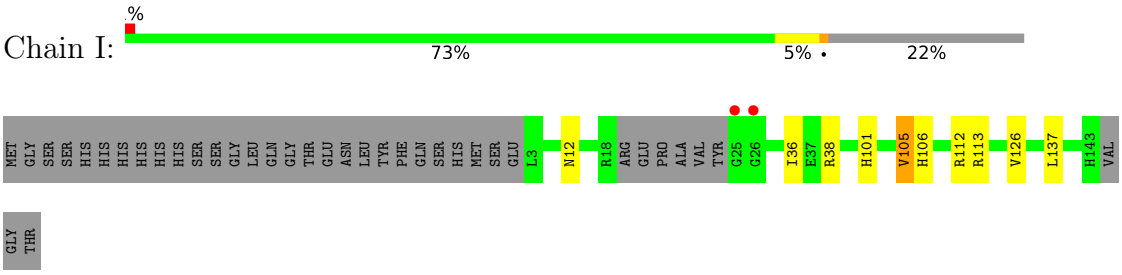
• Molecule 1: 3-dehydroquinate dehydratase

Chain H:



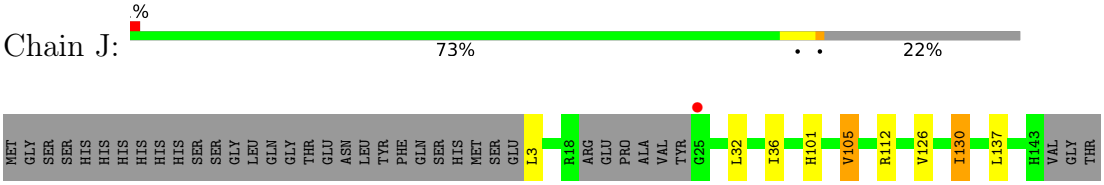
• Molecule 1: 3-dehydroquinate dehydratase

Chain I:



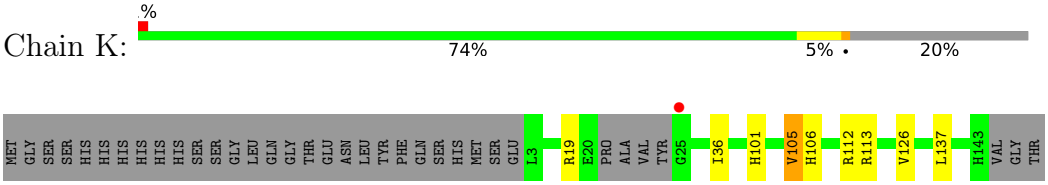
• Molecule 1: 3-dehydroquinate dehydratase

Chain J:



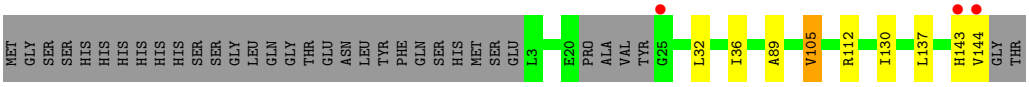
• Molecule 1: 3-dehydroquinate dehydratase

Chain K:

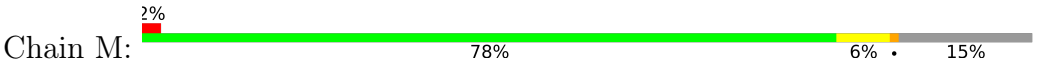


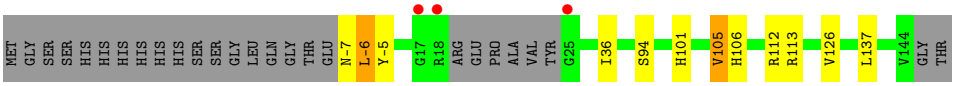
• Molecule 1: 3-dehydroquinate dehydratase

Chain L:

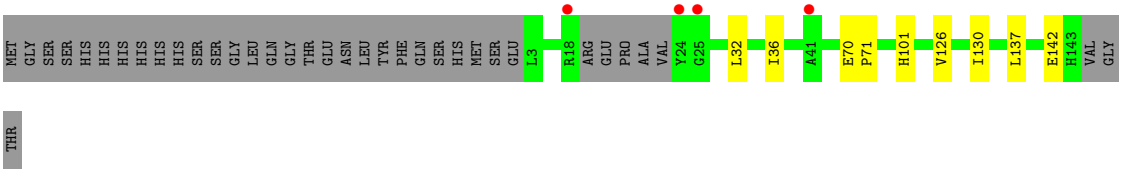


• Molecule 1: 3-dehydroquinate dehydratase

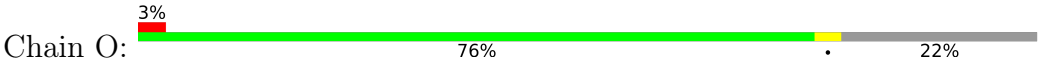


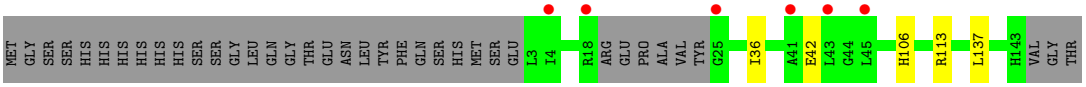


• Molecule 1: 3-dehydroquinate dehydratase

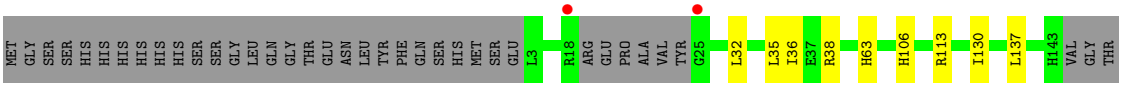


• Molecule 1: 3-dehydroquinate dehydratase

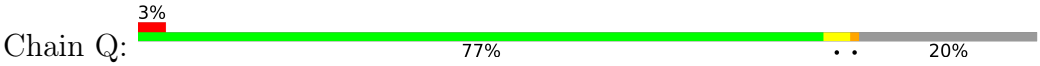


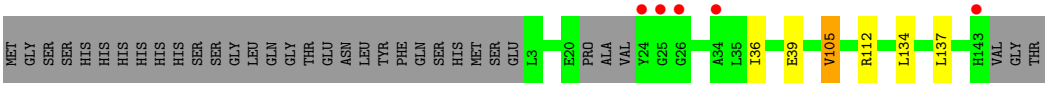


• Molecule 1: 3-dehydroquinate dehydratase

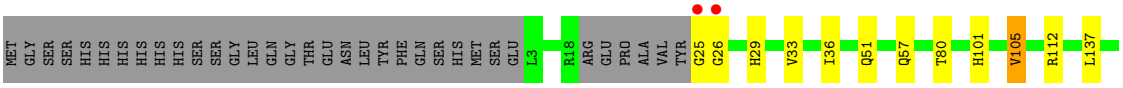


• Molecule 1: 3-dehydroquinate dehydratase



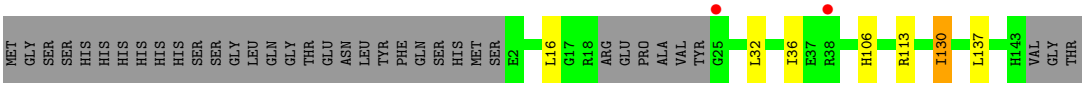


• Molecule 1: 3-dehydroquinate dehydratase



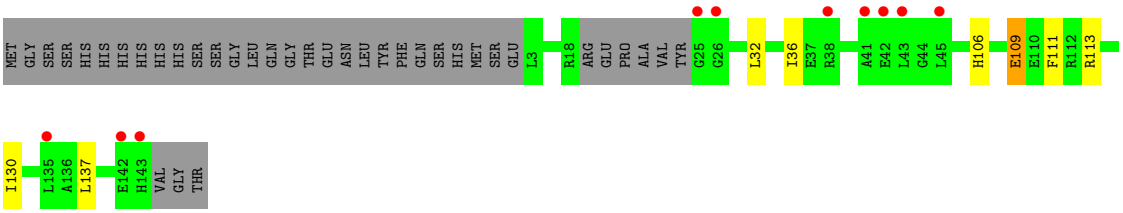
• Molecule 1: 3-dehydroquinate dehydratase

Chain S:



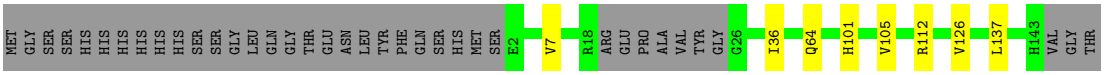
• Molecule 1: 3-dehydroquinate dehydratase

Chain T:



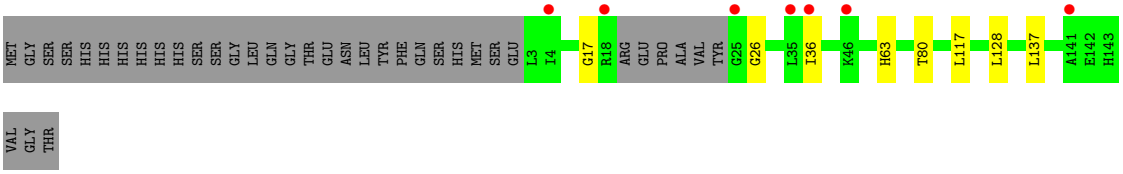
• Molecule 1: 3-dehydroquinate dehydratase

Chain U:



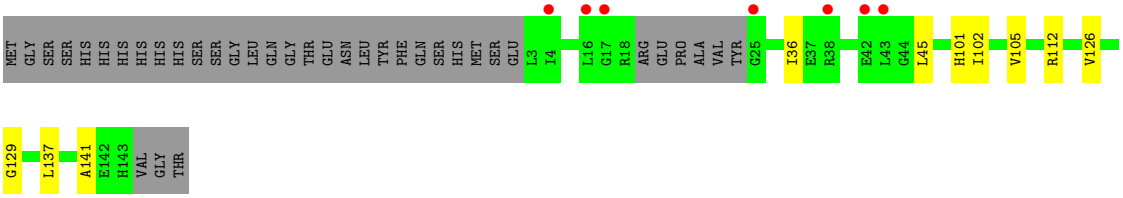
• Molecule 1: 3-dehydroquinate dehydratase

Chain V:



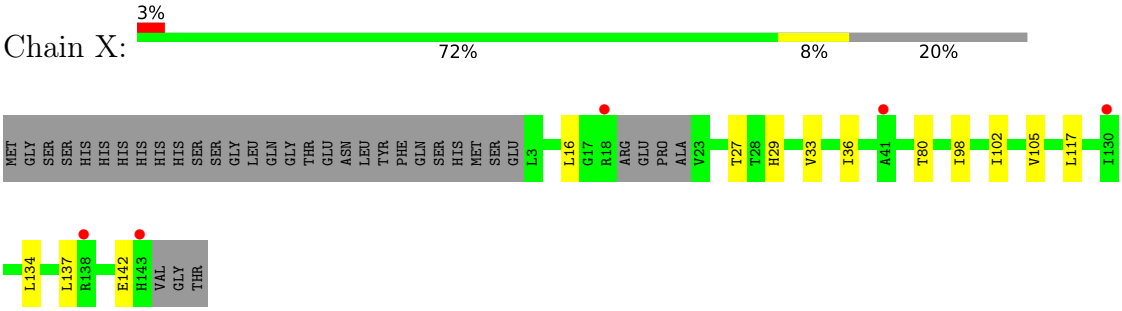
• Molecule 1: 3-dehydroquinate dehydratase

Chain W:



• Molecule 1: 3-dehydroquinate dehydratase

Chain X:


3%
72%
8%
20%
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU GLN GLY THR GLU ASN LEU TYR PHE GLN SER HIS MET SER GLU L3 L16 G17 R18 ARG GLU PRO ALA V23 T27 T28 H29 V33 I36 A41 T80 I98 I102 V105 L117 I130
L134 L137 R138 E142 H143 VAL GLY THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.99Å 137.33Å 148.10Å 90.00° 95.98° 90.00°	Depositor
Resolution (Å)	50.00 – 2.52 49.10 – 2.51	Depositor EDS
% Data completeness (in resolution range)	95.1 (50.00-2.52) 95.1 (49.10-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.89 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.248 0.198 , 0.246	Depositor DCC
R_{free} test set	6267 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26321	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3DS, 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	0.29	0/1063	0.46	0/1446
1	B	0.29	0/1037	0.48	0/1410
1	C	0.29	0/1089	0.48	0/1483
1	D	0.28	0/1051	0.48	0/1429
1	E	0.29	0/1034	0.47	0/1406
1	F	0.29	0/1025	0.47	0/1396
1	G	0.29	0/1102	0.48	0/1503
1	H	0.28	0/1023	0.47	0/1393
1	I	0.28	0/1031	0.48	0/1403
1	J	0.29	0/1027	0.48	0/1397
1	K	0.28	0/1032	0.48	0/1403
1	L	0.29	0/1035	0.48	0/1410
1	M	0.29	0/1121	0.49	0/1525
1	N	0.29	0/1037	0.46	0/1410
1	O	0.28	0/1032	0.47	0/1403
1	P	0.29	0/1038	0.47	0/1410
1	Q	0.28	0/1038	0.45	0/1413
1	R	0.28	0/1037	0.47	0/1410
1	S	0.28	0/1038	0.47	0/1411
1	T	0.28	0/1032	0.46	0/1403
1	U	0.29	0/1039	0.48	0/1412
1	V	0.28	0/1032	0.47	0/1403
1	W	0.28	0/1028	0.46	0/1399
1	X	0.29	0/1042	0.47	0/1417
All	All	0.28	0/25063	0.47	0/34095

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1045	0	1041	4	0
1	B	1022	0	1022	9	0
1	C	1071	0	1072	8	0
1	D	1033	0	1034	5	0
1	E	1019	0	1021	6	0
1	F	1010	0	1007	5	0
1	G	1077	0	1065	7	0
1	H	1008	0	1004	4	0
1	I	1013	0	1018	5	0
1	J	1012	0	1015	4	0
1	K	1017	0	1001	4	0
1	L	1020	0	1001	7	0
1	M	1103	0	1084	8	0
1	N	1022	0	1022	4	0
1	O	1017	0	1020	2	0
1	P	1020	0	1024	6	0
1	Q	1023	0	1006	3	0
1	R	1019	0	1019	6	0
1	S	1023	0	1031	4	0
1	T	1017	0	1020	5	0
1	U	1021	0	1026	5	0
1	V	1017	0	1020	5	0
1	W	1013	0	1009	5	0
1	X	1027	0	1024	6	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	1	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	J	2	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	2	0	0	0	0
2	W	1	0	0	0	0
3	C	12	0	7	0	0
3	G	12	0	7	0	0
4	A	84	0	0	0	0
4	B	88	0	0	0	0
4	C	69	0	0	2	0
4	D	88	0	0	0	0
4	E	69	0	0	0	0
4	F	79	0	0	0	0
4	G	82	0	0	0	0
4	H	62	0	0	0	0
4	I	66	0	0	0	0
4	J	63	0	0	0	0
4	K	77	0	0	0	0
4	L	74	0	0	0	0
4	M	63	0	0	0	0
4	N	74	0	0	0	0
4	O	48	0	0	0	0
4	P	83	0	0	1	0
4	Q	46	0	0	0	0
4	R	79	0	0	0	0
4	S	63	0	0	0	0
4	T	52	0	0	0	0
4	U	67	0	0	0	0
4	V	47	0	0	1	0
4	W	47	0	0	0	0
4	X	34	0	0	0	0
All	All	26321	0	24620	122	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 2.

The worst 5 of 122 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:H:105:VAL:HG22	1:H:112:ARG:HB3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:HIS:HA	1:E:113:ARG:HD3	1.61	0.82
1:B:32:LEU:HD13	1:B:130:ILE:HG12	1.63	0.79
1:G:105:VAL:HG22	1:G:112:ARG:HB3	1.66	0.77
1:D:105:VAL:HG22	1:D:112:ARG:HB3	1.66	0.76

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	136/172 (79%)	133 (98%)	3 (2%)	0	100	100
1	B	132/172 (77%)	129 (98%)	3 (2%)	0	100	100
1	C	140/172 (81%)	136 (97%)	4 (3%)	0	100	100
1	D	135/172 (78%)	132 (98%)	3 (2%)	0	100	100
1	E	132/172 (77%)	130 (98%)	2 (2%)	0	100	100
1	F	131/172 (76%)	129 (98%)	2 (2%)	0	100	100
1	G	142/172 (83%)	138 (97%)	4 (3%)	0	100	100
1	H	131/172 (76%)	128 (98%)	3 (2%)	0	100	100
1	I	132/172 (77%)	129 (98%)	3 (2%)	0	100	100
1	J	131/172 (76%)	129 (98%)	2 (2%)	0	100	100
1	K	133/172 (77%)	129 (97%)	3 (2%)	1 (1%)	19	33
1	L	134/172 (78%)	131 (98%)	3 (2%)	0	100	100
1	M	142/172 (83%)	140 (99%)	2 (1%)	0	100	100
1	N	132/172 (77%)	130 (98%)	2 (2%)	0	100	100
1	O	131/172 (76%)	127 (97%)	4 (3%)	0	100	100
1	P	132/172 (77%)	130 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	134/172 (78%)	131 (98%)	3 (2%)	0	100	100
1	R	132/172 (77%)	127 (96%)	5 (4%)	0	100	100
1	S	132/172 (77%)	131 (99%)	1 (1%)	0	100	100
1	T	131/172 (76%)	129 (98%)	2 (2%)	0	100	100
1	U	131/172 (76%)	130 (99%)	1 (1%)	0	100	100
1	V	131/172 (76%)	129 (98%)	2 (2%)	0	100	100
1	W	131/172 (76%)	128 (98%)	3 (2%)	0	100	100
1	X	133/172 (77%)	128 (96%)	5 (4%)	0	100	100
All	All	3201/4128 (78%)	3133 (98%)	67 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	19	ARG

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	106/137 (77%)	105 (99%)	1 (1%)	78	91
1	B	104/137 (76%)	101 (97%)	3 (3%)	42	67
1	C	108/137 (79%)	105 (97%)	3 (3%)	43	68
1	D	104/137 (76%)	101 (97%)	3 (3%)	42	67
1	E	104/137 (76%)	104 (100%)	0	100	100
1	F	103/137 (75%)	102 (99%)	1 (1%)	76	89
1	G	109/137 (80%)	108 (99%)	1 (1%)	78	91
1	H	102/137 (74%)	100 (98%)	2 (2%)	55	78
1	I	103/137 (75%)	101 (98%)	2 (2%)	57	79
1	J	102/137 (74%)	99 (97%)	3 (3%)	42	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	101/137 (74%)	100 (99%)	1 (1%)	76 89
1	L	101/137 (74%)	100 (99%)	1 (1%)	76 89
1	M	112/137 (82%)	110 (98%)	2 (2%)	59 80
1	N	104/137 (76%)	103 (99%)	1 (1%)	76 89
1	O	104/137 (76%)	103 (99%)	1 (1%)	76 89
1	P	103/137 (75%)	103 (100%)	0	100 100
1	Q	102/137 (74%)	101 (99%)	1 (1%)	76 89
1	R	104/137 (76%)	102 (98%)	2 (2%)	57 79
1	S	104/137 (76%)	103 (99%)	1 (1%)	76 89
1	T	104/137 (76%)	103 (99%)	1 (1%)	76 89
1	U	104/137 (76%)	103 (99%)	1 (1%)	76 89
1	V	104/137 (76%)	104 (100%)	0	100 100
1	W	103/137 (75%)	103 (100%)	0	100 100
1	X	104/137 (76%)	101 (97%)	3 (3%)	42 67
All	All	2499/3288 (76%)	2465 (99%)	34 (1%)	67 85

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	130	ILE
1	T	109	GLU
1	X	105	VAL
1	H	105	VAL
1	G	105	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	114	HIS
1	W	114	HIS
1	T	114	HIS
1	G	114	HIS
1	O	114	HIS

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 26 ligands modelled in this entry, 24 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	3DS	C	147	-	12,12,12	1.74	3 (25%)	14,17,17	1.28	2 (14%)
3	3DS	G	147	-	12,12,12	1.74	3 (25%)	14,17,17	1.36	2 (14%)

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	3DS	C	147	-	-	0/4/20/20	0/1/1/1
3	3DS	G	147	-	-	0/4/20/20	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	147	3DS	CAL-CAI	3.34	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	147	3DS	CAF-CAI	-3.14	1.39	1.46
3	C	147	3DS	CAF-CAI	-3.12	1.39	1.46
3	C	147	3DS	CAL-CAI	3.03	1.54	1.52
3	G	147	3DS	CAF-CAJ	2.13	1.40	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	147	3DS	CAI-CAF-CAJ	-3.58	121.25	123.61
3	C	147	3DS	CAI-CAF-CAJ	-3.13	121.54	123.61
3	C	147	3DS	CAL-CAI-CAF	2.19	120.74	117.30
3	G	147	3DS	CAL-CAI-CAF	2.11	120.62	117.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	139/172 (80%)	-0.26	0 100 100	25, 29, 42, 46	0
1	B	136/172 (79%)	-0.41	2 (1%) 73 76	23, 29, 42, 46	0
1	C	142/172 (82%)	-0.33	0 100 100	27, 33, 45, 46	0
1	D	138/172 (80%)	-0.18	4 (2%) 51 55	24, 29, 41, 48	1 (0%)
1	E	136/172 (79%)	-0.32	1 (0%) 87 89	26, 31, 43, 47	0
1	F	135/172 (78%)	-0.41	1 (0%) 87 89	24, 28, 35, 42	0
1	G	142/172 (82%)	-0.44	1 (0%) 87 89	24, 30, 41, 48	0
1	H	135/172 (78%)	-0.06	3 (2%) 62 65	27, 33, 48, 53	0
1	I	135/172 (78%)	-0.23	2 (1%) 73 76	25, 32, 45, 47	0
1	J	135/172 (78%)	-0.22	1 (0%) 87 89	28, 34, 49, 52	0
1	K	137/172 (79%)	-0.20	1 (0%) 87 89	28, 35, 52, 54	0
1	L	138/172 (80%)	-0.10	3 (2%) 62 65	26, 34, 51, 56	0
1	M	146/172 (84%)	-0.21	3 (2%) 63 67	30, 38, 50, 56	0
1	N	136/172 (79%)	-0.18	4 (2%) 51 55	29, 35, 50, 54	0
1	O	135/172 (78%)	0.19	6 (4%) 34 37	35, 45, 62, 63	0
1	P	135/172 (78%)	-0.32	2 (1%) 73 76	25, 29, 36, 43	0
1	Q	138/172 (80%)	0.16	5 (3%) 42 46	34, 42, 63, 67	0
1	R	135/172 (78%)	-0.15	2 (1%) 73 76	27, 34, 47, 49	0
1	S	136/172 (79%)	-0.15	2 (1%) 73 76	28, 33, 50, 52	0
1	T	135/172 (78%)	0.23	10 (7%) 14 15	35, 44, 62, 65	0
1	U	135/172 (78%)	-0.41	0 100 100	26, 32, 37, 46	0
1	V	135/172 (78%)	0.28	7 (5%) 27 29	38, 48, 64, 65	0
1	W	135/172 (78%)	0.12	7 (5%) 27 29	38, 47, 61, 66	0
1	X	137/172 (79%)	0.31	5 (3%) 42 46	39, 48, 71, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	3286/4128 (79%)	-0.14	72 (2%) 62 65	23, 35, 56, 74	1 (0%)

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	25	GLY	5.6
1	M	25	GLY	5.4
1	V	25	GLY	5.2
1	R	25	GLY	4.8
1	L	144	VAL	4.8

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, 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
3	3DS	C	147	12/12	0.92	0.22	52,52,53,53	0
3	3DS	G	147	12/12	0.95	0.17	38,39,39,39	0
2	CL	M	147	1/1	0.96	0.13	27,27,27,27	0
2	CL	N	147	1/1	0.98	0.11	26,26,26,26	0
2	CL	Q	147	1/1	0.98	0.07	34,34,34,34	0
2	CL	U	147	1/1	0.98	0.18	29,29,29,29	0
2	CL	V	147	1/1	0.98	0.16	28,28,28,28	0
2	CL	J	147	1/1	0.98	0.17	24,24,24,24	0
2	CL	B	148	1/1	0.98	0.09	27,27,27,27	0
2	CL	A	147	1/1	0.99	0.18	19,19,19,19	0
2	CL	J	148	1/1	0.99	0.13	32,32,32,32	0
2	CL	C	148	1/1	0.99	0.14	28,28,28,28	0
2	CL	D	147	1/1	0.99	0.14	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	O	147	1/1	0.99	0.21	31,31,31,31	0
2	CL	P	147	1/1	0.99	0.15	23,23,23,23	0
2	CL	D	148	1/1	0.99	0.20	25,25,25,25	0
2	CL	R	147	1/1	0.99	0.11	23,23,23,23	0
2	CL	T	147	1/1	0.99	0.09	27,27,27,27	0
2	CL	E	147	1/1	0.99	0.11	26,26,26,26	0
2	CL	E	148	1/1	0.99	0.13	23,23,23,23	0
2	CL	V	148	1/1	0.99	0.10	36,36,36,36	0
2	CL	W	147	1/1	0.99	0.16	34,34,34,34	0
2	CL	G	148	1/1	0.99	0.10	22,22,22,22	0
2	CL	H	147	1/1	0.99	0.14	20,20,20,20	0
2	CL	S	147	1/1	1.00	0.15	20,20,20,20	0
2	CL	B	147	1/1	1.00	0.13	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.