Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:09 PM GMT

PDB ID	:	4KIW
Title	:	Design and structural analysis of aromatic inhibitors of type II dehydroquinate dehydratase from Mycobacterium tuberculosis - compound 49e [5-[(3-nitrobenzyl)amino]benzene-1,3-dicarboxylic acid]
Authors	:	Dias, M.V.B; Howard, N.G.; Blundell, T.L.; Abell, C.
Deposited on	:	2013-05-02
Resolution	:	2.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

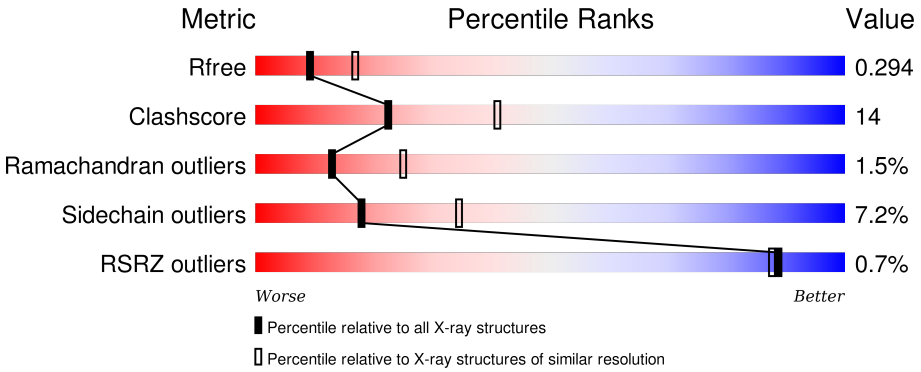
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.57 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}	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	167	% 61% 22% • 16%
1	B	167	60% 21% • 16%
1	C	167	% 59% 21% • 17%
1	D	167	62% 19% •• 18%
1	E	167	62% 19% • 19%

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Mol	Chain	Length	Quality of chain
1	F	167	53% 26% 19%
1	G	167	56% 24% 16%
1	H	167	63% 19% 16%
1	I	167	62% 19% 16%
1	J	167	62% 18% 16%
1	K	167	68% 14% 16%
1	L	167	63% 17% 17%
1	M	167	60% 19% 5% 16%
1	N	167	60% 20% 16%
1	O	167	60% 21% 16%
1	P	167	63% 19% 16%
1	Q	167	52% 25% 19%
1	R	167	4% 62% 19% 17%
1	S	167	56% 26% 16%
1	T	167	55% 27% 16%
1	U	167	63% 20% 16%
1	V	167	58% 22% 18%
1	W	167	62% 17% 16%
1	X	167	56% 23% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KIW	C	201	-	-	-	X
2	KIW	E	201	-	-	-	X
2	KIW	Q	201	-	-	-	X
2	KIW	T	201	-	-	X	-
2	KIW	U	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KIW	V	201	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26969 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	141	Total	C	N	O	S	0	0	0
			1067	672	196	198	1			
1	B	141	Total	C	N	O	S	0	1	0
			1075	677	196	201	1			
1	C	138	Total	C	N	O	S	0	0	0
			1052	661	193	197	1			
1	D	137	Total	C	N	O	S	0	0	0
			1037	653	189	194	1			
1	E	136	Total	C	N	O	S	0	0	0
			1025	644	188	192	1			
1	F	136	Total	C	N	O	S	0	0	0
			1025	644	188	192	1			
1	G	141	Total	C	N	O	S	0	1	0
			1081	680	199	201	1			
1	H	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	I	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			
1	J	141	Total	C	N	O	S	0	0	0
			1069	672	196	200	1			
1	K	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	L	138	Total	C	N	O	S	0	0	0
			1046	658	190	197	1			
1	M	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			
1	N	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	O	141	Total	C	N	O	S	0	0	0
			1061	669	193	198	1			
1	P	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	136	Total	C	N	O	S	0	0	0
			1025	644	188	192	1			
1	R	138	Total	C	N	O	S	0	0	0
			1052	661	193	197	1			
1	S	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			
1	T	140	Total	C	N	O	S	0	0	0
			1059	665	195	198	1			
1	U	141	Total	C	N	O	S	0	0	0
			1071	674	196	200	1			
1	V	137	Total	C	N	O	S	0	0	0
			1037	653	189	194	1			
1	W	141	Total	C	N	O	S	0	0	0
			1065	671	193	200	1			
1	X	138	Total	C	N	O	S	0	0	0
			1042	656	190	195	1			

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
A	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
A	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
A	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
A	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
A	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
A	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
A	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
A	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
A	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
A	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
A	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
A	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
A	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
A	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
A	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
A	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
A	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
A	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
A	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
B	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
B	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
B	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
B	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
B	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
B	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
B	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
B	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
B	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
B	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
B	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
B	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
B	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
B	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
B	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
B	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
B	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
B	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
B	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
C	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
C	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
C	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
C	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
C	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
C	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
C	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
C	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
C	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
C	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
C	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
C	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
C	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
C	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
C	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
C	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
C	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
C	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
C	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
C	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
D	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
D	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
D	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
D	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
D	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
D	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
D	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
D	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
D	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
D	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
D	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
D	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
D	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
D	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
D	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
D	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
D	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
D	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
D	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
E	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
E	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
E	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
E	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
E	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
E	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
E	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
E	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
E	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
E	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
E	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
E	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
E	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
E	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
E	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
E	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
E	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
E	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
E	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
E	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
F	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
F	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
F	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
F	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
F	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
F	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
F	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
F	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
F	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
F	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
F	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
F	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
F	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
F	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
F	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
F	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
F	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
F	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
F	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
G	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
G	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
G	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
G	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
G	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
G	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
G	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
G	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
G	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
G	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
G	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
G	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
G	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
G	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
G	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
G	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
G	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
G	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
G	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
G	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
H	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
H	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
H	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
H	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
H	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
H	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
H	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
H	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
H	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
H	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
H	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
H	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
H	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
H	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
H	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
H	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
H	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
H	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
H	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
I	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
I	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
I	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
I	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
I	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
I	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
I	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
I	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
I	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
I	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
I	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
I	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
I	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
I	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
I	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
I	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
I	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
I	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
I	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
I	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
J	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
J	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
J	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
J	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
J	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
J	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
J	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
J	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
J	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
J	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
J	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
J	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
J	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
J	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
J	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
J	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
J	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
J	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
J	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
K	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
K	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
K	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
K	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
K	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
K	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
K	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
K	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
K	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
K	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
K	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
K	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
K	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
K	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
K	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
K	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
K	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
K	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
K	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
K	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
L	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
L	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
L	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
L	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
L	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
L	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
L	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
L	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
L	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
L	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
L	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
L	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
L	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
L	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
L	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
L	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
L	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
L	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
L	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
M	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
M	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
M	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
M	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
M	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
M	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
M	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
M	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
M	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
M	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
M	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
M	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
M	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
M	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
M	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
M	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
M	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
M	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
M	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
M	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
N	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
N	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
N	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
N	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
N	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
N	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
N	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
N	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
N	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
N	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
N	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
N	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
N	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
N	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
N	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
N	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
N	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
N	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
N	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
O	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
O	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
O	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
O	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
O	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
O	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
O	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
O	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
O	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
O	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
O	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
O	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
O	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
O	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
O	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
O	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
O	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
O	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
O	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
O	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
P	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
P	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
P	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
P	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
P	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
P	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
P	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
P	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
P	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
P	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
P	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
P	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
P	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
P	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
P	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
P	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
P	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
P	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
P	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
Q	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
Q	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
Q	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
Q	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
Q	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
Q	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
Q	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
Q	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
Q	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
Q	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
Q	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
Q	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
Q	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
Q	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
Q	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
Q	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
Q	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
Q	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
Q	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
Q	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
R	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
R	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
R	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
R	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
R	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
R	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
R	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
R	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
R	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
R	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
R	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
R	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
R	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
R	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
R	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
R	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
R	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
R	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
R	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
S	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
S	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
S	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
S	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
S	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
S	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
S	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
S	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
S	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
S	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
S	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
S	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
S	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
S	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
S	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
S	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
S	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
S	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
S	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
S	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
T	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
T	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
T	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
T	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
T	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
T	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
T	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
T	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
T	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
T	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
T	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
T	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
T	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
T	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
T	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
T	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
T	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
T	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
T	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
T	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
U	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
U	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
U	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
U	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
U	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
U	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
U	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
U	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
U	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
U	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
U	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
U	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
U	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
U	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
U	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
U	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
U	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
U	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
U	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
V	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
V	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
V	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
V	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
V	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
V	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
V	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
V	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
V	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
V	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
V	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
V	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
V	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
V	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
V	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
V	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
V	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
V	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
V	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
V	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
W	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
W	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
W	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6

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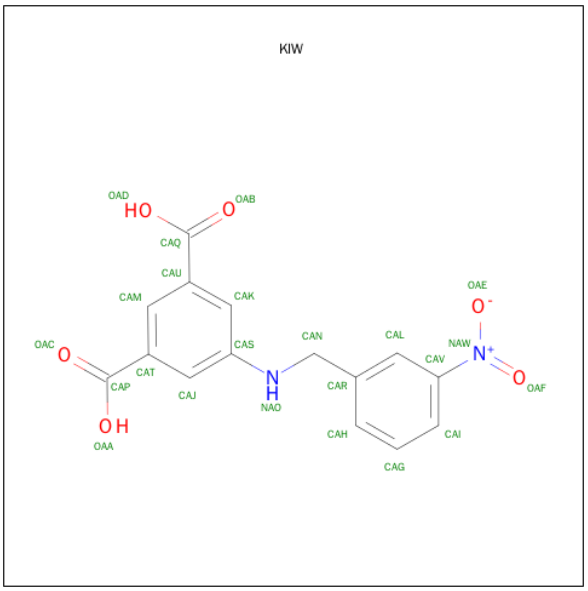
Chain	Residue	Modelled	Actual	Comment	Reference
W	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
W	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
W	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
W	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
W	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
W	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
W	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
W	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
W	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
W	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
W	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
W	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
W	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
W	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
W	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
W	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
W	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6
X	-20	MET	-	EXPRESSION TAG	UNP P0A4Z6
X	-19	GLY	-	EXPRESSION TAG	UNP P0A4Z6
X	-18	SER	-	EXPRESSION TAG	UNP P0A4Z6
X	-17	SER	-	EXPRESSION TAG	UNP P0A4Z6
X	-16	HIS	-	EXPRESSION TAG	UNP P0A4Z6
X	-15	HIS	-	EXPRESSION TAG	UNP P0A4Z6
X	-14	HIS	-	EXPRESSION TAG	UNP P0A4Z6
X	-13	HIS	-	EXPRESSION TAG	UNP P0A4Z6
X	-12	HIS	-	EXPRESSION TAG	UNP P0A4Z6
X	-11	HIS	-	EXPRESSION TAG	UNP P0A4Z6
X	-10	SER	-	EXPRESSION TAG	UNP P0A4Z6
X	-9	SER	-	EXPRESSION TAG	UNP P0A4Z6
X	-8	GLY	-	EXPRESSION TAG	UNP P0A4Z6
X	-7	LEU	-	EXPRESSION TAG	UNP P0A4Z6
X	-6	VAL	-	EXPRESSION TAG	UNP P0A4Z6
X	-5	PRO	-	EXPRESSION TAG	UNP P0A4Z6
X	-4	ARG	-	EXPRESSION TAG	UNP P0A4Z6
X	-3	GLY	-	EXPRESSION TAG	UNP P0A4Z6
X	-2	SER	-	EXPRESSION TAG	UNP P0A4Z6
X	-1	HIS	-	EXPRESSION TAG	UNP P0A4Z6

- Molecule 2 is 5-[(3-NITROBENZYL)AMINO]BENZENE-1,3-DICARBOXYLIC ACID (three-letter code: KIW) (formula: $C_{15}H_{12}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	15	2	6		
2	B	1	Total	C	N	O	0	0
			23	15	2	6		
2	C	1	Total	C	N	O	0	0
			23	15	2	6		
2	D	1	Total	C	N	O	0	0
			23	15	2	6		
2	E	1	Total	C	N	O	0	0
			23	15	2	6		
2	G	1	Total	C	N	O	0	0
			23	15	2	6		
2	H	1	Total	C	N	O	0	0
			23	15	2	6		
2	J	1	Total	C	N	O	0	0
			23	15	2	6		
2	K	1	Total	C	N	O	0	0
			23	15	2	6		
2	L	1	Total	C	N	O	0	0
			23	15	2	6		
2	M	1	Total	C	N	O	0	0
			23	15	2	6		
2	N	1	Total	C	N	O	0	0
			23	15	2	6		
2	O	1	Total	C	N	O	0	0
			23	15	2	6		
2	P	1	Total	C	N	O	0	0
			23	15	2	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Q	1	Total C N O 23 15 2 6	0	0
2	R	1	Total C N O 23 15 2 6	0	0
2	S	1	Total C N O 23 15 2 6	0	0
2	T	1	Total C N O 23 15 2 6	0	0
2	U	1	Total C N O 23 15 2 6	0	0
2	V	1	Total C N O 23 15 2 6	0	0
2	W	1	Total C N O 23 15 2 6	0	0
2	X	1	Total C N O 23 15 2 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	62	Total O 62 62	0	0
3	B	44	Total O 44 44	0	0
3	C	55	Total O 55 55	0	0
3	D	37	Total O 37 37	0	0
3	E	50	Total O 50 50	0	0
3	F	41	Total O 41 41	0	0
3	G	39	Total O 39 39	0	0
3	H	56	Total O 56 56	0	0
3	I	57	Total O 57 57	0	0
3	J	55	Total O 55 55	0	0
3	K	65	Total O 65 65	0	0

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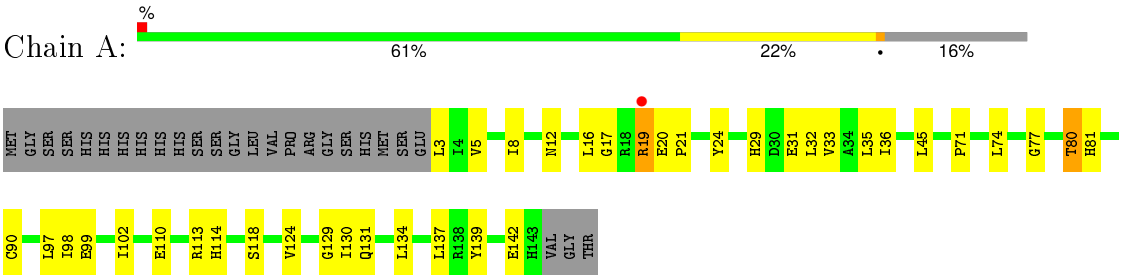
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	55	Total O 55 55	0	0
3	M	37	Total O 37 37	0	0
3	N	68	Total O 68 68	0	0
3	O	52	Total O 52 52	0	0
3	P	21	Total O 21 21	0	0
3	Q	44	Total O 44 44	0	0
3	R	38	Total O 38 38	0	0
3	S	39	Total O 39 39	0	0
3	T	44	Total O 44 44	0	0
3	U	39	Total O 39 39	0	0
3	V	34	Total O 34 34	0	0
3	W	42	Total O 42 42	0	0
3	X	27	Total O 27 27	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

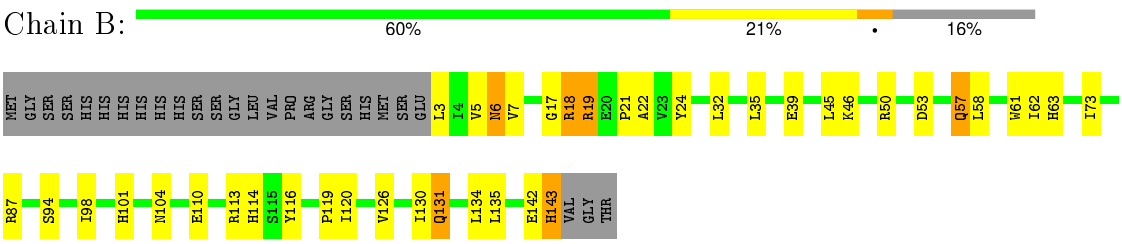
- Molecule 1: 3-dehydroquinate dehydratase

Chain A:



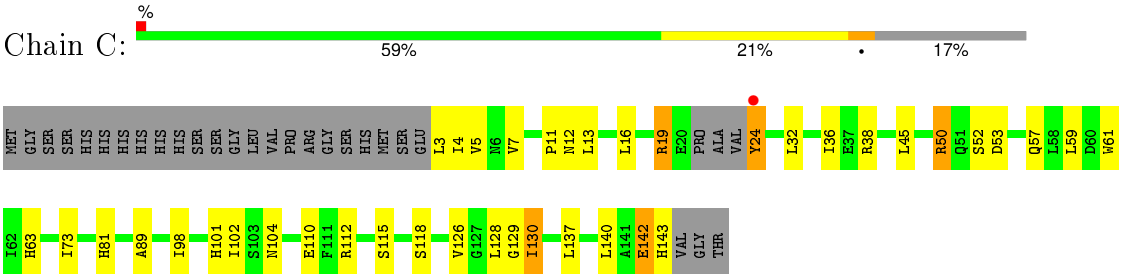
- Molecule 1: 3-dehydroquinate dehydratase

Chain B:



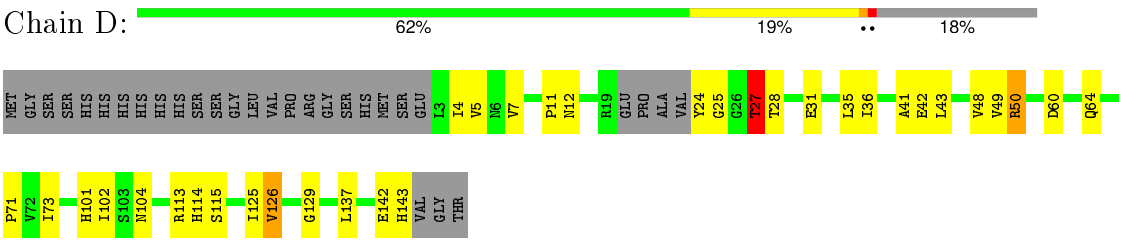
- Molecule 1: 3-dehydroquinate dehydratase

Chain C:



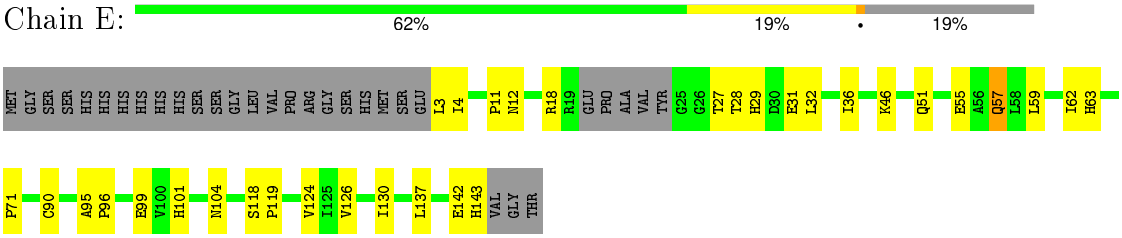
- Molecule 1: 3-dehydroquinate dehydratase

Chain D:



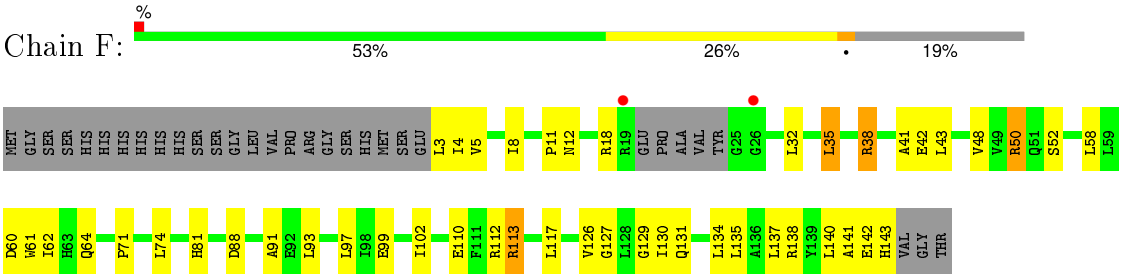
• Molecule 1: 3-dehydroquinate dehydratase

Chain E:



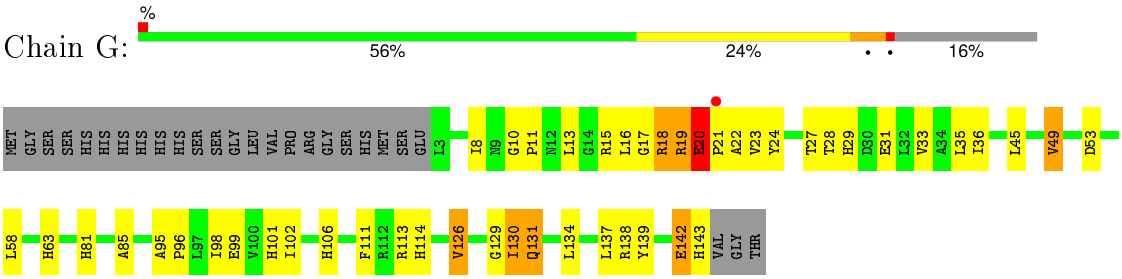
• Molecule 1: 3-dehydroquinate dehydratase

Chain F:



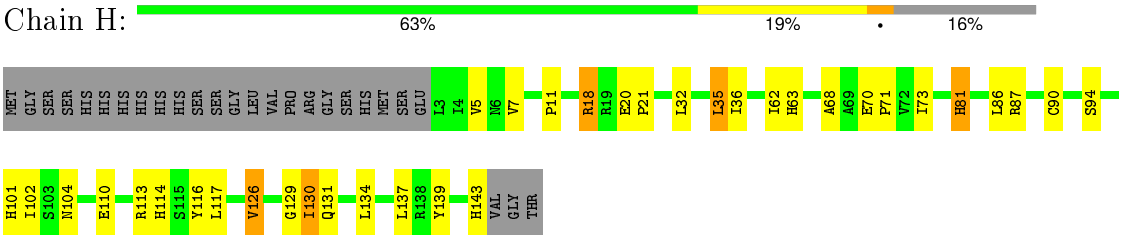
• Molecule 1: 3-dehydroquinate dehydratase

Chain G:



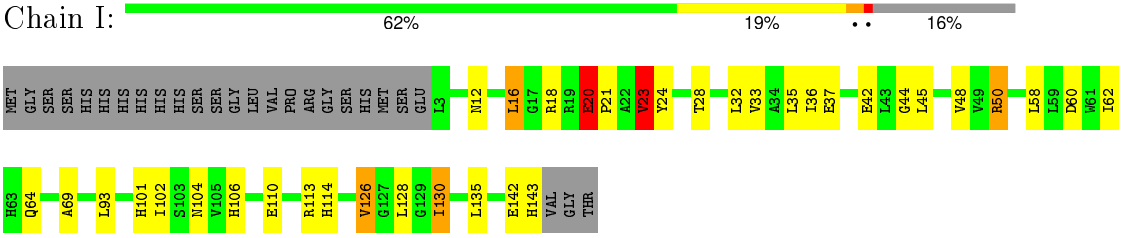
• Molecule 1: 3-dehydroquinate dehydratase

Chain H:



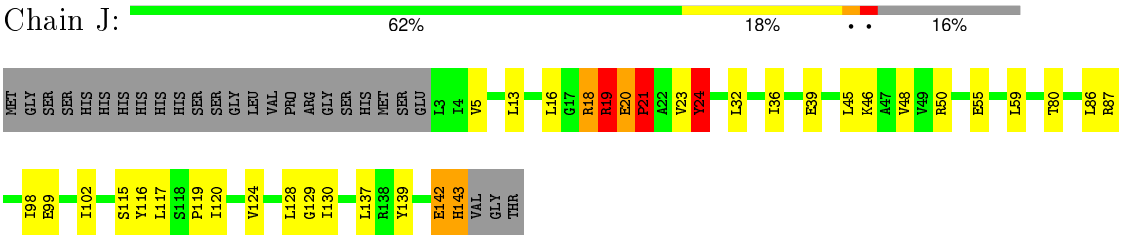
• Molecule 1: 3-dehydroquinate dehydratase

Chain I:



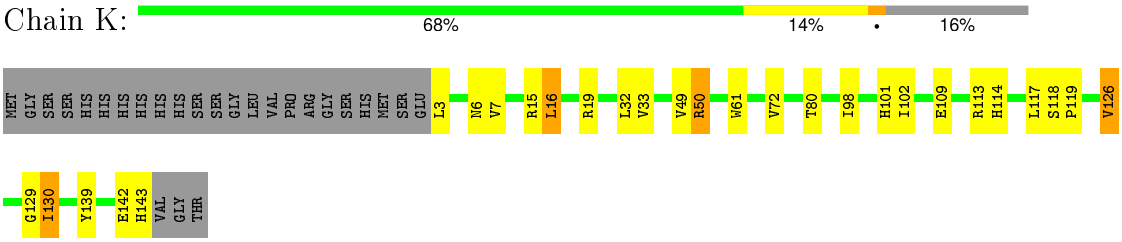
• Molecule 1: 3-dehydroquinate dehydratase

Chain J:



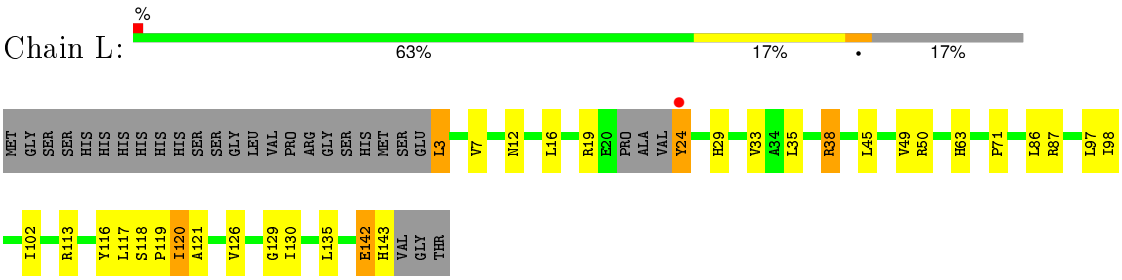
• Molecule 1: 3-dehydroquinate dehydratase

Chain K:



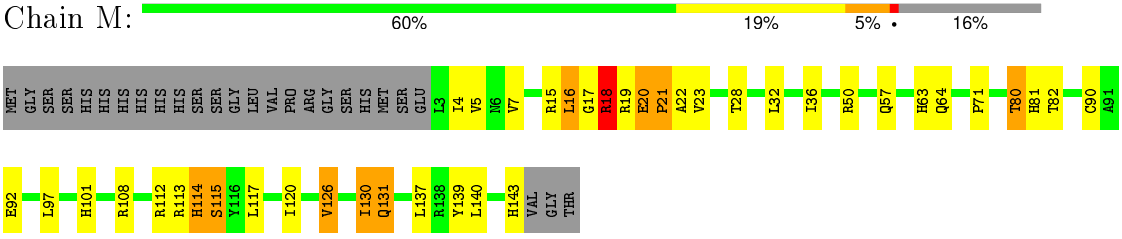
• Molecule 1: 3-dehydroquinate dehydratase

Chain L:



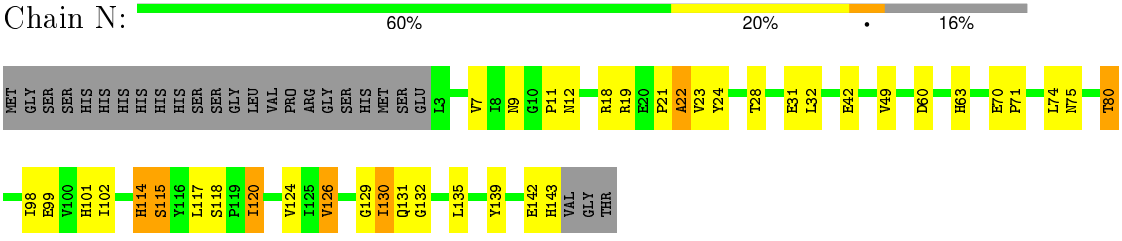
• Molecule 1: 3-dehydroquinate dehydratase

Chain M:



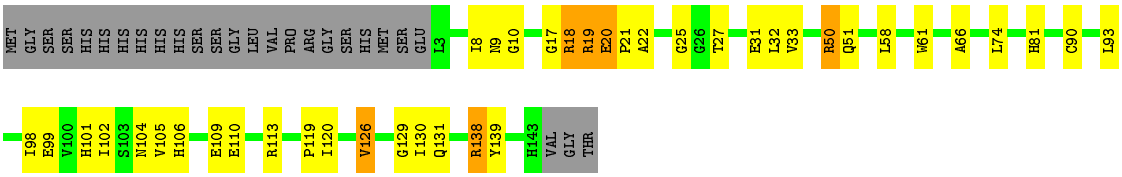
• Molecule 1: 3-dehydroquinate dehydratase

Chain N:



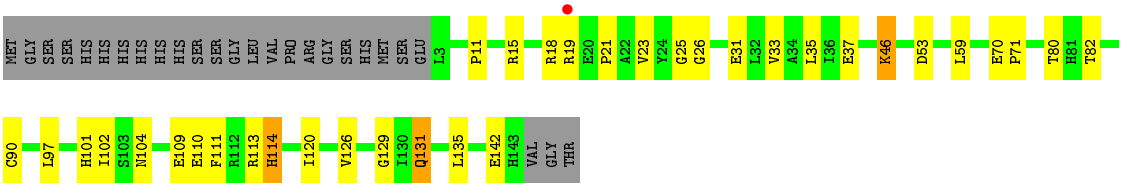
• Molecule 1: 3-dehydroquinate dehydratase

Chain O:



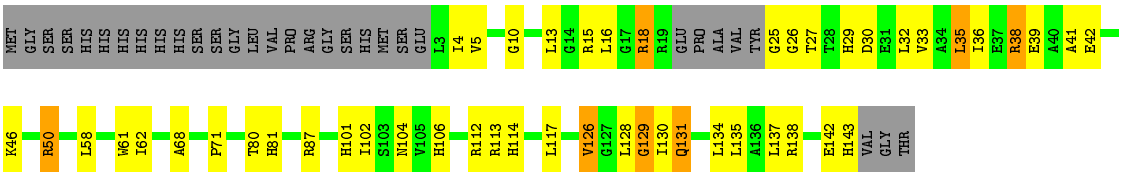
• Molecule 1: 3-dehydroquinate dehydratase

Chain P:



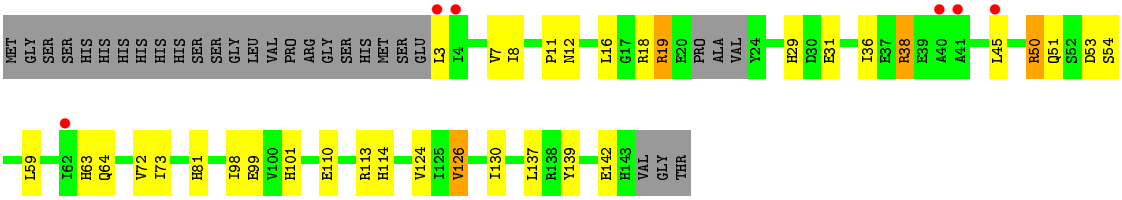
• Molecule 1: 3-dehydroquinate dehydratase

Chain Q:



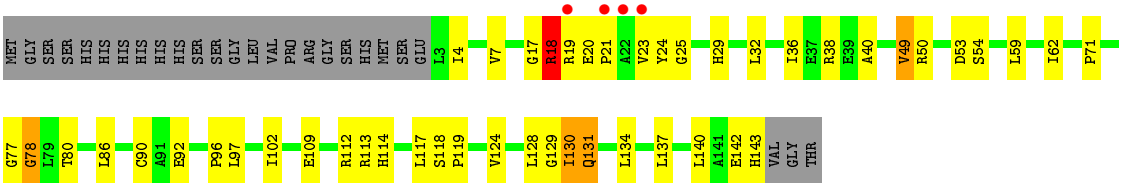
• Molecule 1: 3-dehydroquinate dehydratase

Chain R:



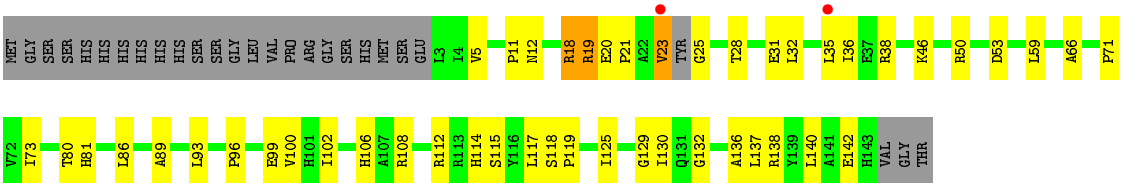
• Molecule 1: 3-dehydroquinate dehydratase

Chain S:



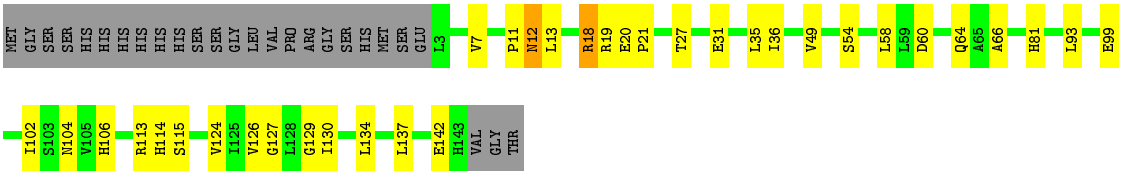
• Molecule 1: 3-dehydroquinate dehydratase

Chain T:



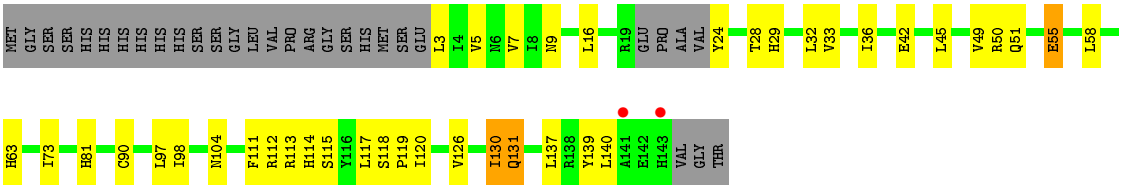
• Molecule 1: 3-dehydroquinate dehydratase

Chain U:



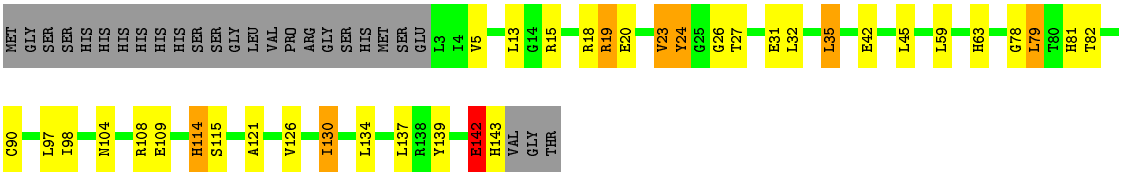
• Molecule 1: 3-dehydroquinate dehydratase

Chain V:



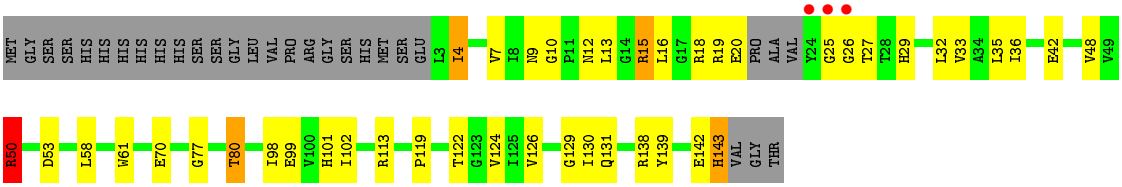
• Molecule 1: 3-dehydroquinate dehydratase

Chain W:



• Molecule 1: 3-dehydroquinate dehydratase

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.71Å 135.22Å 143.91Å 90.00° 97.18° 90.00°	Depositor
Resolution (Å)	67.61 – 2.57 67.61 – 2.57	Depositor EDS
% Data completeness (in resolution range)	85.2 (67.61-2.57) 85.2 (67.61-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.197 , 0.294 0.198 , 0.294	Depositor DCC
R_{free} test set	4996 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 99574 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26969	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 4.08% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: KIW

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	0.52	0/1085	0.73	0/1478
1	B	0.44	0/1094	0.69	0/1491
1	C	0.49	0/1068	0.71	0/1451
1	D	0.51	0/1053	0.71	0/1432
1	E	0.47	0/1040	0.70	0/1414
1	F	0.48	0/1040	0.73	0/1414
1	G	0.50	0/1100	0.81	1/1498 (0.1%)
1	H	0.54	0/1089	0.77	0/1483
1	I	0.53	0/1083	0.76	1/1476 (0.1%)
1	J	0.53	0/1086	0.75	1/1478 (0.1%)
1	K	0.54	0/1089	0.76	0/1483
1	L	0.49	0/1062	0.70	0/1444
1	M	0.44	0/1083	0.70	0/1476
1	N	0.48	0/1089	0.71	0/1483
1	O	0.48	0/1079	0.70	0/1471
1	P	0.47	0/1083	0.72	0/1476
1	Q	0.44	0/1040	0.70	0/1414
1	R	0.46	0/1068	0.73	0/1451
1	S	0.45	0/1083	0.74	0/1476
1	T	0.47	0/1075	0.73	0/1462
1	U	0.48	0/1089	0.72	0/1483
1	V	0.45	0/1053	0.70	0/1432
1	W	0.48	0/1083	0.70	0/1476
1	X	0.47	0/1058	0.71	0/1439
All	All	0.48	0/25772	0.73	3/35081 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	2
1	I	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	21	PRO	N-CA-CB	6.60	111.22	103.30
1	G	23	VAL	C-N-CA	5.91	136.47	121.70
1	I	23	VAL	N-CA-C	-5.39	96.44	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	17	GLY	Peptide
1	G	20	GLU	Peptide
1	I	23	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1067	0	1075	37	0
1	B	1075	0	1074	28	0
1	C	1052	0	1057	35	0
1	D	1037	0	1040	27	0
1	E	1025	0	1031	23	0
1	F	1025	0	1031	33	0
1	G	1081	0	1085	40	0
1	H	1071	0	1079	26	0
1	I	1065	0	1068	28	0
1	J	1069	0	1073	33	0
1	K	1071	0	1079	17	0
1	L	1046	0	1046	28	0
1	M	1065	0	1068	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1071	0	1079	28	0
1	O	1061	0	1064	33	0
1	P	1065	0	1068	27	0
1	Q	1025	0	1031	40	0
1	R	1052	0	1057	28	0
1	S	1065	0	1068	39	0
1	T	1059	0	1069	32	0
1	U	1071	0	1079	24	0
1	V	1037	0	1040	26	0
1	W	1065	0	1068	38	0
1	X	1042	0	1042	34	0
2	A	23	0	10	1	0
2	B	23	0	10	0	0
2	C	23	0	10	2	0
2	D	23	0	10	1	0
2	E	23	0	10	0	0
2	G	23	0	10	1	0
2	H	23	0	10	1	0
2	J	23	0	10	1	0
2	K	23	0	10	0	0
2	L	23	0	10	1	0
2	M	23	0	10	3	0
2	N	23	0	10	0	0
2	O	23	0	10	1	0
2	P	23	0	10	0	0
2	Q	23	0	10	1	0
2	R	23	0	10	2	0
2	S	23	0	10	4	0
2	T	23	0	10	7	0
2	U	23	0	10	3	0
2	V	23	0	10	1	0
2	W	23	0	10	2	0
2	X	23	0	10	1	0
3	A	62	0	0	12	0
3	B	44	0	0	3	0
3	C	55	0	0	13	0
3	D	37	0	0	7	0
3	E	50	0	0	6	0
3	F	41	0	0	4	0
3	G	39	0	0	8	0
3	H	56	0	0	7	0
3	I	57	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	55	0	0	6	0
3	K	65	0	0	5	0
3	L	55	0	0	10	0
3	M	37	0	0	9	0
3	N	68	0	0	1	0
3	O	52	0	0	2	0
3	P	21	0	0	10	0
3	Q	44	0	0	6	0
3	R	38	0	0	6	0
3	S	39	0	0	5	0
3	T	44	0	0	1	0
3	U	39	0	0	2	0
3	V	34	0	0	3	0
3	W	42	0	0	7	0
3	X	27	0	0	4	0
All	All	26969	0	25691	706	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 14.

All (706) 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:K:80:THR:HA	3:K:364:HOH:O	1.23	1.29
1:A:8:ILE:HB	3:A:662:HOH:O	1.25	1.28
1:M:137:LEU:HA	3:M:334:HOH:O	1.36	1.25
1:J:119:PRO:HG3	3:L:353:HOH:O	1.39	1.18
1:D:24:TYR:HB3	1:D:102:ILE:HG21	1.26	1.14
1:C:50:ARG:HH11	1:C:50:ARG:HG3	0.99	1.14
1:R:50:ARG:HG2	1:R:50:ARG:HH11	1.04	1.12
1:J:39:GLU:HG3	3:J:352:HOH:O	1.50	1.11
2:T:201:KIW:H10	2:T:201:KIW:CAJ	1.82	1.09
1:R:38:ARG:HB2	1:R:38:ARG:HH11	1.14	1.09
1:Q:50:ARG:HH11	1:Q:50:ARG:CG	1.65	1.09
1:M:17:GLY:HA3	1:M:18:ARG:O	1.56	1.05
1:X:15:ARG:HH11	1:X:15:ARG:HG2	1.21	1.04
1:B:119:PRO:HG3	3:F:241:HOH:O	1.58	1.03
1:P:114:HIS:HD2	3:P:320:HOH:O	1.41	1.02
1:C:50:ARG:HG3	1:C:50:ARG:NH1	1.57	1.00
1:D:24:TYR:N	1:D:25:GLY:HA3	1.74	0.99
2:T:201:KIW:H2	2:T:201:KIW:H10	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:50:ARG:HH11	1:Q:50:ARG:HG2	0.84	0.98
1:Q:18:ARG:HG2	1:Q:18:ARG:HH11	1.29	0.98
1:D:113:ARG:HD3	3:D:335:HOH:O	1.63	0.97
1:C:81:HIS:HA	3:C:352:HOH:O	1.65	0.95
1:I:42:GLU:HB3	3:I:253:HOH:O	1.66	0.94
1:Q:50:ARG:NH1	1:Q:50:ARG:HG2	1.67	0.94
1:I:24:TYR:HA	3:I:256:HOH:O	1.67	0.93
1:C:50:ARG:CG	1:C:50:ARG:HH11	1.79	0.93
3:A:660:HOH:O	1:K:15:ARG:HB2	1.70	0.92
1:A:3:LEU:HB2	3:A:658:HOH:O	1.70	0.91
1:I:16:LEU:HD11	1:I:130:ILE:HD11	1.51	0.91
1:Q:113:ARG:HD2	3:Q:344:HOH:O	1.70	0.90
1:R:38:ARG:HH11	1:R:38:ARG:CB	1.84	0.90
1:S:130:ILE:HD12	1:S:130:ILE:H	1.37	0.90
1:V:50:ARG:HG2	3:V:333:HOH:O	1.71	0.89
1:N:22:ALA:N	1:N:24:TYR:O	2.08	0.86
1:R:50:ARG:NH1	1:R:50:ARG:HG2	1.74	0.86
1:M:114:HIS:CE1	3:M:332:HOH:O	2.29	0.86
1:S:80:THR:HG23	1:S:117:LEU:HD12	1.56	0.85
1:W:114:HIS:CE1	3:W:327:HOH:O	2.31	0.84
2:T:201:KIW:H2	2:T:201:KIW:CAH	2.07	0.84
1:I:102:ILE:HG22	3:I:256:HOH:O	1.76	0.84
1:C:3:LEU:HG	3:C:355:HOH:O	1.79	0.83
1:D:24:TYR:HB3	1:D:102:ILE:CG2	2.09	0.83
1:P:15:ARG:HA	1:P:18:ARG:NH1	1.93	0.83
1:N:114:HIS:CE1	3:N:366:HOH:O	2.32	0.82
1:E:57:GLN:HG2	3:E:348:HOH:O	1.80	0.82
1:N:131:GLN:OE1	1:R:142:GLU:OE1	1.98	0.82
1:J:18:ARG:O	1:J:19:ARG:O	1.98	0.82
1:R:50:ARG:CG	1:R:50:ARG:HH11	1.88	0.82
1:A:19:ARG:HB3	1:A:21:PRO:HD3	1.63	0.81
1:S:134:LEU:HA	1:S:137:LEU:HD12	1.62	0.81
1:T:18:ARG:O	1:T:19:ARG:HB2	1.78	0.81
1:X:77:GLY:O	1:X:80:THR:OG1	1.99	0.80
1:S:113:ARG:HG3	3:S:338:HOH:O	1.82	0.80
1:A:32:LEU:O	1:A:36:ILE:HG12	1.82	0.80
1:M:139:TYR:HE2	3:M:337:HOH:O	1.65	0.80
1:J:102:ILE:HG23	1:J:129:GLY:HA2	1.63	0.80
1:S:102:ILE:HG23	1:S:129:GLY:HA2	1.62	0.79
1:D:113:ARG:CD	3:D:335:HOH:O	2.24	0.79
1:Q:18:ARG:NH1	1:Q:18:ARG:HG2	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:GLN:HG2	3:F:238:HOH:O	1.82	0.79
1:K:114:HIS:CE1	3:K:360:HOH:O	2.35	0.78
1:G:143:HIS:CE1	3:G:336:HOH:O	2.36	0.78
1:M:64:GLN:HB3	3:M:307:HOH:O	1.84	0.78
1:U:113:ARG:HD2	3:U:333:HOH:O	1.83	0.78
1:F:138:ARG:HH11	1:F:138:ARG:HG3	1.47	0.78
1:J:48:VAL:HG12	1:J:50:ARG:HD2	1.64	0.78
1:J:18:ARG:HD3	1:J:18:ARG:H	1.49	0.77
1:X:131:GLN:HG2	3:X:306:HOH:O	1.84	0.77
1:O:20:GLU:N	1:O:21:PRO:HD2	1.99	0.77
1:R:38:ARG:HB2	1:R:38:ARG:NH1	1.97	0.77
1:D:24:TYR:CB	1:D:102:ILE:HG21	2.13	0.76
1:R:29:HIS:CE1	1:R:51:GLN:HB2	2.21	0.76
1:L:113:ARG:HG3	3:L:352:HOH:O	1.85	0.76
1:A:45:LEU:HD12	3:A:659:HOH:O	1.85	0.76
1:L:16:LEU:HD12	3:L:354:HOH:O	1.86	0.75
1:A:114:HIS:HD2	1:G:113:ARG:HH12	1.34	0.75
1:R:113:ARG:HD2	3:R:336:HOH:O	1.86	0.75
1:L:29:HIS:HA	3:L:354:HOH:O	1.86	0.74
1:P:109:GLU:CB	3:P:321:HOH:O	2.34	0.74
1:W:114:HIS:HB3	3:W:330:HOH:O	1.86	0.74
1:A:32:LEU:HD13	1:A:130:ILE:HG13	1.70	0.74
1:J:87:ARG:HA	1:J:117:LEU:HD21	1.68	0.74
1:O:32:LEU:HD13	1:O:130:ILE:HG13	1.68	0.74
1:E:3:LEU:HA	3:E:345:HOH:O	1.87	0.73
1:B:101:HIS:HB2	1:B:126:VAL:HG22	1.69	0.73
1:N:80:THR:HG23	1:N:117:LEU:HD12	1.70	0.73
1:P:111:PHE:CD2	3:P:321:HOH:O	2.41	0.73
1:M:101:HIS:HB3	2:M:201:KIW:OAD	1.88	0.73
1:T:102:ILE:HG23	1:T:129:GLY:HA2	1.69	0.72
1:E:143:HIS:CE1	3:E:346:HOH:O	2.41	0.72
1:L:113:ARG:CG	3:L:352:HOH:O	2.36	0.72
1:J:99:GLU:HB3	1:J:124:VAL:HG13	1.72	0.72
1:I:142:GLU:O	1:I:143:HIS:HB2	1.90	0.72
1:A:102:ILE:HG23	1:A:129:GLY:HA2	1.72	0.71
1:P:114:HIS:CD2	3:P:320:HOH:O	2.23	0.71
1:J:117:LEU:HD12	3:J:308:HOH:O	1.89	0.71
1:J:87:ARG:HA	1:J:117:LEU:CD2	2.21	0.71
1:H:36:ILE:HG23	1:H:137:LEU:HD11	1.70	0.71
1:D:24:TYR:N	1:D:25:GLY:CA	2.51	0.71
1:A:74:LEU:HD13	3:A:662:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:20:GLU:HA	3:W:339:HOH:O	1.89	0.71
1:N:101:HIS:HB2	1:N:126:VAL:HG22	1.73	0.70
1:F:43:LEU:HD21	1:F:138:ARG:HH12	1.56	0.70
1:K:143:HIS:CE1	3:K:363:HOH:O	2.43	0.70
1:U:81:HIS:HE2	2:U:201:KIW:CAQ	2.05	0.70
1:D:143:HIS:O	3:D:324:HOH:O	2.09	0.70
1:X:10:GLY:HA2	1:X:58:LEU:HD11	1.74	0.70
1:R:3:LEU:HD12	3:R:338:HOH:O	1.92	0.70
1:V:7:VAL:HG22	1:V:73:ILE:HB	1.73	0.70
1:F:41:ALA:C	1:F:43:LEU:H	1.95	0.70
1:P:109:GLU:HB2	3:P:321:HOH:O	1.92	0.69
1:D:104:ASN:HA	1:D:126:VAL:HG13	1.74	0.69
1:W:63:HIS:CE1	1:X:15:ARG:HD2	2.28	0.69
1:F:48:VAL:HG12	1:F:50:ARG:CD	2.23	0.68
1:X:15:ARG:NH1	1:X:15:ARG:HG2	2.00	0.68
1:A:137:LEU:HB3	3:A:659:HOH:O	1.91	0.68
1:X:15:ARG:CG	1:X:15:ARG:HH11	2.04	0.68
1:J:80:THR:HA	3:J:308:HOH:O	1.92	0.68
1:G:36:ILE:HG23	1:G:137:LEU:HD11	1.75	0.68
1:U:18:ARG:HH11	1:U:18:ARG:HG2	1.57	0.68
1:J:142:GLU:O	1:J:143:HIS:HB2	1.94	0.67
1:B:131:GLN:HG2	3:B:344:HOH:O	1.93	0.67
1:D:113:ARG:CG	3:D:335:HOH:O	2.41	0.67
1:G:33:VAL:HG22	1:G:49:VAL:CG2	2.24	0.67
1:W:78:GLY:HA3	3:W:335:HOH:O	1.94	0.67
1:G:111:PHE:HA	3:G:338:HOH:O	1.95	0.67
1:M:101:HIS:HB2	1:M:126:VAL:HG23	1.77	0.67
1:C:102:ILE:HG23	1:C:129:GLY:HA2	1.77	0.67
1:X:99:GLU:HB3	1:X:124:VAL:HG13	1.77	0.67
1:W:63:HIS:ND1	1:X:15:ARG:HD2	2.11	0.66
1:G:15:ARG:O	1:G:18:ARG:O	2.12	0.66
1:J:20:GLU:O	1:J:21:PRO:CB	2.43	0.66
1:M:113:ARG:HH12	1:S:114:HIS:HD2	1.43	0.66
1:G:33:VAL:HG22	1:G:49:VAL:HG22	1.77	0.66
1:K:32:LEU:HD13	1:K:130:ILE:HG13	1.77	0.66
1:J:24:TYR:HB3	1:J:102:ILE:HB	1.78	0.65
1:N:102:ILE:HG23	1:N:129:GLY:HA2	1.79	0.65
1:Q:50:ARG:NH1	1:Q:50:ARG:CG	2.35	0.65
1:U:99:GLU:HB3	1:U:124:VAL:HG13	1.77	0.65
1:F:38:ARG:HH11	1:F:38:ARG:HG3	1.62	0.65
1:G:98:ILE:HD11	1:G:139:TYR:CD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:12:ASN:OD1	1:V:63:HIS:CE1	2.50	0.65
1:H:101:HIS:HB2	1:H:126:VAL:HG22	1.79	0.65
1:M:101:HIS:HB2	1:M:126:VAL:CG2	2.27	0.64
1:G:16:LEU:O	1:G:28:THR:HA	1.97	0.64
1:P:33:VAL:O	1:P:37:GLU:HG3	1.96	0.64
1:G:99:GLU:HG3	3:G:308:HOH:O	1.95	0.64
1:R:101:HIS:HB2	1:R:126:VAL:HG22	1.79	0.64
1:O:104:ASN:HA	1:O:126:VAL:HG13	1.79	0.64
1:G:19:ARG:HG3	1:G:20:GLU:HG2	1.80	0.64
1:G:143:HIS:HE1	3:G:336:HOH:O	1.75	0.64
1:C:36:ILE:HG23	1:C:137:LEU:HD11	1.79	0.63
1:O:101:HIS:HB2	1:O:126:VAL:HG22	1.81	0.63
1:J:32:LEU:HD13	1:J:130:ILE:HD12	1.80	0.63
1:X:19:ARG:HA	1:X:20:GLU:C	2.19	0.63
1:N:99:GLU:HB3	1:N:124:VAL:HG13	1.81	0.63
1:D:101:HIS:HB2	1:D:126:VAL:HG22	1.79	0.63
1:V:113:ARG:HH12	1:X:119:PRO:HG3	1.64	0.63
1:S:131:GLN:HG3	3:S:333:HOH:O	1.98	0.63
1:I:32:LEU:O	1:I:36:ILE:HG13	1.99	0.63
1:C:5:VAL:HG23	3:C:355:HOH:O	1.99	0.62
1:O:99:GLU:OE2	1:O:101:HIS:NE2	2.24	0.62
1:F:60:ASP:OD2	1:F:64:GLN:NE2	2.33	0.62
1:G:20:GLU:C	1:G:22:ALA:H	2.03	0.62
1:X:48:VAL:HG12	1:X:50:ARG:HD2	1.80	0.62
1:O:119:PRO:HB3	1:T:106:HIS:O	1.99	0.62
1:A:139:TYR:HA	1:G:131:GLN:OE1	1.99	0.62
1:M:17:GLY:CA	1:M:18:ARG:O	2.43	0.62
1:T:80:THR:HG23	1:T:117:LEU:HD12	1.82	0.61
1:N:98:ILE:HD11	1:N:139:TYR:CD2	2.35	0.61
1:X:138:ARG:HD3	3:X:310:HOH:O	2.01	0.61
1:M:108:ARG:HH21	1:M:112:ARG:CZ	2.13	0.61
1:F:138:ARG:HG3	1:F:138:ARG:NH1	2.16	0.61
1:O:102:ILE:HG23	1:O:129:GLY:HA2	1.83	0.61
1:B:135:LEU:HD22	1:F:135:LEU:HB3	1.82	0.61
1:E:101:HIS:HB2	1:E:126:VAL:HG22	1.81	0.61
1:C:32:LEU:HD13	1:C:130:ILE:HG13	1.83	0.61
1:F:62:ILE:HG23	1:F:93:LEU:HD21	1.82	0.61
1:C:5:VAL:CG2	3:C:355:HOH:O	2.49	0.60
1:G:134:LEU:O	1:G:138:ARG:HG3	2.01	0.60
1:G:113:ARG:HD2	3:G:335:HOH:O	2.02	0.60
1:U:36:ILE:HG23	1:U:137:LEU:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:17:GLY:HA2	1:M:28:THR:HG22	1.83	0.60
1:M:139:TYR:CE2	3:M:337:HOH:O	2.47	0.60
1:O:19:ARG:O	1:O:20:GLU:CB	2.49	0.60
1:V:98:ILE:HD11	1:V:139:TYR:CD2	2.36	0.60
1:I:16:LEU:O	1:I:28:THR:HA	2.02	0.60
1:U:134:LEU:HA	1:U:137:LEU:HD12	1.82	0.60
1:D:5:VAL:HG22	1:D:71:PRO:HG2	1.84	0.60
1:S:23:VAL:N	1:S:25:GLY:H	2.00	0.60
1:J:102:ILE:CG2	1:J:129:GLY:HA2	2.32	0.59
1:G:18:ARG:HG3	1:G:19:ARG:HB3	1.84	0.59
1:G:143:HIS:C	3:G:306:HOH:O	2.40	0.59
1:V:29:HIS:O	1:V:33:VAL:HG23	2.02	0.59
1:R:36:ILE:HG23	1:R:137:LEU:HD11	1.84	0.59
1:N:32:LEU:HD13	1:N:130:ILE:HG12	1.85	0.59
1:G:20:GLU:C	1:G:22:ALA:N	2.55	0.59
1:S:23:VAL:H	1:S:25:GLY:H	1.50	0.59
1:R:63:HIS:HD2	3:R:330:HOH:O	1.85	0.59
1:I:69:ALA:HB2	1:W:31:GLU:HA	1.84	0.59
1:M:32:LEU:HD13	1:M:130:ILE:CG1	2.33	0.59
1:R:81:HIS:HE2	2:R:201:KIW:CAQ	2.16	0.58
1:K:117:LEU:HD12	3:K:364:HOH:O	2.02	0.58
1:K:113:ARG:HD2	3:K:354:HOH:O	2.03	0.58
1:J:46:LYS:HA	3:J:309:HOH:O	2.03	0.58
1:A:19:ARG:CZ	1:A:21:PRO:HA	2.34	0.58
1:T:32:LEU:HD13	1:T:130:ILE:HG13	1.84	0.58
1:N:142:GLU:O	1:N:143:HIS:HB2	2.03	0.58
1:L:12:ASN:HB3	3:L:351:HOH:O	2.02	0.58
1:Q:42:GLU:HB3	3:Q:337:HOH:O	2.02	0.58
1:M:143:HIS:CD2	3:M:336:HOH:O	2.57	0.58
1:I:101:HIS:HB2	1:I:126:VAL:HG22	1.85	0.58
1:S:7:VAL:HB	1:S:49:VAL:HB	1.86	0.58
1:W:13:LEU:HD23	2:W:201:KIW:H9	1.85	0.58
1:V:111:PHE:CE1	1:V:112:ARG:HG3	2.39	0.57
1:J:87:ARG:NH1	1:J:116:TYR:O	2.37	0.57
3:Q:343:HOH:O	1:W:139:TYR:HE1	1.88	0.57
1:M:117:LEU:O	1:M:120:ILE:HG13	2.05	0.57
1:X:143:HIS:HE1	3:X:321:HOH:O	1.87	0.57
1:M:140:LEU:HD12	3:M:334:HOH:O	2.05	0.57
1:W:98:ILE:HD11	1:W:139:TYR:CD2	2.40	0.57
1:I:48:VAL:HG12	1:I:50:ARG:HD2	1.87	0.57
1:J:115:SER:H	1:L:113:ARG:HH22	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:18:ARG:HH11	1:S:18:ARG:HG2	1.71	0.56
1:A:24:TYR:HB2	3:A:641:HOH:O	2.04	0.56
1:U:54:SER:O	1:U:58:LEU:HG	2.06	0.56
1:M:137:LEU:HD23	3:M:334:HOH:O	2.05	0.56
1:T:23:VAL:HG13	1:T:108:ARG:NH2	2.21	0.56
1:H:131:GLN:HB3	3:H:348:HOH:O	2.05	0.56
1:B:32:LEU:HD13	1:B:130:ILE:CG2	2.36	0.56
1:C:59:LEU:HD22	1:C:89:ALA:HB2	1.86	0.56
1:B:50:ARG:HB3	1:B:61:TRP:CZ3	2.40	0.56
3:C:302:HOH:O	1:E:18:ARG:HD3	2.06	0.56
1:H:131:GLN:HG2	3:H:307:HOH:O	2.06	0.56
1:V:7:VAL:HB	1:V:49:VAL:HG22	1.88	0.56
1:M:63:HIS:HB3	1:W:15:ARG:NH1	2.20	0.56
1:J:19:ARG:HA	1:W:26:GLY:HA3	1.88	0.55
1:W:108:ARG:HB3	1:W:109:GLU:OE1	2.06	0.55
1:Q:101:HIS:HB2	1:Q:126:VAL:HG22	1.88	0.55
1:T:11:PRO:HA	1:T:53:ASP:HA	1.86	0.55
1:M:21:PRO:O	1:M:23:VAL:N	2.38	0.55
1:J:18:ARG:HH11	1:W:19:ARG:H	1.55	0.55
1:O:8:ILE:O	1:O:74:LEU:HD12	2.06	0.55
1:R:18:ARG:HA	3:R:324:HOH:O	2.05	0.55
1:Q:104:ASN:HA	1:Q:126:VAL:HG13	1.89	0.55
1:U:20:GLU:N	1:U:21:PRO:HD3	2.21	0.55
3:D:332:HOH:O	1:G:85:ALA:HB2	2.07	0.55
1:N:22:ALA:HA	1:N:23:VAL:C	2.27	0.55
1:P:15:ARG:HA	1:P:18:ARG:HH12	1.68	0.55
1:M:19:ARG:O	1:M:20:GLU:HB2	2.07	0.55
1:V:131:GLN:HB2	3:V:326:HOH:O	2.07	0.55
1:R:59:LEU:HD12	1:S:53:ASP:HB3	1.89	0.55
1:A:74:LEU:CD1	3:A:662:HOH:O	2.52	0.55
1:F:11:PRO:O	1:F:12:ASN:HB2	2.07	0.55
1:C:101:HIS:HB2	1:C:126:VAL:HG22	1.87	0.55
1:B:130:ILE:HD12	1:B:130:ILE:H	1.72	0.54
1:O:120:ILE:O	1:O:120:ILE:HD12	2.06	0.54
1:L:24:TYR:CD1	1:L:24:TYR:N	2.74	0.54
1:H:87:ARG:HG3	1:H:116:TYR:O	2.07	0.54
1:U:60:ASP:OD1	1:U:64:GLN:NE2	2.36	0.54
1:L:113:ARG:HD2	3:L:352:HOH:O	2.06	0.54
1:D:113:ARG:HG3	3:D:335:HOH:O	2.07	0.54
1:X:101:HIS:HB2	1:X:126:VAL:HG22	1.89	0.54
1:S:130:ILE:N	1:S:130:ILE:HD12	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LEU:HD22	3:C:354:HOH:O	2.08	0.54
1:P:102:ILE:HG23	1:P:129:GLY:HA2	1.89	0.54
1:S:19:ARG:CB	2:S:201:KIW:OAF	2.55	0.54
1:H:20:GLU:N	1:H:21:PRO:HD3	2.23	0.54
1:F:99:GLU:HG3	3:F:211:HOH:O	2.07	0.54
1:P:15:ARG:HA	1:P:18:ARG:HH11	1.71	0.54
1:A:36:ILE:HG23	1:A:137:LEU:HD11	1.90	0.54
1:W:32:LEU:HD13	1:W:130:ILE:CG1	2.37	0.54
1:M:17:GLY:HA3	1:M:18:ARG:C	2.26	0.54
1:G:33:VAL:HG13	1:G:49:VAL:HG13	1.90	0.54
1:W:78:GLY:CA	3:W:335:HOH:O	2.53	0.54
1:B:87:ARG:HD2	1:B:116:TYR:O	2.08	0.54
1:C:19:ARG:HB3	1:C:19:ARG:NH1	2.22	0.54
1:T:23:VAL:O	2:T:201:KIW:H11	2.07	0.54
1:X:10:GLY:H	1:X:13:LEU:HD12	1.72	0.53
1:Q:35:LEU:HD23	1:Q:38:ARG:HH12	1.72	0.53
1:O:20:GLU:N	1:O:21:PRO:CD	2.70	0.53
1:I:142:GLU:O	1:I:143:HIS:CB	2.57	0.53
1:G:98:ILE:HD11	1:G:139:TYR:HD2	1.73	0.53
1:G:27:THR:HB	1:G:130:ILE:HD13	1.89	0.53
1:D:50:ARG:HG2	1:D:50:ARG:HH11	1.73	0.53
1:T:12:ASN:OD1	1:V:63:HIS:HE1	1.91	0.53
1:J:130:ILE:HG12	3:J:330:HOH:O	2.07	0.53
1:S:23:VAL:HB	1:S:24:TYR:HB2	1.90	0.53
1:M:21:PRO:C	1:M:23:VAL:H	2.12	0.53
1:F:134:LEU:HA	1:F:137:LEU:HD12	1.91	0.53
1:O:81:HIS:NE2	2:O:201:KIW:OAA	2.42	0.53
1:F:50:ARG:HB3	1:F:61:TRP:CZ3	2.44	0.53
1:F:48:VAL:HG12	1:F:50:ARG:HD2	1.90	0.53
1:A:142:GLU:HB2	3:A:661:HOH:O	2.08	0.53
1:E:118:SER:HB2	1:E:119:PRO:HD3	1.90	0.53
1:U:11:PRO:O	1:U:12:ASN:HB2	2.09	0.53
1:O:90:CYS:O	1:O:93:LEU:HG	2.08	0.53
1:F:74:LEU:HD23	1:F:117:LEU:HD13	1.91	0.53
1:A:113:ARG:HG3	3:A:656:HOH:O	2.08	0.53
1:H:104:ASN:HA	1:H:126:VAL:HG13	1.90	0.52
1:C:24:TYR:HA	3:C:348:HOH:O	2.09	0.52
1:U:7:VAL:HB	1:U:49:VAL:HG22	1.92	0.52
1:F:138:ARG:O	1:F:141:ALA:HB3	2.10	0.52
1:S:59:LEU:HD21	1:S:86:LEU:HA	1.91	0.52
1:W:78:GLY:N	3:W:335:HOH:O	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:ILE:HG23	1:E:137:LEU:HD11	1.89	0.52
1:G:101:HIS:HB2	1:G:126:VAL:HG22	1.92	0.52
1:A:45:LEU:CD1	3:A:659:HOH:O	2.51	0.52
1:H:5:VAL:HG22	1:H:71:PRO:HG2	1.92	0.52
1:B:131:GLN:NE2	1:F:142:GLU:HG2	2.23	0.52
1:F:38:ARG:CG	1:F:38:ARG:HH11	2.23	0.52
1:Q:10:GLY:HA2	1:Q:58:LEU:HD11	1.90	0.52
1:C:11:PRO:HA	1:C:53:ASP:OD1	2.09	0.52
1:X:12:ASN:HB2	2:X:201:KIW:H7	1.92	0.52
2:T:201:KIW:CAJ	2:T:201:KIW:CAH	2.69	0.52
1:C:142:GLU:O	1:C:143:HIS:HB2	2.10	0.52
1:O:21:PRO:O	1:O:22:ALA:HB3	2.09	0.52
1:M:143:HIS:HD2	3:M:336:HOH:O	1.91	0.52
1:N:28:THR:OG1	1:N:31:GLU:HG3	2.09	0.52
1:U:27:THR:HG23	1:U:31:GLU:HB3	1.91	0.52
1:H:62:ILE:HD13	1:H:90:CYS:SG	2.49	0.52
1:K:33:VAL:HG22	1:K:49:VAL:HG11	1.92	0.52
1:S:59:LEU:CD2	1:S:86:LEU:HA	2.40	0.52
1:R:38:ARG:CG	1:R:38:ARG:HH11	2.22	0.51
1:H:32:LEU:HD13	1:H:130:ILE:HG13	1.91	0.51
1:C:98:ILE:HD11	1:C:140:LEU:HD21	1.92	0.51
1:Q:32:LEU:HD13	1:Q:130:ILE:HD12	1.92	0.51
1:J:102:ILE:HG23	1:J:129:GLY:CA	2.37	0.51
1:W:35:LEU:HD22	1:W:134:LEU:HD11	1.93	0.51
1:T:102:ILE:CG2	1:T:129:GLY:HA2	2.37	0.51
1:I:93:LEU:HB3	3:I:254:HOH:O	2.10	0.51
1:S:18:ARG:NH1	1:S:18:ARG:HG2	2.25	0.51
1:V:90:CYS:HB3	1:V:97:LEU:HD22	1.92	0.51
1:X:98:ILE:HD11	1:X:139:TYR:CD2	2.46	0.51
1:S:124:VAL:HB	3:S:322:HOH:O	2.11	0.51
1:E:28:THR:OG1	1:E:31:GLU:HG3	2.11	0.51
1:H:143:HIS:HA	3:H:354:HOH:O	2.11	0.51
1:B:7:VAL:HG22	1:B:73:ILE:HB	1.93	0.51
1:U:13:LEU:HD23	2:U:201:KIW:H9	1.93	0.51
1:A:19:ARG:HE	1:Q:68:ALA:HA	1.75	0.51
1:B:53:ASP:HB3	1:E:59:LEU:HD12	1.92	0.51
1:R:11:PRO:O	1:R:12:ASN:HB2	2.11	0.51
1:C:143:HIS:CE1	3:C:354:HOH:O	2.64	0.51
3:R:315:HOH:O	2:S:201:KIW:H11	2.11	0.51
1:G:102:ILE:HG23	1:G:129:GLY:HA2	1.92	0.51
1:T:81:HIS:NE2	1:T:112:ARG:HG2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:20:GLU:H	1:O:21:PRO:HD2	1.75	0.50
1:E:27:THR:HG23	1:E:31:GLU:HB2	1.92	0.50
1:A:77:GLY:O	1:A:80:THR:OG1	2.25	0.50
1:G:143:HIS:CE1	3:G:307:HOH:O	2.64	0.50
1:U:18:ARG:HH11	1:U:18:ARG:CG	2.24	0.50
1:O:66:ALA:HB2	1:O:93:LEU:HD23	1.94	0.50
1:V:36:ILE:HG23	1:V:137:LEU:HD11	1.92	0.50
1:D:7:VAL:HB	1:D:49:VAL:HG22	1.92	0.50
1:E:63:HIS:HD2	3:E:347:HOH:O	1.92	0.50
1:D:11:PRO:O	1:D:12:ASN:HB2	2.11	0.50
1:N:102:ILE:HG12	1:N:130:ILE:HD12	1.94	0.50
1:A:99:GLU:HB3	1:A:124:VAL:HG13	1.93	0.50
1:G:29:HIS:O	1:G:33:VAL:HG23	2.12	0.50
1:C:32:LEU:HD13	1:C:130:ILE:CG1	2.41	0.50
1:L:113:ARG:CZ	3:L:353:HOH:O	2.60	0.50
1:M:81:HIS:HE2	2:M:201:KIW:CAP	2.24	0.50
1:V:115:SER:H	1:X:113:ARG:HH22	1.59	0.50
1:I:58:LEU:O	1:I:62:ILE:HD12	2.12	0.50
1:U:81:HIS:NE2	2:U:201:KIW:OAB	2.40	0.50
1:W:59:LEU:HD12	1:X:53:ASP:HB3	1.94	0.50
1:H:63:HIS:HE1	1:I:12:ASN:OD1	1.93	0.50
1:T:36:ILE:HG23	1:T:137:LEU:HD11	1.92	0.50
1:R:8:ILE:HD12	1:R:72:VAL:HG13	1.92	0.50
1:G:142:GLU:O	1:G:143:HIS:HB2	2.12	0.49
1:E:104:ASN:HA	1:E:126:VAL:HG13	1.94	0.49
1:X:7:VAL:HG11	1:X:36:ILE:HD13	1.94	0.49
1:P:131:GLN:O	1:P:135:LEU:HG	2.13	0.49
1:L:97:LEU:HD23	1:L:121:ALA:HA	1.94	0.49
1:Q:50:ARG:HB3	1:Q:61:TRP:CZ3	2.48	0.49
1:E:27:THR:HB	3:E:340:HOH:O	2.12	0.49
1:O:131:GLN:HG2	3:O:340:HOH:O	2.12	0.49
1:L:113:ARG:CD	3:L:352:HOH:O	2.60	0.49
1:R:64:GLN:HB3	3:R:311:HOH:O	2.12	0.49
1:Q:80:THR:HG23	1:Q:117:LEU:HD12	1.95	0.49
1:F:113:ARG:HG3	3:F:226:HOH:O	2.13	0.49
1:I:104:ASN:HA	1:I:126:VAL:HG13	1.93	0.49
1:F:41:ALA:C	1:F:43:LEU:N	2.65	0.49
1:A:98:ILE:HD11	1:A:139:TYR:CD2	2.48	0.49
1:U:114:HIS:CE1	3:U:308:HOH:O	2.66	0.49
2:T:201:KIW:CAL	3:T:343:HOH:O	2.60	0.48
1:N:21:PRO:HA	1:N:24:TYR:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:81:HIS:NE2	2:R:201:KIW:OAB	2.42	0.48
1:M:80:THR:HG23	1:M:117:LEU:HD12	1.93	0.48
1:F:102:ILE:HG23	1:F:129:GLY:HA2	1.94	0.48
1:Q:134:LEU:HA	1:Q:137:LEU:HD12	1.94	0.48
1:R:7:VAL:HG22	1:R:73:ILE:HB	1.96	0.48
1:A:17:GLY:O	1:A:20:GLU:CB	2.61	0.48
1:F:93:LEU:CD1	1:F:97:LEU:HD13	2.44	0.48
1:Q:39:GLU:OE2	1:Q:138:ARG:NH2	2.46	0.48
1:A:110:GLU:HG2	3:A:639:HOH:O	2.12	0.48
1:R:101:HIS:HB2	1:R:126:VAL:CG2	2.43	0.48
1:W:27:THR:HG23	1:W:31:GLU:HB3	1.95	0.48
1:M:5:VAL:HG22	1:M:71:PRO:HG2	1.93	0.48
1:S:109:GLU:OE1	1:S:112:ARG:NE	2.39	0.48
1:M:90:CYS:HB3	1:M:97:LEU:HD22	1.95	0.48
1:M:115:SER:H	1:S:113:ARG:HH22	1.62	0.48
1:Q:36:ILE:HG23	1:Q:137:LEU:HD11	1.95	0.48
1:D:115:SER:H	1:I:113:ARG:HH22	1.61	0.48
1:E:32:LEU:CD1	1:E:130:ILE:HG23	2.44	0.48
1:W:5:VAL:HG11	1:W:137:LEU:HD21	1.96	0.48
1:O:106:HIS:HA	1:O:113:ARG:HG2	1.96	0.48
1:X:143:HIS:CE1	3:X:321:HOH:O	2.64	0.48
1:M:63:HIS:CE1	1:W:15:ARG:HD3	2.49	0.48
1:E:62:ILE:HD13	1:E:90:CYS:SG	2.54	0.48
1:C:81:HIS:NE2	2:C:201:KIW:OAC	2.47	0.48
1:S:17:GLY:O	1:S:18:ARG:HB3	2.13	0.48
1:A:12:ASN:OD1	1:L:63:HIS:HE1	1.97	0.48
1:B:6:ASN:N	1:B:6:ASN:HD22	2.11	0.48
1:H:18:ARG:HG3	1:H:18:ARG:NH1	2.29	0.48
1:Q:104:ASN:ND2	1:W:121:ALA:O	2.47	0.48
1:P:113:ARG:HH22	1:U:115:SER:H	1.62	0.48
1:L:7:VAL:HB	1:L:49:VAL:HG22	1.94	0.48
1:C:57:GLN:HG2	3:C:339:HOH:O	2.13	0.48
1:A:81:HIS:NE2	2:A:500:KIW:OAB	2.46	0.48
1:C:3:LEU:HD23	1:C:45:LEU:CD2	2.43	0.47
1:N:32:LEU:HD13	1:N:130:ILE:CG1	2.43	0.47
1:J:128:LEU:HD21	1:L:98:ILE:HD12	1.95	0.47
1:G:81:HIS:NE2	2:G:201:KIW:OAB	2.46	0.47
1:N:117:LEU:O	1:N:120:ILE:HD13	2.14	0.47
1:J:117:LEU:HD22	1:J:120:ILE:HD11	1.96	0.47
1:N:132:GLY:HA2	1:N:135:LEU:HD12	1.96	0.47
1:B:63:HIS:HE1	1:C:12:ASN:OD1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:ALA:HB1	1:E:96:PRO:CD	2.44	0.47
1:P:111:PHE:CG	3:P:321:HOH:O	2.67	0.47
1:T:81:HIS:CE1	1:T:112:ARG:HA	2.49	0.47
1:T:66:ALA:HB2	1:T:93:LEU:HD23	1.95	0.47
1:G:11:PRO:HA	1:G:53:ASP:HA	1.96	0.47
1:F:5:VAL:HG22	1:F:71:PRO:HB2	1.96	0.47
1:O:98:ILE:HD11	1:O:139:TYR:CD2	2.49	0.47
1:V:16:LEU:O	1:V:28:THR:HA	2.13	0.47
1:T:23:VAL:HG13	1:T:108:ARG:CZ	2.44	0.47
1:Q:113:ARG:HH22	1:W:115:SER:H	1.62	0.47
1:C:143:HIS:HE1	3:C:354:HOH:O	1.97	0.47
1:T:32:LEU:HD13	1:T:130:ILE:CG1	2.45	0.47
1:N:98:ILE:HD11	1:N:139:TYR:HD2	1.78	0.47
1:B:5:VAL:C	1:B:6:ASN:HD22	2.18	0.47
1:W:142:GLU:O	1:W:143:HIS:HB2	2.14	0.47
1:T:130:ILE:C	1:T:132:GLY:N	2.67	0.47
1:H:102:ILE:HG23	1:H:129:GLY:HA2	1.97	0.47
1:G:63:HIS:HD2	3:G:301:HOH:O	1.97	0.47
1:I:60:ASP:HB2	3:J:301:HOH:O	2.15	0.47
2:T:201:KIW:H10	2:T:201:KIW:CAS	2.42	0.47
1:M:92:GLU:HG3	1:W:20:GLU:OE1	2.15	0.47
1:W:81:HIS:NE2	2:W:201:KIW:OAB	2.48	0.47
1:P:101:HIS:HB2	1:P:126:VAL:HG22	1.97	0.47
1:L:142:GLU:O	1:L:143:HIS:HB2	2.15	0.47
1:D:60:ASP:OD2	1:D:64:GLN:NE2	2.48	0.47
1:L:118:SER:HB2	1:L:119:PRO:HD3	1.97	0.47
1:B:101:HIS:HB2	1:B:126:VAL:CG2	2.41	0.46
1:W:35:LEU:CD2	1:W:134:LEU:HD11	2.45	0.46
1:M:7:VAL:HG21	1:M:36:ILE:HD13	1.96	0.46
1:H:7:VAL:HG22	1:H:73:ILE:HB	1.96	0.46
1:I:106:HIS:HA	1:I:113:ARG:HG2	1.97	0.46
1:I:110:GLU:O	1:I:113:ARG:HB2	2.16	0.46
1:O:27:THR:CG2	1:O:31:GLU:HB3	2.45	0.46
1:F:88:ASP:O	1:F:91:ALA:HB3	2.16	0.46
1:O:18:ARG:HB3	1:O:18:ARG:HH11	1.79	0.46
1:D:102:ILE:HG23	1:D:129:GLY:HA2	1.96	0.46
1:B:50:ARG:HB3	1:B:61:TRP:CH2	2.51	0.46
1:P:104:ASN:HA	1:P:126:VAL:HG13	1.97	0.46
1:B:17:GLY:O	1:B:19:ARG:N	2.48	0.46
1:A:102:ILE:HG12	1:A:130:ILE:HD12	1.96	0.46
1:O:138:ARG:CG	1:O:138:ARG:HH11	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:104:ASN:HA	1:V:126:VAL:HG13	1.98	0.46
1:L:86:LEU:O	1:L:87:ARG:C	2.54	0.46
1:M:131:GLN:HA	1:M:131:GLN:HE21	1.80	0.46
1:H:68:ALA:HB3	1:H:70:GLU:HG3	1.96	0.46
1:B:17:GLY:O	1:B:18:ARG:C	2.53	0.46
1:T:73:ILE:HD13	1:T:136:ALA:HB3	1.96	0.46
1:V:32:LEU:HD13	1:V:130:ILE:HG12	1.98	0.46
1:K:98:ILE:HD11	1:K:139:TYR:CD1	2.50	0.46
1:D:25:GLY:HA2	3:D:305:HOH:O	2.16	0.46
1:J:36:ILE:HG23	1:J:137:LEU:HD11	1.97	0.46
1:I:16:LEU:HD23	1:I:16:LEU:HA	1.80	0.46
1:L:29:HIS:O	1:L:33:VAL:HG23	2.16	0.46
1:P:109:GLU:HB3	3:P:321:HOH:O	2.04	0.46
1:T:28:THR:HG23	1:T:31:GLU:OE2	2.15	0.46
1:O:50:ARG:HD2	3:O:344:HOH:O	2.14	0.46
1:B:46:LYS:O	1:B:46:LYS:HG3	2.16	0.46
1:N:115:SER:HB3	1:N:118:SER:H	1.81	0.46
1:T:118:SER:N	1:T:119:PRO:CD	2.79	0.46
1:A:31:GLU:O	1:A:35:LEU:HG	2.16	0.46
1:B:39:GLU:OE1	1:B:134:LEU:HD13	2.16	0.46
1:C:3:LEU:N	3:C:327:HOH:O	2.50	0.45
1:B:131:GLN:HE22	1:F:142:GLU:HG2	1.81	0.45
1:G:33:VAL:HG22	1:G:49:VAL:HG21	1.94	0.45
1:X:102:ILE:HG23	1:X:129:GLY:HA2	1.98	0.45
1:C:3:LEU:HD23	1:C:45:LEU:HD21	1.98	0.45
1:D:27:THR:HA	1:D:31:GLU:OE1	2.16	0.45
1:C:7:VAL:HG22	1:C:73:ILE:HD12	1.98	0.45
1:X:9:ASN:HB3	1:X:13:LEU:CB	2.47	0.45
1:A:29:HIS:O	1:A:33:VAL:HG23	2.17	0.45
1:I:23:VAL:O	1:I:23:VAL:HG23	2.16	0.45
1:S:77:GLY:HA2	2:S:201:KIW:CAJ	2.46	0.45
1:P:113:ARG:HD2	3:P:319:HOH:O	2.15	0.45
1:O:138:ARG:HD3	1:T:138:ARG:NE	2.31	0.45
1:V:117:LEU:O	1:V:120:ILE:HG13	2.17	0.45
1:M:15:ARG:O	1:M:16:LEU:C	2.55	0.45
1:Q:5:VAL:HG22	1:Q:71:PRO:HG2	1.97	0.45
1:X:15:ARG:NH1	1:X:15:ARG:CG	2.68	0.45
1:Q:106:HIS:HA	1:Q:113:ARG:HG2	1.97	0.45
1:Q:29:HIS:O	1:Q:33:VAL:HG23	2.17	0.45
1:C:128:LEU:HD22	1:H:139:TYR:CD1	2.52	0.45
1:T:96:PRO:HB2	1:T:140:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:99:GLU:HB3	1:R:124:VAL:HG13	1.99	0.45
1:D:41:ALA:C	1:D:43:LEU:H	2.19	0.45
1:X:9:ASN:HB3	1:X:13:LEU:HD13	1.98	0.45
1:W:32:LEU:HD13	1:W:130:ILE:HG13	1.98	0.45
1:H:18:ARG:HH11	1:H:18:ARG:HG3	1.81	0.45
1:L:87:ARG:HG3	1:L:116:TYR:O	2.17	0.45
1:P:11:PRO:HA	1:P:53:ASP:HA	1.99	0.45
1:S:118:SER:N	1:S:119:PRO:CD	2.79	0.45
1:G:95:ALA:HB1	1:G:96:PRO:CD	2.47	0.45
1:E:27:THR:CG2	1:E:31:GLU:HB2	2.47	0.45
1:V:5:VAL:HG11	1:V:137:LEU:HD23	1.99	0.45
1:Q:41:ALA:HA	3:Q:306:HOH:O	2.16	0.45
1:A:5:VAL:HG22	1:A:71:PRO:HG2	1.99	0.45
1:O:105:VAL:HG22	1:O:126:VAL:HG21	1.99	0.45
1:S:128:LEU:O	1:S:131:GLN:HB2	2.16	0.45
1:V:9:ASN:O	1:V:51:GLN:HA	2.17	0.45
1:P:120:ILE:HA	3:P:309:HOH:O	2.16	0.45
1:B:24:TYR:HB2	3:B:342:HOH:O	2.17	0.45
1:C:112:ARG:HD3	2:C:201:KIW:OAA	2.17	0.44
1:O:104:ASN:HA	1:O:126:VAL:CG1	2.47	0.44
1:T:80:THR:HG21	1:T:99:GLU:OE2	2.17	0.44
1:E:71:PRO:HB3	1:E:96:PRO:HD2	1.98	0.44
1:X:16:LEU:HB3	1:X:27:THR:O	2.17	0.44
1:F:81:HIS:CE1	1:F:112:ARG:HA	2.52	0.44
1:B:142:GLU:O	1:B:143:HIS:HB2	2.17	0.44
1:K:50:ARG:HB3	1:K:61:TRP:CH2	2.52	0.44
1:N:7:VAL:HB	1:N:49:VAL:HG22	1.99	0.44
1:A:134:LEU:O	1:A:137:LEU:HB2	2.17	0.44
1:D:125:ILE:HD11	1:I:128:LEU:HD11	2.00	0.44
1:J:55:GLU:O	1:J:59:LEU:HG	2.18	0.44
1:U:27:THR:HG23	1:U:31:GLU:CB	2.48	0.44
1:I:135:LEU:HA	1:I:135:LEU:HD23	1.78	0.44
1:R:38:ARG:NH1	1:R:38:ARG:CB	2.67	0.44
1:L:3:LEU:HD23	1:N:22:ALA:HB3	1.98	0.44
1:T:5:VAL:HG22	1:T:71:PRO:HG2	1.99	0.44
1:V:24:TYR:HE2	3:V:334:HOH:O	2.00	0.44
1:U:104:ASN:HA	1:U:126:VAL:HG13	1.99	0.44
1:J:20:GLU:HB3	1:J:23:VAL:O	2.18	0.44
1:H:21:PRO:HD2	3:H:337:HOH:O	2.17	0.44
1:I:44:GLY:O	1:I:45:LEU:HD23	2.17	0.44
1:V:118:SER:HB2	1:V:119:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:ILE:HA	1:E:46:LYS:O	2.17	0.44
1:Q:16:LEU:HB3	1:Q:27:THR:O	2.18	0.44
1:N:11:PRO:O	1:N:12:ASN:HB2	2.18	0.44
1:Q:142:GLU:O	1:Q:143:HIS:HB2	2.18	0.44
1:Q:81:HIS:CE1	1:Q:112:ARG:HA	2.53	0.44
1:M:82:THR:O	1:W:82:THR:HG21	2.17	0.44
1:P:21:PRO:C	1:P:23:VAL:H	2.20	0.44
1:N:80:THR:HG22	1:N:115:SER:OG	2.17	0.43
1:W:15:ARG:H	1:W:15:ARG:HG2	1.72	0.43
1:F:35:LEU:HD22	1:F:134:LEU:HD11	2.00	0.43
1:S:29:HIS:O	1:S:32:LEU:HB3	2.18	0.43
1:P:59:LEU:HD12	1:R:53:ASP:HB3	1.99	0.43
1:V:5:VAL:HG11	1:V:137:LEU:CD2	2.48	0.43
1:J:98:ILE:HD11	1:J:139:TYR:CD1	2.53	0.43
1:D:36:ILE:HG23	1:D:137:LEU:HD11	1.99	0.43
1:L:117:LEU:O	1:L:120:ILE:HD13	2.19	0.43
1:N:9:ASN:OD1	1:N:75:ASN:HB3	2.18	0.43
1:S:38:ARG:HA	3:S:327:HOH:O	2.18	0.43
1:S:90:CYS:HB3	1:S:97:LEU:HD22	2.01	0.43
1:U:66:ALA:HB2	1:U:93:LEU:HD23	1.99	0.43
1:H:113:ARG:HD2	3:H:313:HOH:O	2.18	0.43
1:R:98:ILE:HD11	1:R:139:TYR:CD2	2.53	0.43
1:H:134:LEU:HA	1:H:137:LEU:HD12	2.00	0.43
1:K:101:HIS:HB2	1:K:126:VAL:HG22	2.00	0.43
1:W:90:CYS:HB3	1:W:97:LEU:HD22	1.99	0.43
1:O:9:ASN:O	1:O:51:GLN:HA	2.19	0.43
1:S:143:HIS:CE1	3:S:337:HOH:O	2.71	0.43
1:S:40:ALA:HB2	1:S:137:LEU:HD22	2.00	0.43
1:B:104:ASN:HA	1:B:126:VAL:HG13	2.00	0.43
1:P:15:ARG:NH2	1:S:92:GLU:OE1	2.49	0.43
1:J:19:ARG:HG2	1:J:20:GLU:H	1.84	0.43
1:D:48:VAL:HG12	1:D:50:ARG:HD3	2.00	0.43
1:K:7:VAL:HB	1:K:49:VAL:HG22	2.01	0.43
1:P:15:ARG:HE	1:P:15:ARG:HB3	1.68	0.43
1:V:55:GLU:HA	1:V:58:LEU:HD12	2.01	0.43
1:M:101:HIS:HB2	1:M:126:VAL:HG22	2.01	0.42
1:G:20:GLU:O	1:G:22:ALA:N	2.52	0.42
1:X:29:HIS:O	1:X:33:VAL:HG23	2.19	0.42
1:P:70:GLU:HA	1:P:71:PRO:HD3	1.95	0.42
1:L:3:LEU:HD22	1:L:3:LEU:HA	1.76	0.42
1:S:77:GLY:HA2	2:S:201:KIW:CAS	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:LEU:O	1:F:137:LEU:HB2	2.19	0.42
1:H:81:HIS:NE2	2:H:201:KIW:OAB	2.52	0.42
1:T:59:LEU:HD22	1:T:89:ALA:HB2	2.00	0.42
1:I:33:VAL:O	1:I:37:GLU:HB2	2.19	0.42
1:W:23:VAL:O	1:W:24:TYR:CB	2.67	0.42
1:A:90:CYS:HB3	1:A:97:LEU:HD22	2.02	0.42
1:L:3:LEU:HB3	1:L:45:LEU:HD23	2.00	0.42
1:U:106:HIS:HA	1:U:113:ARG:HG2	2.00	0.42
1:G:19:ARG:HG3	1:G:20:GLU:CG	2.48	0.42
1:X:142:GLU:N	1:X:142:GLU:OE1	2.51	0.42
1:B:18:ARG:O	1:B:19:ARG:CB	2.68	0.42
1:U:102:ILE:O	1:U:127:GLY:HA2	2.20	0.42
1:Q:13:LEU:HD23	2:Q:201:KIW:H9	2.00	0.42
1:H:117:LEU:HG	3:H:349:HOH:O	2.19	0.42
1:M:32:LEU:HD13	1:M:130:ILE:HG12	2.00	0.42
1:Q:58:LEU:O	1:Q:62:ILE:HG12	2.19	0.42
1:B:58:LEU:O	1:B:62:ILE:HG12	2.19	0.42
1:S:134:LEU:O	1:S:137:LEU:HB2	2.20	0.42
1:D:4:ILE:O	1:D:71:PRO:HD2	2.19	0.42
1:C:52:SER:HB2	1:C:61:TRP:CH2	2.54	0.42
1:Q:46:LYS:HD2	3:Q:340:HOH:O	2.19	0.42
1:N:70:GLU:HA	1:N:71:PRO:HD2	1.88	0.42
1:X:142:GLU:O	1:X:143:HIS:HB2	2.20	0.42
1:J:13:LEU:HD23	2:J:201:KIW:H9	2.00	0.42
1:K:102:ILE:HG23	1:K:129:GLY:HA2	2.02	0.42
1:K:6:ASN:HB2	1:K:72:VAL:HG22	2.02	0.42
1:A:114:HIS:CD2	1:G:113:ARG:HH12	2.23	0.42
1:U:102:ILE:HG23	1:U:129:GLY:HA2	2.02	0.42
1:X:25:GLY:HA3	1:X:26:GLY:HA2	1.65	0.42
1:E:11:PRO:O	1:E:12:ASN:HB2	2.20	0.42
1:S:4:ILE:O	1:S:71:PRO:HD2	2.19	0.42
1:B:113:ARG:NH1	3:B:308:HOH:O	2.44	0.42
1:Q:113:ARG:CD	3:Q:344:HOH:O	2.47	0.42
1:I:60:ASP:OD2	1:I:64:GLN:NE2	2.53	0.42
1:V:81:HIS:NE2	2:V:201:KIW:OAD	2.53	0.42
1:X:4:ILE:HB	1:X:70:GLU:OE2	2.20	0.42
1:E:99:GLU:HB3	1:E:124:VAL:HG13	2.00	0.42
1:A:19:ARG:HB3	1:A:20:GLU:HA	2.02	0.42
1:N:115:SER:H	1:R:113:ARG:HH22	1.68	0.42
1:F:140:LEU:O	1:F:143:HIS:N	2.38	0.42
1:K:118:SER:HB2	1:K:119:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:114:HIS:HB2	3:W:338:HOH:O	2.19	0.41
1:K:98:ILE:HD11	1:K:139:TYR:HD1	1.85	0.41
1:C:115:SER:HG	1:C:118:SER:H	1.68	0.41
1:C:5:VAL:HG22	3:C:355:HOH:O	2.19	0.41
1:S:36:ILE:HG23	1:S:137:LEU:HD11	2.02	0.41
1:S:77:GLY:O	1:S:78:GLY:C	2.59	0.41
1:Q:32:LEU:HD13	1:Q:130:ILE:HG23	2.02	0.41
1:D:7:VAL:HG22	1:D:73:ILE:HB	2.01	0.41
1:T:100:VAL:HA	1:T:125:ILE:O	2.20	0.41
1:B:57:GLN:HE21	1:B:57:GLN:HA	1.84	0.41
1:I:23:VAL:HB	3:I:256:HOH:O	2.19	0.41
1:T:130:ILE:C	1:T:132:GLY:H	2.22	0.41
1:P:82:THR:HA	3:P:308:HOH:O	2.20	0.41
1:T:86:LEU:HD23	1:T:117:LEU:HD11	2.02	0.41
1:T:32:LEU:CD1	1:T:130:ILE:HG13	2.49	0.41
1:H:143:HIS:CD2	3:H:354:HOH:O	2.73	0.41
1:O:98:ILE:HD11	1:O:139:TYR:HD2	1.85	0.41
1:O:27:THR:HG22	1:O:31:GLU:HB3	2.01	0.41
1:J:59:LEU:CD2	1:J:86:LEU:HA	2.51	0.41
1:G:10:GLY:O	1:G:13:LEU:HB2	2.21	0.41
1:S:7:VAL:O	1:S:49:VAL:HA	2.20	0.41
1:Q:102:ILE:HG23	1:Q:129:GLY:HA2	2.01	0.41
1:Q:15:ARG:O	1:Q:18:ARG:HG3	2.20	0.41
1:N:60:ASP:O	1:N:63:HIS:HB2	2.21	0.41
1:S:20:GLU:HG3	1:S:24:TYR:CD2	2.55	0.41
1:F:52:SER:HB3	1:F:58:LEU:HD23	2.02	0.41
1:L:102:ILE:HG23	1:L:129:GLY:HA2	2.02	0.41
1:Q:131:GLN:O	1:Q:135:LEU:HG	2.20	0.41
1:K:16:LEU:HD11	1:K:130:ILE:HD11	2.02	0.41
1:C:63:HIS:HB2	3:C:351:HOH:O	2.20	0.41
1:P:46:LYS:HB3	1:P:46:LYS:NZ	2.36	0.41
1:G:27:THR:HG23	1:G:31:GLU:HB2	2.03	0.41
1:O:138:ARG:CG	1:O:138:ARG:NH1	2.84	0.41
1:O:50:ARG:HB3	1:O:61:TRP:CH2	2.55	0.41
1:P:90:CYS:HB3	1:P:97:LEU:HD22	2.03	0.41
1:O:10:GLY:HA2	1:O:58:LEU:HD11	2.03	0.41
1:I:20:GLU:HA	1:I:21:PRO:HD3	1.85	0.41
1:V:140:LEU:HD23	1:V:140:LEU:HA	1.98	0.41
1:J:5:VAL:HG21	1:J:45:LEU:HD13	2.03	0.41
1:O:17:GLY:HA2	1:O:25:GLY:O	2.21	0.41
1:U:18:ARG:CG	1:U:18:ARG:NH1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:32:LEU:HD13	1:W:130:ILE:HG12	2.02	0.41
1:L:71:PRO:HD2	3:L:310:HOH:O	2.20	0.41
1:Q:25:GLY:HA2	1:Q:26:GLY:HA2	1.73	0.41
1:X:50:ARG:NH2	1:X:61:TRP:CD1	2.89	0.40
1:L:86:LEU:HD12	1:L:86:LEU:HA	1.80	0.40
1:Q:30:ASP:OD1	1:Q:30:ASP:N	2.54	0.40
1:H:86:LEU:HA	1:H:86:LEU:HD12	1.87	0.40
1:Q:128:LEU:HB3	1:W:139:TYR:CD1	2.56	0.40
1:F:102:ILE:O	1:F:127:GLY:HA2	2.21	0.40
1:W:79:LEU:HA	1:W:82:THR:OG1	2.20	0.40
1:X:32:LEU:HA	1:X:35:LEU:HD23	2.03	0.40
1:L:38:ARG:HE	1:L:38:ARG:HB3	1.67	0.40
2:D:201:KIW:H2	2:D:201:KIW:H8	1.93	0.40
2:M:201:KIW:H5	2:M:201:KIW:H8	1.89	0.40
1:H:35:LEU:CD1	1:H:134:LEU:HD11	2.51	0.40
1:T:80:THR:HG22	1:T:115:SER:OG	2.22	0.40
1:L:87:ARG:HB2	1:L:116:TYR:HB3	2.02	0.40
1:W:104:ASN:HA	1:W:126:VAL:HG13	2.02	0.40
1:T:21:PRO:HA	1:T:25:GLY:HA2	2.03	0.40
1:A:118:SER:HB3	1:G:106:HIS:CB	2.52	0.40
1:S:140:LEU:C	1:S:142:GLU:H	2.24	0.40
1:N:74:LEU:HD23	1:N:117:LEU:HD13	2.04	0.40
1:E:3:LEU:HD12	3:E:345:HOH:O	2.21	0.40
1:V:90:CYS:HB3	1:V:97:LEU:CD2	2.51	0.40
1:G:8:ILE:CG2	1:G:58:LEU:HD22	2.52	0.40
1:F:50:ARG:HB3	1:F:61:TRP:CH2	2.56	0.40
1:C:104:ASN:HA	1:C:126:VAL:HG13	2.04	0.40
1:Q:87:ARG:HG2	1:Q:87:ARG:O	2.22	0.40
2:L:201:KIW:H2	2:L:201:KIW:H8	1.66	0.40
1:E:29:HIS:CE1	1:E:51:GLN:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	139/167 (83%)	129 (93%)	8 (6%)	2 (1%)	14 27
1	B	140/167 (84%)	123 (88%)	13 (9%)	4 (3%)	6 9
1	C	134/167 (80%)	126 (94%)	7 (5%)	1 (1%)	26 49
1	D	133/167 (80%)	128 (96%)	3 (2%)	2 (2%)	13 25
1	E	132/167 (79%)	124 (94%)	8 (6%)	0	100 100
1	F	132/167 (79%)	124 (94%)	7 (5%)	1 (1%)	24 45
1	G	140/167 (84%)	124 (89%)	12 (9%)	4 (3%)	6 9
1	H	139/167 (83%)	130 (94%)	9 (6%)	0	100 100
1	I	139/167 (83%)	133 (96%)	5 (4%)	1 (1%)	26 49
1	J	139/167 (83%)	129 (93%)	6 (4%)	4 (3%)	6 9
1	K	139/167 (83%)	124 (89%)	14 (10%)	1 (1%)	26 49
1	L	134/167 (80%)	127 (95%)	5 (4%)	2 (2%)	13 25
1	M	139/167 (83%)	124 (89%)	11 (8%)	4 (3%)	6 9
1	N	139/167 (83%)	134 (96%)	3 (2%)	2 (1%)	14 27
1	O	139/167 (83%)	130 (94%)	5 (4%)	4 (3%)	6 9
1	P	139/167 (83%)	130 (94%)	6 (4%)	3 (2%)	8 15
1	Q	132/167 (79%)	125 (95%)	6 (4%)	1 (1%)	24 45
1	R	134/167 (80%)	129 (96%)	4 (3%)	1 (1%)	26 49
1	S	139/167 (83%)	117 (84%)	17 (12%)	5 (4%)	4 6
1	T	136/167 (81%)	123 (90%)	11 (8%)	2 (2%)	13 25
1	U	139/167 (83%)	133 (96%)	5 (4%)	1 (1%)	26 49
1	V	133/167 (80%)	123 (92%)	10 (8%)	0	100 100
1	W	139/167 (83%)	122 (88%)	14 (10%)	3 (2%)	8 15
1	X	134/167 (80%)	121 (90%)	11 (8%)	2 (2%)	13 25
All	All	3282/4008 (82%)	3032 (92%)	200 (6%)	50 (2%)	13 25

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	B	18	ARG
1	B	19	ARG

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Mol	Chain	Res	Type
1	B	21	PRO
1	G	20	GLU
1	G	21	PRO
1	G	24	TYR
1	J	19	ARG
1	J	20	GLU
1	J	21	PRO
1	L	19	ARG
1	M	18	ARG
1	M	20	GLU
1	N	22	ALA
1	O	19	ARG
1	O	20	GLU
1	P	19	ARG
1	B	22	ALA
1	D	27	THR
1	F	42	GLU
1	J	24	TYR
1	M	22	ALA
1	P	25	GLY
1	P	26	GLY
1	S	18	ARG
1	T	19	ARG
1	W	24	TYR
1	C	19	ARG
1	D	42	GLU
1	K	109	GLU
1	N	19	ARG
1	S	21	PRO
1	W	19	ARG
1	I	20	GLU
1	M	21	PRO
1	R	19	ARG
1	S	78	GLY
1	U	12	ASN
1	W	142	GLU
1	X	50	ARG
1	Q	129	GLY
1	S	96	PRO
1	T	20	GLU
1	X	42	GLU
1	A	16	LEU

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Mol	Chain	Res	Type
1	O	109	GLU
1	S	130	ILE
1	O	33	VAL
1	G	130	ILE
1	L	130	ILE

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	109/132 (83%)	107 (98%)	2 (2%)	66 86
1	B	110/132 (83%)	97 (88%)	13 (12%)	6 11
1	C	108/132 (82%)	99 (92%)	9 (8%)	14 26
1	D	106/132 (80%)	99 (93%)	7 (7%)	21 39
1	E	105/132 (80%)	102 (97%)	3 (3%)	50 76
1	F	105/132 (80%)	93 (89%)	12 (11%)	7 12
1	G	111/132 (84%)	101 (91%)	10 (9%)	12 22
1	H	110/132 (83%)	101 (92%)	9 (8%)	14 27
1	I	109/132 (83%)	100 (92%)	9 (8%)	14 26
1	J	109/132 (83%)	103 (94%)	6 (6%)	27 50
1	K	110/132 (83%)	103 (94%)	7 (6%)	22 42
1	L	107/132 (81%)	98 (92%)	9 (8%)	14 25
1	M	109/132 (83%)	98 (90%)	11 (10%)	9 16
1	N	110/132 (83%)	102 (93%)	8 (7%)	17 34
1	O	108/132 (82%)	103 (95%)	5 (5%)	33 59
1	P	109/132 (83%)	101 (93%)	8 (7%)	17 34
1	Q	105/132 (80%)	97 (92%)	8 (8%)	16 31
1	R	108/132 (82%)	97 (90%)	11 (10%)	9 16
1	S	109/132 (83%)	103 (94%)	6 (6%)	27 50
1	T	109/132 (83%)	101 (93%)	8 (7%)	17 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	110/132 (83%)	105 (96%)	5 (4%)	34	60
1	V	106/132 (80%)	99 (93%)	7 (7%)	21	39
1	W	109/132 (83%)	100 (92%)	9 (8%)	14	26
1	X	106/132 (80%)	98 (92%)	8 (8%)	17	32
All	All	2597/3168 (82%)	2407 (93%)	190 (7%)	18	34

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	THR
1	A	131	GLN
1	B	3	LEU
1	B	6	ASN
1	B	35	LEU
1	B	45	LEU
1	B	57	GLN
1	B	94	SER
1	B	98	ILE
1	B	110	GLU
1	B	114[A]	HIS
1	B	114[B]	HIS
1	B	120	ILE
1	B	131	GLN
1	B	143	HIS
1	C	4	ILE
1	C	13	LEU
1	C	16	LEU
1	C	24	TYR
1	C	38	ARG
1	C	50	ARG
1	C	110	GLU
1	C	130	ILE
1	C	142	GLU
1	D	27	THR
1	D	28	THR
1	D	35	LEU
1	D	50	ARG
1	D	114	HIS
1	D	126	VAL
1	D	142	GLU
1	E	55	GLU

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Mol	Chain	Res	Type
1	E	57	GLN
1	E	142	GLU
1	F	3	LEU
1	F	4	ILE
1	F	8	ILE
1	F	18	ARG
1	F	32	LEU
1	F	35	LEU
1	F	38	ARG
1	F	50	ARG
1	F	110	GLU
1	F	113	ARG
1	F	126	VAL
1	F	130	ILE
1	G	18	ARG
1	G	19	ARG
1	G	35	LEU
1	G	45	LEU
1	G	49	VAL
1	G	114[A]	HIS
1	G	114[B]	HIS
1	G	126	VAL
1	G	131	GLN
1	G	142	GLU
1	H	11	PRO
1	H	18	ARG
1	H	35	LEU
1	H	81	HIS
1	H	94	SER
1	H	110	GLU
1	H	114	HIS
1	H	126	VAL
1	H	130	ILE
1	I	16	LEU
1	I	18	ARG
1	I	20	GLU
1	I	23	VAL
1	I	35	LEU
1	I	50	ARG
1	I	114	HIS
1	I	126	VAL
1	I	130	ILE

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Mol	Chain	Res	Type
1	J	16	LEU
1	J	18	ARG
1	J	19	ARG
1	J	24	TYR
1	J	142	GLU
1	J	143	HIS
1	K	3	LEU
1	K	16	LEU
1	K	19	ARG
1	K	50	ARG
1	K	126	VAL
1	K	130	ILE
1	K	142	GLU
1	L	3	LEU
1	L	24	TYR
1	L	35	LEU
1	L	38	ARG
1	L	50	ARG
1	L	120	ILE
1	L	126	VAL
1	L	135	LEU
1	L	142	GLU
1	M	4	ILE
1	M	16	LEU
1	M	18	ARG
1	M	50	ARG
1	M	57	GLN
1	M	80	THR
1	M	114	HIS
1	M	115	SER
1	M	126	VAL
1	M	130	ILE
1	M	131	GLN
1	N	18	ARG
1	N	42	GLU
1	N	80	THR
1	N	114	HIS
1	N	115	SER
1	N	120	ILE
1	N	126	VAL
1	N	130	ILE
1	O	18	ARG

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Mol	Chain	Res	Type
1	O	50	ARG
1	O	110	GLU
1	O	126	VAL
1	O	138	ARG
1	P	31	GLU
1	P	35	LEU
1	P	46	LYS
1	P	80	THR
1	P	110	GLU
1	P	114	HIS
1	P	131	GLN
1	P	142	GLU
1	Q	4	ILE
1	Q	18	ARG
1	Q	35	LEU
1	Q	38	ARG
1	Q	50	ARG
1	Q	114	HIS
1	Q	126	VAL
1	Q	131	GLN
1	R	16	LEU
1	R	19	ARG
1	R	31	GLU
1	R	38	ARG
1	R	45	LEU
1	R	50	ARG
1	R	54	SER
1	R	110	GLU
1	R	114	HIS
1	R	126	VAL
1	R	130	ILE
1	S	18	ARG
1	S	49	VAL
1	S	50	ARG
1	S	54	SER
1	S	62	ILE
1	S	131	GLN
1	T	18	ARG
1	T	23	VAL
1	T	35	LEU
1	T	38	ARG
1	T	46	LYS

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Mol	Chain	Res	Type
1	T	50	ARG
1	T	114	HIS
1	T	142	GLU
1	U	18	ARG
1	U	19	ARG
1	U	35	LEU
1	U	130	ILE
1	U	142	GLU
1	V	3	LEU
1	V	42	GLU
1	V	45	LEU
1	V	55	GLU
1	V	114	HIS
1	V	130	ILE
1	V	131	GLN
1	W	18	ARG
1	W	23	VAL
1	W	35	LEU
1	W	42	GLU
1	W	45	LEU
1	W	79	LEU
1	W	114	HIS
1	W	130	ILE
1	W	142	GLU
1	X	4	ILE
1	X	15	ARG
1	X	18	ARG
1	X	50	ARG
1	X	80	THR
1	X	122	THR
1	X	130	ILE
1	X	143	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	131	GLN
1	A	143	HIS
1	B	6	ASN
1	B	57	GLN
1	B	63	HIS

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Mol	Chain	Res	Type
1	B	131	GLN
1	C	63	HIS
1	D	57	GLN
1	D	64	GLN
1	D	143	HIS
1	E	57	GLN
1	F	63	HIS
1	F	64	GLN
1	G	64	GLN
1	G	143	HIS
1	H	63	HIS
1	I	51	GLN
1	I	63	HIS
1	I	64	GLN
1	I	143	HIS
1	J	12	ASN
1	K	114	HIS
1	K	143	HIS
1	L	63	HIS
1	M	63	HIS
1	M	114	HIS
1	M	131	GLN
1	N	6	ASN
1	N	63	HIS
1	N	114	HIS
1	O	63	HIS
1	P	6	ASN
1	P	114	HIS
1	P	131	GLN
1	Q	63	HIS
1	Q	131	GLN
1	S	114	HIS
1	T	63	HIS
1	V	63	HIS
1	V	114	HIS
1	W	12	ASN
1	X	64	GLN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	KIW	A	500	-	16,24,24	1.85	1 (6%)	21,33,33	1.08	2 (9%)
2	KIW	B	201	-	16,24,24	1.81	1 (6%)	21,33,33	1.14	2 (9%)
2	KIW	C	201	-	16,24,24	1.96	1 (6%)	21,33,33	1.46	3 (14%)
2	KIW	D	201	-	16,24,24	2.01	1 (6%)	21,33,33	0.88	0
2	KIW	E	201	-	16,24,24	1.82	1 (6%)	21,33,33	0.95	0
2	KIW	G	201	-	16,24,24	2.04	1 (6%)	21,33,33	1.15	2 (9%)
2	KIW	H	201	-	16,24,24	1.92	1 (6%)	21,33,33	1.35	2 (9%)
2	KIW	J	201	-	16,24,24	1.88	1 (6%)	21,33,33	1.05	1 (4%)
2	KIW	K	201	-	16,24,24	2.02	1 (6%)	21,33,33	1.77	3 (14%)
2	KIW	L	201	-	16,24,24	1.94	2 (12%)	21,33,33	0.88	0
2	KIW	M	201	-	16,24,24	1.95	1 (6%)	21,33,33	0.92	0
2	KIW	N	201	-	16,24,24	1.78	1 (6%)	21,33,33	0.91	0
2	KIW	O	201	-	16,24,24	1.89	1 (6%)	21,33,33	1.30	2 (9%)
2	KIW	P	201	-	16,24,24	1.90	1 (6%)	21,33,33	1.54	4 (19%)
2	KIW	Q	201	-	16,24,24	1.92	1 (6%)	21,33,33	1.05	0
2	KIW	R	201	-	16,24,24	1.82	1 (6%)	21,33,33	1.30	1 (4%)
2	KIW	S	201	-	16,24,24	1.79	1 (6%)	21,33,33	1.47	3 (14%)
2	KIW	T	201	-	16,24,24	2.18	2 (12%)	21,33,33	1.14	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	KIW	U	201	-	16,24,24	1.96	1 (6%)	21,33,33	1.20	2 (9%)
2	KIW	V	201	-	16,24,24	1.87	1 (6%)	21,33,33	0.86	1 (4%)
2	KIW	W	201	-	16,24,24	1.88	1 (6%)	21,33,33	0.93	0
2	KIW	X	201	-	16,24,24	2.06	1 (6%)	21,33,33	1.26	1 (4%)

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	KIW	A	500	-	-	0/9/17/17	0/2/2/2
2	KIW	B	201	-	-	0/9/17/17	0/2/2/2
2	KIW	C	201	-	-	0/9/17/17	0/2/2/2
2	KIW	D	201	-	-	0/9/17/17	0/2/2/2
2	KIW	E	201	-	-	2/9/17/17	0/2/2/2
2	KIW	G	201	-	-	0/9/17/17	0/2/2/2
2	KIW	H	201	-	-	0/9/17/17	0/2/2/2
2	KIW	J	201	-	-	0/9/17/17	0/2/2/2
2	KIW	K	201	-	-	0/9/17/17	0/2/2/2
2	KIW	L	201	-	-	0/9/17/17	0/2/2/2
2	KIW	M	201	-	-	0/9/17/17	0/2/2/2
2	KIW	N	201	-	-	0/9/17/17	0/2/2/2
2	KIW	O	201	-	-	0/9/17/17	0/2/2/2
2	KIW	P	201	-	-	0/9/17/17	0/2/2/2
2	KIW	Q	201	-	-	0/9/17/17	0/2/2/2
2	KIW	R	201	-	-	0/9/17/17	0/2/2/2
2	KIW	S	201	-	-	0/9/17/17	0/2/2/2
2	KIW	T	201	-	-	0/9/17/17	0/2/2/2
2	KIW	U	201	-	-	0/9/17/17	0/2/2/2
2	KIW	V	201	-	-	0/9/17/17	0/2/2/2
2	KIW	W	201	-	-	0/9/17/17	0/2/2/2
2	KIW	X	201	-	-	0/9/17/17	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	201	KIW	CAS-NAO	-2.03	1.32	1.38
2	T	201	KIW	CAN-CAR	2.04	1.56	1.51
2	N	201	KIW	OAF-NAW	6.70	1.36	1.22
2	S	201	KIW	OAF-NAW	6.72	1.36	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	201	KIW	OAF-NAW	6.78	1.36	1.22
2	E	201	KIW	OAF-NAW	6.85	1.36	1.22
2	B	201	KIW	OAF-NAW	6.86	1.36	1.22
2	A	500	KIW	OAF-NAW	6.89	1.36	1.22
2	V	201	KIW	OAF-NAW	6.92	1.36	1.22
2	D	201	KIW	OAF-NAW	7.03	1.36	1.22
2	J	201	KIW	OAF-NAW	7.05	1.36	1.22
2	W	201	KIW	OAF-NAW	7.07	1.36	1.22
2	P	201	KIW	OAF-NAW	7.08	1.36	1.22
2	O	201	KIW	OAF-NAW	7.08	1.36	1.22
2	H	201	KIW	OAF-NAW	7.13	1.36	1.22
2	Q	201	KIW	OAF-NAW	7.22	1.37	1.22
2	M	201	KIW	OAF-NAW	7.24	1.37	1.22
2	L	201	KIW	OAF-NAW	7.26	1.37	1.22
2	U	201	KIW	OAF-NAW	7.30	1.37	1.22
2	C	201	KIW	OAF-NAW	7.30	1.37	1.22
2	G	201	KIW	OAF-NAW	7.53	1.37	1.22
2	K	201	KIW	OAF-NAW	7.60	1.37	1.22
2	X	201	KIW	OAF-NAW	7.61	1.37	1.22
2	T	201	KIW	OAF-NAW	7.79	1.38	1.22

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	201	KIW	CAR-CAN-NAO	-3.87	104.74	113.73
2	K	201	KIW	CAN-CAR-CAL	-3.16	115.02	120.62
2	S	201	KIW	CAU-CAK-CAS	-2.85	118.86	121.52
2	C	201	KIW	CAL-CAV-NAW	-2.82	116.33	118.80
2	C	201	KIW	CAR-CAN-NAO	-2.79	107.26	113.73
2	J	201	KIW	CAT-CAJ-CAS	-2.62	119.08	121.52
2	P	201	KIW	CAR-CAN-NAO	-2.61	107.69	113.73
2	S	201	KIW	CAJ-CAS-NAO	-2.56	116.04	120.74
2	O	201	KIW	CAR-CAN-NAO	-2.40	108.16	113.73
2	B	201	KIW	CAT-CAJ-CAS	-2.38	119.30	121.52
2	P	201	KIW	CAT-CAJ-CAS	-2.28	119.39	121.52
2	B	201	KIW	CAR-CAN-NAO	-2.26	108.48	113.73
2	H	201	KIW	CAK-CAS-NAO	-2.19	116.72	120.74
2	A	500	KIW	CAK-CAS-NAO	-2.15	116.80	120.74
2	U	201	KIW	CAK-CAS-NAO	-2.13	116.84	120.74
2	G	201	KIW	CAT-CAJ-CAS	-2.12	119.54	121.52
2	V	201	KIW	CAR-CAN-NAO	-2.12	108.83	113.73
2	P	201	KIW	CAK-CAS-NAO	-2.04	116.99	120.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	201	KIW	CAK-CAS-NAO	-2.03	117.02	120.74
2	A	500	KIW	CAJ-CAS-NAO	2.01	124.42	120.74
2	U	201	KIW	CAL-CAV-NAW	2.10	120.64	118.80
2	G	201	KIW	CAM-CAT-CAJ	2.19	121.65	118.29
2	T	201	KIW	CAL-CAV-NAW	2.40	120.91	118.80
2	O	201	KIW	CAL-CAV-NAW	2.76	121.22	118.80
2	C	201	KIW	CAI-CAV-NAW	2.86	121.79	119.48
2	X	201	KIW	CAL-CAV-NAW	2.90	121.35	118.80
2	H	201	KIW	CAI-CAV-NAW	2.91	121.83	119.48
2	R	201	KIW	CAI-CAV-NAW	3.13	122.01	119.48
2	P	201	KIW	CAL-CAV-NAW	4.07	122.37	118.80
2	K	201	KIW	CAI-CAV-NAW	5.23	123.70	119.48

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	201	KIW	CAL-CAV-NAW-OAF
2	E	201	KIW	CAI-CAV-NAW-OAF

There are no ring outliers.

17 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	KIW	1	0
2	C	201	KIW	2	0
2	D	201	KIW	1	0
2	G	201	KIW	1	0
2	H	201	KIW	1	0
2	J	201	KIW	1	0
2	L	201	KIW	1	0
2	M	201	KIW	3	0
2	O	201	KIW	1	0
2	Q	201	KIW	1	0
2	R	201	KIW	2	0
2	S	201	KIW	4	0
2	T	201	KIW	7	0
2	U	201	KIW	3	0
2	V	201	KIW	1	0
2	W	201	KIW	2	0
2	X	201	KIW	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	141/167 (84%)	-0.25	1 (0%) 89 87	17, 28, 54, 85	10 (7%)
1	B	141/167 (84%)	0.02	0 100 100	30, 40, 66, 80	8 (5%)
1	C	138/167 (82%)	-0.19	1 (0%) 89 87	18, 33, 58, 76	9 (6%)
1	D	137/167 (82%)	-0.16	0 100 100	19, 29, 60, 69	9 (6%)
1	E	136/167 (81%)	-0.15	0 100 100	19, 33, 59, 78	9 (6%)
1	F	136/167 (81%)	0.01	2 (1%) 76 73	27, 37, 62, 96	9 (6%)
1	G	141/167 (84%)	-0.20	1 (0%) 89 87	19, 32, 57, 92	1 (0%)
1	H	141/167 (84%)	-0.25	0 100 100	16, 25, 37, 61	9 (6%)
1	I	141/167 (84%)	-0.25	0 100 100	17, 27, 48, 66	9 (6%)
1	J	141/167 (84%)	-0.25	0 100 100	18, 26, 52, 66	9 (6%)
1	K	141/167 (84%)	-0.24	0 100 100	17, 26, 40, 65	9 (6%)
1	L	138/167 (82%)	-0.25	1 (0%) 89 87	16, 26, 59, 75	9 (6%)
1	M	141/167 (84%)	-0.17	0 100 100	25, 41, 65, 86	10 (7%)
1	N	141/167 (84%)	-0.18	0 100 100	26, 35, 48, 73	9 (6%)
1	O	141/167 (84%)	-0.26	0 100 100	21, 35, 58, 85	10 (7%)
1	P	141/167 (84%)	-0.13	1 (0%) 89 87	22, 33, 63, 104	9 (6%)
1	Q	136/167 (81%)	-0.24	0 100 100	29, 40, 62, 69	9 (6%)
1	R	138/167 (82%)	0.20	6 (4%) 39 33	25, 37, 60, 80	9 (6%)
1	S	141/167 (84%)	0.02	4 (2%) 56 52	28, 38, 71, 129	1 (0%)
1	T	140/167 (83%)	-0.05	2 (1%) 78 75	19, 34, 64, 81	9 (6%)
1	U	141/167 (84%)	-0.23	0 100 100	20, 31, 49, 78	9 (6%)
1	V	137/167 (82%)	0.21	2 (1%) 76 73	27, 38, 66, 78	9 (6%)
1	W	141/167 (84%)	-0.03	0 100 100	30, 41, 57, 79	9 (6%)
1	X	138/167 (82%)	-0.00	3 (2%) 65 61	28, 42, 68, 107	9 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	3348/4008 (83%)	-0.13	24 (0%)	89	87	16, 34, 61, 129	202 (6%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	21	PRO	5.9
1	X	25	GLY	4.0
1	X	26	GLY	3.8
1	X	24	TYR	3.2
1	R	40	ALA	3.0
1	P	19	ARG	2.8
1	F	26	GLY	2.8
1	S	22	ALA	2.7
1	T	23	VAL	2.7
1	V	143	HIS	2.6
1	F	19	ARG	2.6
1	R	62	ILE	2.5
1	S	19	ARG	2.5
1	R	41	ALA	2.5
1	S	23	VAL	2.4
1	G	21	PRO	2.4
1	A	19	ARG	2.3
1	R	45	LEU	2.2
1	T	35	LEU	2.2
1	C	24	TYR	2.1
1	L	24	TYR	2.1
1	R	3	LEU	2.0
1	V	141	ALA	2.0
1	R	4	ILE	2.0

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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	KIW	Q	201	23/23	0.94	0.21	2.82	41,52,86,89	0
2	KIW	C	201	23/23	0.91	0.20	2.47	47,58,72,76	0
2	KIW	E	201	23/23	0.94	0.22	2.35	40,49,67,70	0
2	KIW	V	201	23/23	0.95	0.22	2.17	39,43,59,62	0
2	KIW	U	201	23/23	0.97	0.23	2.12	29,38,66,68	0
2	KIW	B	201	23/23	0.95	0.19	1.58	46,52,67,69	0
2	KIW	O	201	23/23	0.95	0.18	1.56	31,39,69,76	0
2	KIW	A	500	23/23	0.96	0.17	1.40	28,35,49,52	0
2	KIW	W	201	23/23	0.95	0.18	1.37	32,39,66,68	0
2	KIW	S	201	23/23	0.92	0.23	1.04	55,66,87,94	0
2	KIW	T	201	23/23	0.92	0.23	0.98	32,38,74,79	0
2	KIW	X	201	23/23	0.93	0.20	0.93	50,60,66,71	0
2	KIW	H	201	23/23	0.97	0.15	0.82	22,29,39,40	0
2	KIW	R	201	23/23	0.96	0.18	0.73	37,44,61,66	0
2	KIW	D	201	23/23	0.96	0.16	0.62	33,38,59,64	0
2	KIW	L	201	23/23	0.96	0.18	0.60	35,44,72,79	0
2	KIW	N	201	23/23	0.95	0.16	0.54	35,38,42,47	0
2	KIW	P	201	23/23	0.95	0.17	0.51	40,47,77,83	0
2	KIW	M	201	23/23	0.96	0.16	0.48	40,49,65,73	0
2	KIW	K	201	23/23	0.97	0.15	0.47	21,28,33,34	0
2	KIW	J	201	23/23	0.97	0.15	0.23	32,35,43,45	0
2	KIW	G	201	23/23	0.95	0.15	-0.08	37,40,57,60	0

6.5 Other polymers

There are no such residues in this entry.