Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 11:51 PM EDT

PDB ID	:	6CV6
Title	:	Crystal structure of 3-dehydroquinate dehydratase, type II, from Burkholderia phymatum STM815
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2018-03-27
Resolution	:	2.60 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

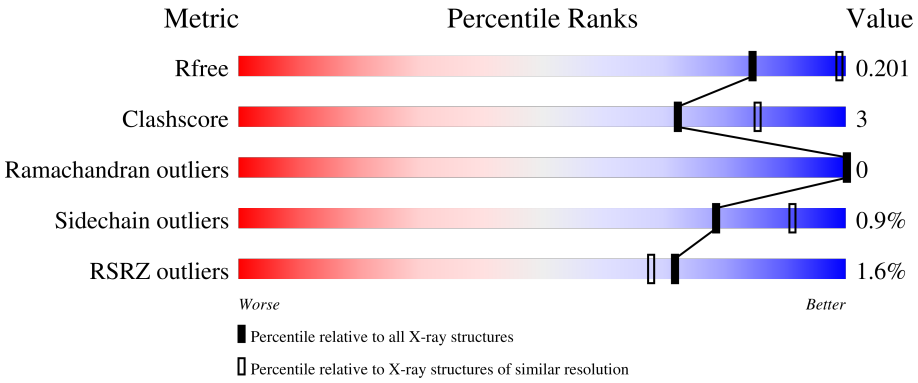
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	166	81% 6% • 13%
1	B	166	81% 6% 13%
1	C	166	% 83% • • 13%
1	D	166	80% 7% • 13%
1	E	166	% 83% 5% 13%

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Mol	Chain	Length	Quality of chain
1	F	166	80% 8% 13%
1	G	166	84% 13%
1	H	166	81% 6% 13%
1	I	166	84% 12%
1	J	166	78% 8% 13%
1	K	166	9% 81% 5% 13%
1	L	166	84% 13%

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	TLA	D	201	-	X	-	-
2	TLA	F	201	-	X	-	-
2	TLA	G	201	-	X	-	-
2	TLA	L	201	-	X	-	-
3	TAR	A	202	-	-	-	X
3	TAR	B	203	-	-	-	X
3	TAR	C	202	-	-	-	X
3	TAR	G	202	-	-	-	X
3	TAR	H	202	-	-	-	X
3	TAR	J	202	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14369 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	145	Total	C	N	O	S	0	0	0
			1125	707	202	206	10			
1	B	145	Total	C	N	O	S	0	0	0
			1127	708	202	207	10			
1	C	145	Total	C	N	O	S	0	0	0
			1127	708	202	207	10			
1	D	144	Total	C	N	O	S	0	0	0
			1113	699	199	205	10			
1	E	145	Total	C	N	O	S	0	0	0
			1113	700	197	206	10			
1	F	145	Total	C	N	O	S	0	0	0
			1125	707	202	206	10			
1	G	145	Total	C	N	O	S	0	0	0
			1125	707	202	206	10			
1	H	145	Total	C	N	O	S	0	0	0
			1121	704	201	206	10			
1	I	146	Total	C	N	O	S	0	0	0
			1120	703	201	206	10			
1	J	144	Total	C	N	O	S	0	0	0
			1097	689	194	204	10			
1	K	144	Total	C	N	O	S	0	0	0
			1077	675	192	200	10			
1	L	144	Total	C	N	O	S	0	0	0
			1101	692	195	204	10			

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	HIS	-	expression tag	UNP B2JVW0
A	-17	HIS	-	expression tag	UNP B2JVW0
A	-16	HIS	-	expression tag	UNP B2JVW0
A	-15	HIS	-	expression tag	UNP B2JVW0
A	-14	HIS	-	expression tag	UNP B2JVW0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	HIS	-	expression tag	UNP B2JVW0
A	-12	MET	-	expression tag	UNP B2JVW0
A	-11	GLY	-	expression tag	UNP B2JVW0
A	-10	THR	-	expression tag	UNP B2JVW0
A	-9	LEU	-	expression tag	UNP B2JVW0
A	-8	GLU	-	expression tag	UNP B2JVW0
A	-7	ALA	-	expression tag	UNP B2JVW0
A	-6	GLN	-	expression tag	UNP B2JVW0
A	-5	THR	-	expression tag	UNP B2JVW0
A	-4	GLN	-	expression tag	UNP B2JVW0
A	-3	GLY	-	expression tag	UNP B2JVW0
A	-2	PRO	-	expression tag	UNP B2JVW0
A	-1	GLY	-	expression tag	UNP B2JVW0
A	0	SER	-	expression tag	UNP B2JVW0
B	-18	HIS	-	expression tag	UNP B2JVW0
B	-17	HIS	-	expression tag	UNP B2JVW0
B	-16	HIS	-	expression tag	UNP B2JVW0
B	-15	HIS	-	expression tag	UNP B2JVW0
B	-14	HIS	-	expression tag	UNP B2JVW0
B	-13	HIS	-	expression tag	UNP B2JVW0
B	-12	MET	-	expression tag	UNP B2JVW0
B	-11	GLY	-	expression tag	UNP B2JVW0
B	-10	THR	-	expression tag	UNP B2JVW0
B	-9	LEU	-	expression tag	UNP B2JVW0
B	-8	GLU	-	expression tag	UNP B2JVW0
B	-7	ALA	-	expression tag	UNP B2JVW0
B	-6	GLN	-	expression tag	UNP B2JVW0
B	-5	THR	-	expression tag	UNP B2JVW0
B	-4	GLN	-	expression tag	UNP B2JVW0
B	-3	GLY	-	expression tag	UNP B2JVW0
B	-2	PRO	-	expression tag	UNP B2JVW0
B	-1	GLY	-	expression tag	UNP B2JVW0
B	0	SER	-	expression tag	UNP B2JVW0
C	-18	HIS	-	expression tag	UNP B2JVW0
C	-17	HIS	-	expression tag	UNP B2JVW0
C	-16	HIS	-	expression tag	UNP B2JVW0
C	-15	HIS	-	expression tag	UNP B2JVW0
C	-14	HIS	-	expression tag	UNP B2JVW0
C	-13	HIS	-	expression tag	UNP B2JVW0
C	-12	MET	-	expression tag	UNP B2JVW0
C	-11	GLY	-	expression tag	UNP B2JVW0
C	-10	THR	-	expression tag	UNP B2JVW0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	LEU	-	expression tag	UNP B2JVW0
C	-8	GLU	-	expression tag	UNP B2JVW0
C	-7	ALA	-	expression tag	UNP B2JVW0
C	-6	GLN	-	expression tag	UNP B2JVW0
C	-5	THR	-	expression tag	UNP B2JVW0
C	-4	GLN	-	expression tag	UNP B2JVW0
C	-3	GLY	-	expression tag	UNP B2JVW0
C	-2	PRO	-	expression tag	UNP B2JVW0
C	-1	GLY	-	expression tag	UNP B2JVW0
C	0	SER	-	expression tag	UNP B2JVW0
D	-18	HIS	-	expression tag	UNP B2JVW0
D	-17	HIS	-	expression tag	UNP B2JVW0
D	-16	HIS	-	expression tag	UNP B2JVW0
D	-15	HIS	-	expression tag	UNP B2JVW0
D	-14	HIS	-	expression tag	UNP B2JVW0
D	-13	HIS	-	expression tag	UNP B2JVW0
D	-12	MET	-	expression tag	UNP B2JVW0
D	-11	GLY	-	expression tag	UNP B2JVW0
D	-10	THR	-	expression tag	UNP B2JVW0
D	-9	LEU	-	expression tag	UNP B2JVW0
D	-8	GLU	-	expression tag	UNP B2JVW0
D	-7	ALA	-	expression tag	UNP B2JVW0
D	-6	GLN	-	expression tag	UNP B2JVW0
D	-5	THR	-	expression tag	UNP B2JVW0
D	-4	GLN	-	expression tag	UNP B2JVW0
D	-3	GLY	-	expression tag	UNP B2JVW0
D	-2	PRO	-	expression tag	UNP B2JVW0
D	-1	GLY	-	expression tag	UNP B2JVW0
D	0	SER	-	expression tag	UNP B2JVW0
E	-18	HIS	-	expression tag	UNP B2JVW0
E	-17	HIS	-	expression tag	UNP B2JVW0
E	-16	HIS	-	expression tag	UNP B2JVW0
E	-15	HIS	-	expression tag	UNP B2JVW0
E	-14	HIS	-	expression tag	UNP B2JVW0
E	-13	HIS	-	expression tag	UNP B2JVW0
E	-12	MET	-	expression tag	UNP B2JVW0
E	-11	GLY	-	expression tag	UNP B2JVW0
E	-10	THR	-	expression tag	UNP B2JVW0
E	-9	LEU	-	expression tag	UNP B2JVW0
E	-8	GLU	-	expression tag	UNP B2JVW0
E	-7	ALA	-	expression tag	UNP B2JVW0
E	-6	GLN	-	expression tag	UNP B2JVW0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	THR	-	expression tag	UNP B2JVW0
E	-4	GLN	-	expression tag	UNP B2JVW0
E	-3	GLY	-	expression tag	UNP B2JVW0
E	-2	PRO	-	expression tag	UNP B2JVW0
E	-1	GLY	-	expression tag	UNP B2JVW0
E	0	SER	-	expression tag	UNP B2JVW0
F	-18	HIS	-	expression tag	UNP B2JVW0
F	-17	HIS	-	expression tag	UNP B2JVW0
F	-16	HIS	-	expression tag	UNP B2JVW0
F	-15	HIS	-	expression tag	UNP B2JVW0
F	-14	HIS	-	expression tag	UNP B2JVW0
F	-13	HIS	-	expression tag	UNP B2JVW0
F	-12	MET	-	expression tag	UNP B2JVW0
F	-11	GLY	-	expression tag	UNP B2JVW0
F	-10	THR	-	expression tag	UNP B2JVW0
F	-9	LEU	-	expression tag	UNP B2JVW0
F	-8	GLU	-	expression tag	UNP B2JVW0
F	-7	ALA	-	expression tag	UNP B2JVW0
F	-6	GLN	-	expression tag	UNP B2JVW0
F	-5	THR	-	expression tag	UNP B2JVW0
F	-4	GLN	-	expression tag	UNP B2JVW0
F	-3	GLY	-	expression tag	UNP B2JVW0
F	-2	PRO	-	expression tag	UNP B2JVW0
F	-1	GLY	-	expression tag	UNP B2JVW0
F	0	SER	-	expression tag	UNP B2JVW0
G	-18	HIS	-	expression tag	UNP B2JVW0
G	-17	HIS	-	expression tag	UNP B2JVW0
G	-16	HIS	-	expression tag	UNP B2JVW0
G	-15	HIS	-	expression tag	UNP B2JVW0
G	-14	HIS	-	expression tag	UNP B2JVW0
G	-13	HIS	-	expression tag	UNP B2JVW0
G	-12	MET	-	expression tag	UNP B2JVW0
G	-11	GLY	-	expression tag	UNP B2JVW0
G	-10	THR	-	expression tag	UNP B2JVW0
G	-9	LEU	-	expression tag	UNP B2JVW0
G	-8	GLU	-	expression tag	UNP B2JVW0
G	-7	ALA	-	expression tag	UNP B2JVW0
G	-6	GLN	-	expression tag	UNP B2JVW0
G	-5	THR	-	expression tag	UNP B2JVW0
G	-4	GLN	-	expression tag	UNP B2JVW0
G	-3	GLY	-	expression tag	UNP B2JVW0
G	-2	PRO	-	expression tag	UNP B2JVW0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP B2JVW0
G	0	SER	-	expression tag	UNP B2JVW0
H	-18	HIS	-	expression tag	UNP B2JVW0
H	-17	HIS	-	expression tag	UNP B2JVW0
H	-16	HIS	-	expression tag	UNP B2JVW0
H	-15	HIS	-	expression tag	UNP B2JVW0
H	-14	HIS	-	expression tag	UNP B2JVW0
H	-13	HIS	-	expression tag	UNP B2JVW0
H	-12	MET	-	expression tag	UNP B2JVW0
H	-11	GLY	-	expression tag	UNP B2JVW0
H	-10	THR	-	expression tag	UNP B2JVW0
H	-9	LEU	-	expression tag	UNP B2JVW0
H	-8	GLU	-	expression tag	UNP B2JVW0
H	-7	ALA	-	expression tag	UNP B2JVW0
H	-6	GLN	-	expression tag	UNP B2JVW0
H	-5	THR	-	expression tag	UNP B2JVW0
H	-4	GLN	-	expression tag	UNP B2JVW0
H	-3	GLY	-	expression tag	UNP B2JVW0
H	-2	PRO	-	expression tag	UNP B2JVW0
H	-1	GLY	-	expression tag	UNP B2JVW0
H	0	SER	-	expression tag	UNP B2JVW0
I	-18	HIS	-	expression tag	UNP B2JVW0
I	-17	HIS	-	expression tag	UNP B2JVW0
I	-16	HIS	-	expression tag	UNP B2JVW0
I	-15	HIS	-	expression tag	UNP B2JVW0
I	-14	HIS	-	expression tag	UNP B2JVW0
I	-13	HIS	-	expression tag	UNP B2JVW0
I	-12	MET	-	expression tag	UNP B2JVW0
I	-11	GLY	-	expression tag	UNP B2JVW0
I	-10	THR	-	expression tag	UNP B2JVW0
I	-9	LEU	-	expression tag	UNP B2JVW0
I	-8	GLU	-	expression tag	UNP B2JVW0
I	-7	ALA	-	expression tag	UNP B2JVW0
I	-6	GLN	-	expression tag	UNP B2JVW0
I	-5	THR	-	expression tag	UNP B2JVW0
I	-4	GLN	-	expression tag	UNP B2JVW0
I	-3	GLY	-	expression tag	UNP B2JVW0
I	-2	PRO	-	expression tag	UNP B2JVW0
I	-1	GLY	-	expression tag	UNP B2JVW0
I	0	SER	-	expression tag	UNP B2JVW0
J	-18	HIS	-	expression tag	UNP B2JVW0
J	-17	HIS	-	expression tag	UNP B2JVW0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-16	HIS	-	expression tag	UNP B2JVW0
J	-15	HIS	-	expression tag	UNP B2JVW0
J	-14	HIS	-	expression tag	UNP B2JVW0
J	-13	HIS	-	expression tag	UNP B2JVW0
J	-12	MET	-	expression tag	UNP B2JVW0
J	-11	GLY	-	expression tag	UNP B2JVW0
J	-10	THR	-	expression tag	UNP B2JVW0
J	-9	LEU	-	expression tag	UNP B2JVW0
J	-8	GLU	-	expression tag	UNP B2JVW0
J	-7	ALA	-	expression tag	UNP B2JVW0
J	-6	GLN	-	expression tag	UNP B2JVW0
J	-5	THR	-	expression tag	UNP B2JVW0
J	-4	GLN	-	expression tag	UNP B2JVW0
J	-3	GLY	-	expression tag	UNP B2JVW0
J	-2	PRO	-	expression tag	UNP B2JVW0
J	-1	GLY	-	expression tag	UNP B2JVW0
J	0	SER	-	expression tag	UNP B2JVW0
K	-18	HIS	-	expression tag	UNP B2JVW0
K	-17	HIS	-	expression tag	UNP B2JVW0
K	-16	HIS	-	expression tag	UNP B2JVW0
K	-15	HIS	-	expression tag	UNP B2JVW0
K	-14	HIS	-	expression tag	UNP B2JVW0
K	-13	HIS	-	expression tag	UNP B2JVW0
K	-12	MET	-	expression tag	UNP B2JVW0
K	-11	GLY	-	expression tag	UNP B2JVW0
K	-10	THR	-	expression tag	UNP B2JVW0
K	-9	LEU	-	expression tag	UNP B2JVW0
K	-8	GLU	-	expression tag	UNP B2JVW0
K	-7	ALA	-	expression tag	UNP B2JVW0
K	-6	GLN	-	expression tag	UNP B2JVW0
K	-5	THR	-	expression tag	UNP B2JVW0
K	-4	GLN	-	expression tag	UNP B2JVW0
K	-3	GLY	-	expression tag	UNP B2JVW0
K	-2	PRO	-	expression tag	UNP B2JVW0
K	-1	GLY	-	expression tag	UNP B2JVW0
K	0	SER	-	expression tag	UNP B2JVW0
L	-18	HIS	-	expression tag	UNP B2JVW0
L	-17	HIS	-	expression tag	UNP B2JVW0
L	-16	HIS	-	expression tag	UNP B2JVW0
L	-15	HIS	-	expression tag	UNP B2JVW0
L	-14	HIS	-	expression tag	UNP B2JVW0
L	-13	HIS	-	expression tag	UNP B2JVW0

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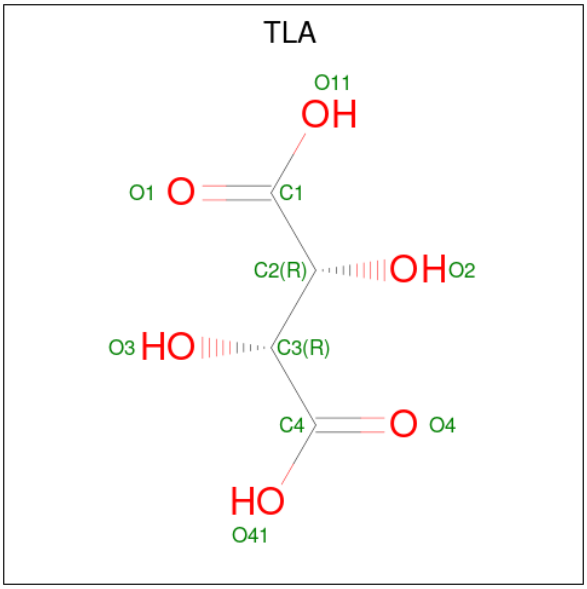
Chain	Residue	Modelled	Actual	Comment	Reference
L	-12	MET	-	expression tag	UNP B2JVW0
L	-11	GLY	-	expression tag	UNP B2JVW0
L	-10	THR	-	expression tag	UNP B2JVW0
L	-9	LEU	-	expression tag	UNP B2JVW0
L	-8	GLU	-	expression tag	UNP B2JVW0
L	-7	ALA	-	expression tag	UNP B2JVW0
L	-6	GLN	-	expression tag	UNP B2JVW0
L	-5	THR	-	expression tag	UNP B2JVW0
L	-4	GLN	-	expression tag	UNP B2JVW0
L	-3	GLY	-	expression tag	UNP B2JVW0
L	-2	PRO	-	expression tag	UNP B2JVW0
L	-1	GLY	-	expression tag	UNP B2JVW0
L	0	SER	-	expression tag	UNP B2JVW0

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 4 6	0	0
2	A	1	Total C O 10 4 6	0	0
2	B	1	Total C O 10 4 6	0	0
2	B	1	Total C O 10 4 6	0	0
2	C	1	Total C O 10 4 6	0	0

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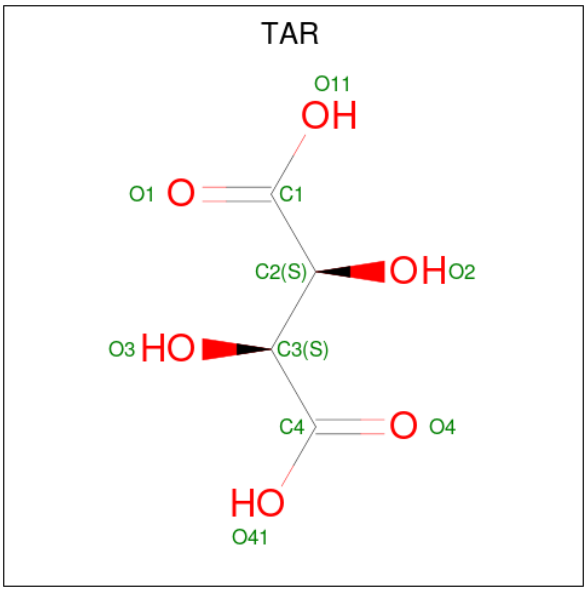
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 10 4 6	0	0
2	D	1	Total C O 10 4 6	0	0
2	D	1	Total C O 10 4 6	0	0
2	E	1	Total C O 10 4 6	0	0
2	E	1	Total C O 10 4 6	0	0
2	F	1	Total C O 10 4 6	0	0
2	F	1	Total C O 10 4 6	0	0
2	G	1	Total C O 10 4 6	0	0
2	G	1	Total C O 10 4 6	0	0
2	H	1	Total C O 10 4 6	0	0
2	H	1	Total C O 10 4 6	0	0
2	I	1	Total C O 10 4 6	0	0
2	I	1	Total C O 10 4 6	0	0
2	J	1	Total C O 10 4 6	0	0
2	J	1	Total C O 10 4 6	0	0
2	K	1	Total C O 10 4 6	0	0
2	K	1	Total C O 10 4 6	0	0
2	L	1	Total C O 10 4 6	0	0
2	L	1	Total C O 10 4 6	0	0

- Molecule 3 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 4 6	0	0
3	B	1	Total C O 10 4 6	0	0
3	C	1	Total C O 10 4 6	0	0
3	D	1	Total C O 10 4 6	0	0
3	E	1	Total C O 10 4 6	0	0
3	F	1	Total C O 10 4 6	0	0
3	G	1	Total C O 10 4 6	0	0
3	H	1	Total C O 10 4 6	0	0
3	I	1	Total C O 10 4 6	0	0
3	J	1	Total C O 10 4 6	0	0
3	K	1	Total C O 10 4 6	0	0
3	L	1	Total C O 10 4 6	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0

- Molecule 5 is water.

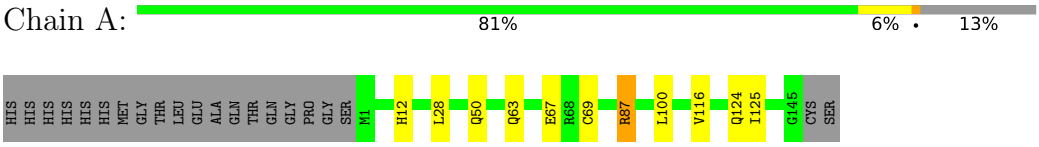
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	77	Total O 77 77	0	0
5	B	94	Total O 94 94	0	0
5	C	86	Total O 86 86	0	0
5	D	84	Total O 86 86	0	2
5	E	65	Total O 66 66	0	1
5	F	70	Total O 70 70	0	0
5	G	59	Total O 59 59	0	0
5	H	42	Total O 42 42	0	0
5	I	30	Total O 30 30	0	0
5	J	10	Total O 10 10	0	0
5	K	6	Total O 6 6	0	0
5	L	11	Total O 11 11	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.

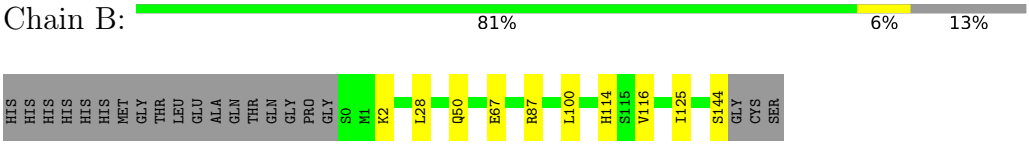
• Molecule 1: 3-dehydroquinate dehydratase

Chain A:



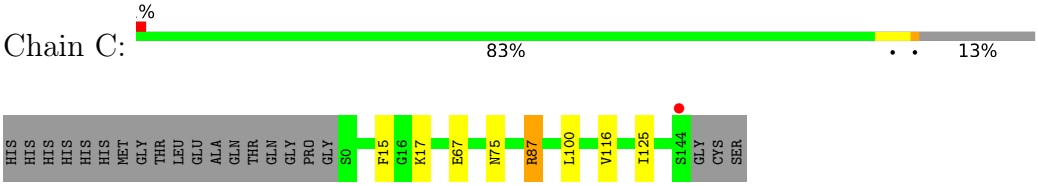
• Molecule 1: 3-dehydroquinate dehydratase

Chain B:



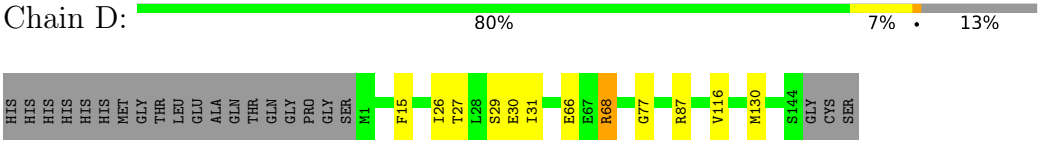
• Molecule 1: 3-dehydroquinate dehydratase

Chain C:



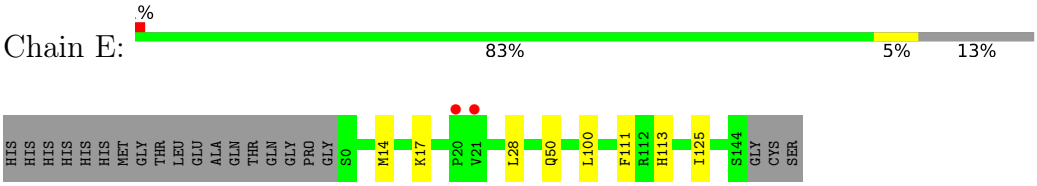
• Molecule 1: 3-dehydroquinate dehydratase

Chain D:



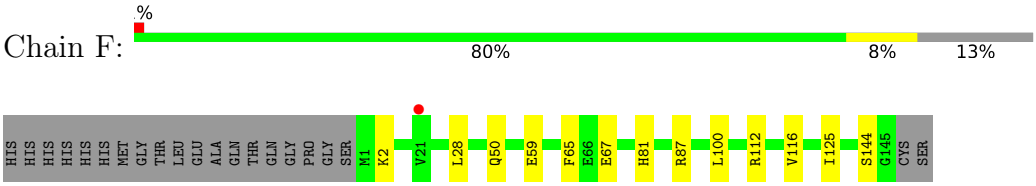
• Molecule 1: 3-dehydroquinate dehydratase

Chain E:



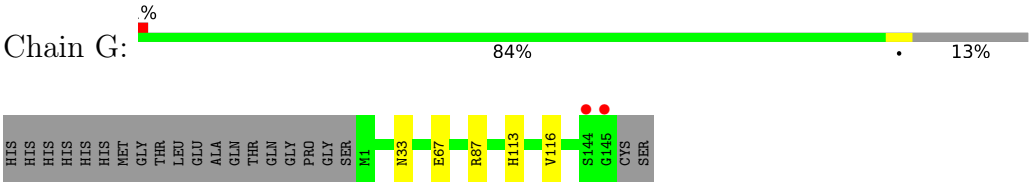
• Molecule 1: 3-dehydroquinate dehydratase

Chain F:



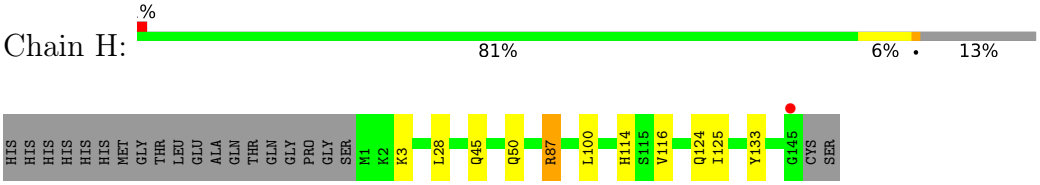
• Molecule 1: 3-dehydroquinate dehydratase

Chain G:



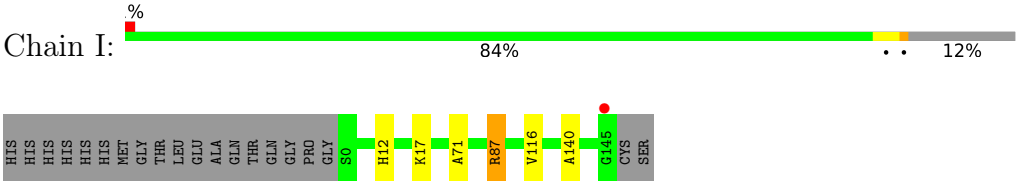
• Molecule 1: 3-dehydroquinate dehydratase

Chain H:



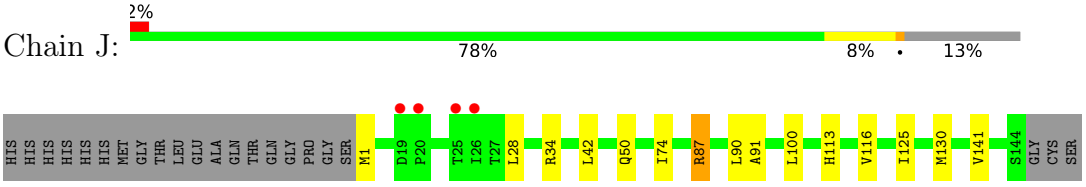
• Molecule 1: 3-dehydroquinate dehydratase

Chain I:



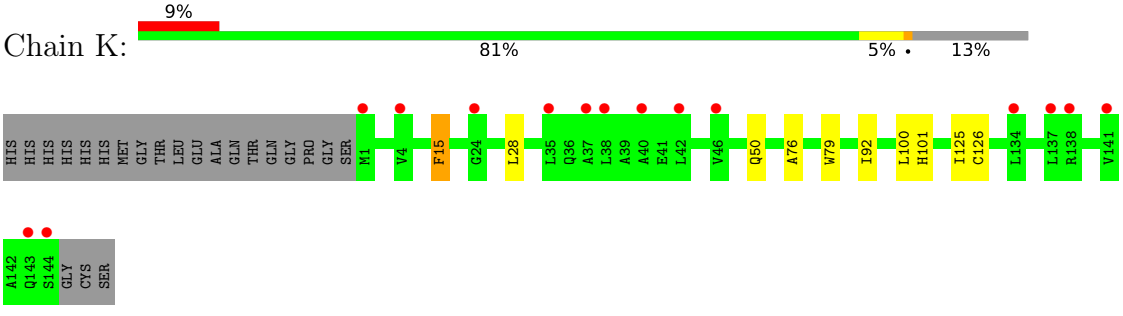
• Molecule 1: 3-dehydroquinate dehydratase

Chain J:



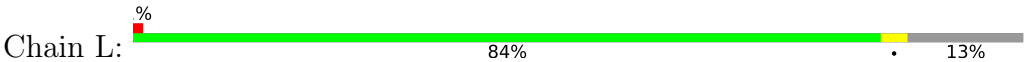
• Molecule 1: 3-dehydroquinate dehydratase

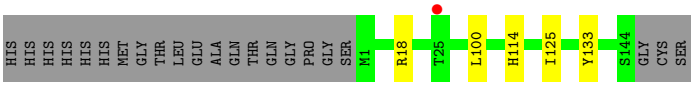
Chain K:



• Molecule 1: 3-dehydroquinate dehydratase

Chain L:




HIS
HIS
HIS
HIS
HIS
MET
GLY
THR
LEU
GLU
ALA
GLN
THR
GLN
GLY
PRO
GLY
SER
M1
R18
T25
L100
H114
I125
Y133
S144
GLY
CYS
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	152.39Å 152.39Å 177.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.52 – 2.60 48.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.52-2.60) 99.8 (48.85-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 2.61Å)	Xtriage
Refinement program	PHENIX (dev_3063)	Depositor
R, R_{free}	0.156 , 0.201 0.156 , 0.201	Depositor DCC
R_{free} test set	2071 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14369	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: CL, TLA, TAR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.30	0/1147	0.48	0/1550
1	B	0.29	0/1149	0.48	0/1553
1	C	0.30	0/1149	0.50	0/1553
1	D	0.29	0/1135	0.51	0/1537
1	E	0.28	0/1135	0.49	0/1537
1	F	0.28	0/1147	0.47	0/1550
1	G	0.29	0/1147	0.48	0/1550
1	H	0.28	0/1143	0.48	0/1546
1	I	0.27	0/1142	0.46	0/1545
1	J	0.26	0/1119	0.44	0/1518
1	K	0.25	0/1098	0.41	0/1490
1	L	0.25	0/1123	0.44	0/1522
All	All	0.28	0/13634	0.47	0/18451

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1125	0	1106	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1127	0	1108	6	0
1	C	1127	0	1108	7	0
1	D	1113	0	1081	9	0
1	E	1113	0	1080	5	0
1	F	1125	0	1106	9	0
1	G	1125	0	1106	3	0
1	H	1121	0	1095	8	0
1	I	1120	0	1084	4	0
1	J	1097	0	1046	8	0
1	K	1077	0	1013	6	0
1	L	1101	0	1057	4	0
2	A	20	0	8	3	0
2	B	20	0	8	4	0
2	C	20	0	8	1	0
2	D	20	0	8	1	0
2	E	20	0	8	2	0
2	F	20	0	8	1	0
2	G	20	0	8	1	0
2	H	20	0	8	1	0
2	I	20	0	8	1	0
2	J	20	0	8	1	0
2	K	20	0	8	0	0
2	L	20	0	8	0	0
3	A	10	0	4	0	0
3	B	10	0	4	1	0
3	C	10	0	4	0	0
3	D	10	0	4	1	0
3	E	10	0	4	2	0
3	F	10	0	4	2	0
3	G	10	0	4	3	0
3	H	10	0	4	2	0
3	I	10	0	4	1	0
3	J	10	0	4	3	0
3	K	10	0	4	0	0
3	L	10	0	4	1	0
4	B	1	0	0	0	0
5	A	77	0	0	1	0
5	B	94	0	0	3	0
5	C	86	0	0	2	0
5	D	86	0	0	1	0
5	E	66	0	0	2	0
5	F	70	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	59	0	0	3	0
5	H	42	0	0	1	0
5	I	30	0	0	1	0
5	J	10	0	0	2	0
5	K	6	0	0	0	0
5	L	11	0	0	0	0
All	All	14369	0	13134	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (91) 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)
2:B:202:TLA:O41	5:B:301:HOH:O	2.01	0.78
2:E:201:TLA:O41	5:E:301:HOH:O	2.01	0.77
2:G:201:TLA:O2	5:G:301:HOH:O	2.02	0.77
1:C:67:GLU:OE1	5:C:301:HOH:O	2.10	0.70
2:E:201:TLA:O2	5:E:302:HOH:O	2.10	0.70
1:G:67:GLU:OE1	5:G:302:HOH:O	2.15	0.65
1:J:91:ALA:O	5:J:301:HOH:O	2.13	0.65
1:B:114:HIS:NE2	2:B:201:TLA:O11	2.25	0.64
2:F:201:TLA:O2	5:F:301:HOH:O	2.16	0.61
1:H:3:LYS:HG2	1:H:45:GLN:HE21	1.65	0.61
2:A:201:TLA:O4	5:A:301:HOH:O	2.17	0.59
1:I:12:HIS:NE2	2:I:201:TLA:O3	2.37	0.58
1:D:26:ILE:HG13	1:D:30:GLU:OE2	2.03	0.58
3:J:202:TAR:O4	3:J:202:TAR:O2	2.19	0.55
1:C:17:LYS:HD3	1:F:65:PHE:HE2	1.72	0.54
1:J:34:ARG:HG3	1:J:130:MET:HE3	1.90	0.54
1:D:31:ILE:HA	1:D:130:MET:HE1	1.90	0.54
2:B:202:TLA:O2	5:B:302:HOH:O	2.18	0.53
1:H:114:HIS:NE2	2:H:200:TLA:O1	2.34	0.53
1:D:77:GLY:HA2	2:D:201:TLA:H2	1.90	0.53
3:F:202:TAR:O2	3:F:202:TAR:O4	2.27	0.52
1:A:87:ARG:HG3	1:A:116:VAL:O	2.09	0.52
1:A:67:GLU:HB2	1:D:68:ARG:HD3	1.93	0.51
1:A:63:GLN:NE2	1:D:66:GLU:HB3	2.27	0.50
3:J:202:TAR:O11	3:J:202:TAR:O3	2.23	0.50
1:A:12:HIS:HE2	2:A:201:TLA:HB	1.57	0.50
1:F:28:LEU:HD21	1:F:50:GLN:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:28:LEU:HD21	1:H:50:GLN:HG3	1.94	0.49
1:E:113:HIS:O	3:E:202:TAR:O2	2.30	0.49
1:F:2:LYS:HE2	1:F:144:SER:HB3	1.93	0.49
1:F:67:GLU:OE1	5:F:302:HOH:O	2.20	0.49
1:A:100:LEU:HA	1:A:125:ILE:O	2.13	0.49
3:H:202:TAR:O1	3:H:202:TAR:O3	2.25	0.49
2:J:201:TLA:O2	5:J:302:HOH:O	2.20	0.49
1:J:28:LEU:HD21	1:J:50:GLN:HG3	1.94	0.48
1:L:114:HIS:ND1	3:L:202:TAR:O1	2.44	0.48
3:G:202:TAR:O2	3:G:202:TAR:O4	2.31	0.48
1:E:14:MET:HA	1:E:17:LYS:HD2	1.95	0.48
1:K:76:ALA:HB1	1:K:79:TRP:HB2	1.95	0.48
1:H:124:GLN:NE2	5:H:306:HOH:O	2.46	0.47
1:B:67:GLU:OE1	5:B:303:HOH:O	2.20	0.47
1:J:113:HIS:O	3:J:202:TAR:O2	2.32	0.47
1:C:87:ARG:HG3	1:C:116:VAL:O	2.15	0.47
1:J:87:ARG:HG3	1:J:116:VAL:O	2.15	0.46
1:G:113:HIS:O	3:G:202:TAR:O2	2.32	0.46
3:I:202:TAR:O11	3:I:202:TAR:O3	2.26	0.46
1:F:100:LEU:HA	1:F:125:ILE:O	2.15	0.46
3:B:203:TAR:O2	3:B:203:TAR:O41	2.34	0.46
1:D:27:THR:OG1	1:D:30:GLU:HG3	2.16	0.46
1:J:100:LEU:HA	1:J:125:ILE:O	2.16	0.45
1:E:28:LEU:HD21	1:E:50:GLN:HG3	1.98	0.45
1:H:100:LEU:HD11	1:H:133:TYR:CE1	2.52	0.45
1:B:28:LEU:HD21	1:B:50:GLN:HG3	1.99	0.44
1:A:12:HIS:NE2	2:A:201:TLA:O3	2.44	0.44
1:B:100:LEU:HA	1:B:125:ILE:O	2.18	0.44
1:K:100:LEU:HA	1:K:125:ILE:O	2.17	0.44
1:H:100:LEU:HA	1:H:125:ILE:O	2.18	0.44
1:B:87:ARG:HG3	1:B:116:VAL:O	2.18	0.44
1:J:42:LEU:HD13	1:J:141:VAL:HG21	1.99	0.43
1:H:87:ARG:HG3	1:H:116:VAL:O	2.19	0.43
1:I:17:LYS:NZ	5:I:307:HOH:O	2.50	0.43
1:L:100:LEU:HA	1:L:125:ILE:O	2.19	0.43
1:I:87:ARG:HG3	1:I:116:VAL:O	2.19	0.43
1:B:2:LYS:HE2	1:B:144:SER:HB3	2.00	0.42
1:D:30:GLU:HB3	5:D:353:HOH:O	2.19	0.42
3:D:202:TAR:O2	3:D:202:TAR:O4	2.35	0.42
1:I:71:ALA:HB1	1:I:140:ALA:HB1	2.01	0.42
2:B:201:TLA:H3	1:E:111:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ASN:OD1	2:C:201:TLA:O2	2.38	0.42
5:C:369:HOH:O	1:F:59:GLU:HG2	2.19	0.42
1:A:28:LEU:HD21	1:A:50:GLN:HG3	2.02	0.42
1:E:100:LEU:HA	1:E:125:ILE:O	2.19	0.42
1:C:17:LYS:HD3	1:F:65:PHE:CE2	2.54	0.41
3:E:202:TAR:O2	3:E:202:TAR:O4	2.33	0.41
1:F:81:HIS:CE1	1:F:112:ARG:HA	2.55	0.41
1:K:28:LEU:HD21	1:K:50:GLN:HG3	2.03	0.41
1:K:92:ILE:HG23	1:L:18:ARG:HG2	2.02	0.41
1:K:101:HIS:O	1:K:126:CYS:HA	2.21	0.41
1:C:100:LEU:HA	1:C:125:ILE:O	2.21	0.41
1:L:100:LEU:HD11	1:L:133:TYR:CE1	2.56	0.41
1:F:87:ARG:HG3	1:F:116:VAL:O	2.21	0.41
1:D:31:ILE:HA	1:D:130:MET:CE	2.50	0.41
3:F:202:TAR:O11	3:F:202:TAR:O3	2.30	0.40
3:G:202:TAR:O11	5:G:303:HOH:O	2.22	0.40
3:H:202:TAR:O4	3:H:202:TAR:O2	2.25	0.40
1:J:74:ILE:HD13	1:J:90:LEU:HD11	2.03	0.40
1:D:87:ARG:HG3	1:D:116:VAL:O	2.22	0.40
1:K:15:PHE:HD1	1:K:15:PHE:HA	1.76	0.40
1:C:15:PHE:HD1	1:C:15:PHE:HA	1.76	0.40
1:H:28:LEU:HD12	1:H:28:LEU:HA	1.97	0.40
1:G:87:ARG:HG3	1:G:116:VAL:O	2.21	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	143/166 (86%)	140 (98%)	3 (2%)	0	100	100
1	B	143/166 (86%)	140 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	143/166 (86%)	140 (98%)	3 (2%)	0	100	100
1	D	142/166 (86%)	139 (98%)	3 (2%)	0	100	100
1	E	143/166 (86%)	140 (98%)	3 (2%)	0	100	100
1	F	143/166 (86%)	140 (98%)	3 (2%)	0	100	100
1	G	143/166 (86%)	140 (98%)	3 (2%)	0	100	100
1	H	143/166 (86%)	140 (98%)	3 (2%)	0	100	100
1	I	144/166 (87%)	141 (98%)	3 (2%)	0	100	100
1	J	142/166 (86%)	139 (98%)	3 (2%)	0	100	100
1	K	142/166 (86%)	136 (96%)	6 (4%)	0	100	100
1	L	142/166 (86%)	139 (98%)	3 (2%)	0	100	100
All	All	1713/1992 (86%)	1674 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	119/136 (88%)	116 (98%)	3 (2%)	47	73
1	B	120/136 (88%)	120 (100%)	0	100	100
1	C	120/136 (88%)	119 (99%)	1 (1%)	81	92
1	D	117/136 (86%)	114 (97%)	3 (3%)	46	72
1	E	117/136 (86%)	117 (100%)	0	100	100
1	F	119/136 (88%)	119 (100%)	0	100	100
1	G	119/136 (88%)	118 (99%)	1 (1%)	81	92
1	H	118/136 (87%)	117 (99%)	1 (1%)	81	92
1	I	116/136 (85%)	115 (99%)	1 (1%)	78	91
1	J	113/136 (83%)	111 (98%)	2 (2%)	59	80
1	K	108/136 (79%)	107 (99%)	1 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	114/136 (84%)	114 (100%)	0	100 100
All	All	1400/1632 (86%)	1387 (99%)	13 (1%)	78 91

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	CYS
1	A	87	ARG
1	A	124	GLN
1	C	87	ARG
1	D	15	PHE
1	D	29	SER
1	D	68	ARG
1	G	33	ASN
1	H	87	ARG
1	I	87	ARG
1	J	1	MET
1	J	87	ARG
1	K	15	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	45	GLN
1	L	22	GLN
1	L	33	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TLA	A	201	-	9,9,9	1.07	0	12,12,12	1.89	4 (33%)
2	TLA	K	201	-	9,9,9	1.08	0	12,12,12	1.48	2 (16%)
2	TLA	E	200	-	9,9,9	1.08	0	12,12,12	1.21	2 (16%)
2	TLA	G	200	-	9,9,9	1.21	0	12,12,12	0.99	1 (8%)
2	TLA	H	201	-	9,9,9	1.08	0	12,12,12	1.53	3 (25%)
2	TLA	C	201	-	9,9,9	1.09	0	12,12,12	2.13	4 (33%)
3	TAR	H	202	3	9,9,9	1.21	0	12,12,12	0.98	0
3	TAR	D	202	-	9,9,9	1.21	0	12,12,12	0.99	0
2	TLA	I	200	-	9,9,9	1.21	0	12,12,12	1.08	1 (8%)
2	TLA	L	200	-	9,9,9	1.14	0	12,12,12	1.07	1 (8%)
2	TLA	F	200	-	9,9,9	1.26	0	12,12,12	0.89	0
3	TAR	A	202	3	9,9,9	1.21	0	12,12,12	1.01	0
2	TLA	D	200	-	9,9,9	1.14	0	12,12,12	1.13	2 (16%)
2	TLA	F	201	-	9,9,9	1.02	0	12,12,12	1.69	3 (25%)
3	TAR	I	202	3	9,9,9	1.20	0	12,12,12	0.94	0
3	TAR	C	202	3	9,9,9	1.20	0	12,12,12	0.99	0
2	TLA	E	201	-	9,9,9	1.09	0	12,12,12	1.51	2 (16%)
2	TLA	G	201	-	9,9,9	1.08	0	12,12,12	1.80	4 (33%)
2	TLA	J	200	-	9,9,9	1.19	0	12,12,12	1.12	1 (8%)
3	TAR	L	202	3	9,9,9	1.19	0	12,12,12	1.06	2 (16%)
2	TLA	H	200	-	9,9,9	1.14	0	12,12,12	1.08	1 (8%)
3	TAR	B	203	-	9,9,9	1.22	0	12,12,12	0.98	0
3	TAR	J	202	3	9,9,9	1.20	0	12,12,12	0.95	0
2	TLA	I	201	-	9,9,9	1.10	0	12,12,12	1.25	2 (16%)
2	TLA	A	200	-	9,9,9	1.13	0	12,12,12	1.19	1 (8%)
2	TLA	B	201	-	9,9,9	1.21	0	12,12,12	0.95	1 (8%)
3	TAR	F	202	3	9,9,9	1.21	0	12,12,12	0.98	0
2	TLA	K	200	-	9,9,9	1.19	0	12,12,12	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	TLA	B	202	-	9,9,9	1.08	0	12,12,12	1.42	3 (25%)
2	TLA	L	201	-	9,9,9	1.11	0	12,12,12	1.55	4 (33%)
2	TLA	C	200	-	9,9,9	1.10	0	12,12,12	1.22	1 (8%)
2	TLA	D	201	-	9,9,9	1.07	0	12,12,12	2.52	5 (41%)
3	TAR	E	202	3	9,9,9	1.23	0	12,12,12	0.95	0
3	TAR	G	202	-	9,9,9	1.22	0	12,12,12	0.95	0
3	TAR	K	202	-	9,9,9	1.20	0	12,12,12	1.02	2 (16%)
2	TLA	J	201	-	9,9,9	1.19	0	12,12,12	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TLA	A	201	-	-	6/12/12/12	-
2	TLA	K	201	-	-	6/12/12/12	-
2	TLA	E	200	-	-	8/12/12/12	-
2	TLA	G	200	-	-	8/12/12/12	-
2	TLA	H	201	-	-	10/12/12/12	-
2	TLA	C	201	-	-	8/12/12/12	-
3	TAR	H	202	3	-	8/12/12/12	-
3	TAR	D	202	-	-	8/12/12/12	-
2	TLA	I	200	-	-	7/12/12/12	-
2	TLA	L	200	-	-	8/12/12/12	-
2	TLA	F	200	-	-	8/12/12/12	-
3	TAR	A	202	3	-	8/12/12/12	-
2	TLA	D	200	-	-	8/12/12/12	-
2	TLA	F	201	-	-	11/12/12/12	-
3	TAR	I	202	3	-	8/12/12/12	-
3	TAR	C	202	3	-	8/12/12/12	-
2	TLA	E	201	-	-	11/12/12/12	-
2	TLA	G	201	-	-	10/12/12/12	-
2	TLA	J	200	-	-	8/12/12/12	-
3	TAR	L	202	3	-	8/12/12/12	-
2	TLA	H	200	-	-	4/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TAR	B	203	-	-	8/12/12/12	-
3	TAR	J	202	3	-	10/12/12/12	-
2	TLA	I	201	-	-	8/12/12/12	-
2	TLA	A	200	-	-	8/12/12/12	-
2	TLA	B	201	-	-	0/12/12/12	-
3	TAR	F	202	3	-	8/12/12/12	-
2	TLA	K	200	-	-	8/12/12/12	-
2	TLA	B	202	-	-	8/12/12/12	-
2	TLA	L	201	-	-	10/12/12/12	-
2	TLA	C	200	-	-	7/12/12/12	-
2	TLA	D	201	-	-	12/12/12/12	-
3	TAR	E	202	3	-	6/12/12/12	-
3	TAR	G	202	-	-	8/12/12/12	-
3	TAR	K	202	-	-	8/12/12/12	-
2	TLA	J	201	-	-	10/12/12/12	-

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	201	TLA	C2-C3-C4	5.73	122.66	109.87
2	C	201	TLA	C3-C2-C1	4.99	121.02	109.87
2	A	201	TLA	C2-C3-C4	3.60	117.92	109.87
2	D	201	TLA	C3-C2-C1	3.52	117.74	109.87
2	C	201	TLA	C2-C3-C4	3.44	117.56	109.87
2	E	201	TLA	C2-C3-C4	3.30	117.24	109.87
2	G	201	TLA	C3-C2-C1	3.28	117.19	109.87
2	F	201	TLA	C2-C3-C4	3.26	117.15	109.87
2	A	201	TLA	O41-C4-C3	3.17	121.84	113.27
2	G	201	TLA	C2-C3-C4	3.15	116.90	109.87
2	F	201	TLA	C3-C2-C1	2.96	116.49	109.87
2	E	201	TLA	C3-C2-C1	2.88	116.31	109.87
2	B	202	TLA	C2-C3-C4	2.84	116.22	109.87
2	A	201	TLA	C3-C2-C1	2.83	116.20	109.87
2	I	201	TLA	C2-C3-C4	2.82	116.18	109.87
2	C	200	TLA	O11-C1-C2	2.73	120.66	113.27
2	K	201	TLA	C3-C2-C1	2.70	115.89	109.87
2	H	201	TLA	C2-C3-C4	2.69	115.89	109.87
2	D	201	TLA	O3-C3-C2	-2.65	104.97	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	201	TLA	O11-C1-C2	2.64	120.41	113.27
2	D	201	TLA	O11-C1-C2	2.61	120.32	113.27
2	L	201	TLA	C2-C3-C4	2.59	115.67	109.87
2	F	201	TLA	O11-C1-C2	2.53	120.11	113.27
2	L	201	TLA	C3-C2-C1	2.50	115.45	109.87
2	D	201	TLA	O41-C4-C3	2.47	119.94	113.27
2	B	202	TLA	O11-C1-C2	2.41	119.80	113.27
2	J	200	TLA	O11-C1-C2	2.40	119.75	113.27
2	C	201	TLA	O11-C1-C2	2.39	119.73	113.27
2	G	201	TLA	O41-C4-C3	2.38	119.71	113.27
2	H	201	TLA	O11-C1-C2	2.38	119.71	113.27
2	E	200	TLA	O11-C1-C2	2.34	119.61	113.27
2	L	200	TLA	O11-C1-C2	2.29	119.47	113.27
2	H	201	TLA	C3-C2-C1	2.28	114.97	109.87
2	G	201	TLA	O11-C1-C2	2.28	119.43	113.27
2	L	201	TLA	O11-C1-C2	2.26	119.39	113.27
2	B	202	TLA	C3-C2-C1	2.26	114.93	109.87
2	H	200	TLA	O11-C1-C2	2.25	119.35	113.27
2	D	200	TLA	O11-C1-C2	2.23	119.29	113.27
2	L	201	TLA	O41-C4-C3	2.18	119.16	113.27
2	G	200	TLA	O11-C1-C2	2.12	119.00	113.27
2	E	200	TLA	O41-C4-C3	2.10	118.94	113.27
2	C	201	TLA	O2-C2-C3	-2.09	106.07	110.23
2	A	201	TLA	O4-C4-C3	-2.09	116.15	121.63
3	L	202	TAR	O41-C4-C3	2.08	118.89	113.27
3	L	202	TAR	O11-C1-C2	2.06	118.85	113.27
2	I	201	TLA	C3-C2-C1	2.06	114.46	109.87
2	I	200	TLA	O11-C1-C2	2.04	118.79	113.27
2	D	200	TLA	O41-C4-C3	2.03	118.77	113.27
2	A	200	TLA	O41-C4-C3	2.03	118.77	113.27
3	K	202	TAR	O11-C1-C2	2.02	118.72	113.27
2	B	201	TLA	O41-C4-C3	2.01	118.71	113.27
3	K	202	TAR	O41-C4-C3	2.01	118.70	113.27

There are no chirality outliers.

All (288) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	200	TLA	C1-C2-C3-O3
2	A	200	TLA	C1-C2-C3-C4
2	A	200	TLA	O2-C2-C3-O3
2	A	200	TLA	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	A	201	TLA	C1-C2-C3-O3
2	A	201	TLA	C1-C2-C3-C4
2	A	201	TLA	O2-C2-C3-O3
2	A	201	TLA	O2-C2-C3-C4
2	A	201	TLA	O3-C3-C4-O4
2	A	201	TLA	O3-C3-C4-O41
2	B	202	TLA	C1-C2-C3-O3
2	B	202	TLA	C1-C2-C3-C4
2	B	202	TLA	O2-C2-C3-C4
2	C	200	TLA	C1-C2-C3-O3
2	C	200	TLA	C1-C2-C3-C4
2	C	200	TLA	O2-C2-C3-O3
2	C	200	TLA	O2-C2-C3-C4
2	C	201	TLA	C1-C2-C3-C4
2	C	201	TLA	O2-C2-C3-O3
2	C	201	TLA	C2-C3-C4-O41
2	D	200	TLA	C1-C2-C3-O3
2	D	200	TLA	C1-C2-C3-C4
2	D	200	TLA	O2-C2-C3-O3
2	D	200	TLA	O2-C2-C3-C4
2	D	201	TLA	O1-C1-C2-C3
2	D	201	TLA	C1-C2-C3-C4
2	D	201	TLA	O2-C2-C3-O3
2	D	201	TLA	O2-C2-C3-C4
2	E	200	TLA	C1-C2-C3-O3
2	E	200	TLA	C1-C2-C3-C4
2	E	200	TLA	O2-C2-C3-O3
2	E	200	TLA	O2-C2-C3-C4
2	E	201	TLA	C1-C2-C3-O3
2	E	201	TLA	C1-C2-C3-C4
2	E	201	TLA	O2-C2-C3-O3
2	E	201	TLA	O2-C2-C3-C4
2	F	200	TLA	C1-C2-C3-O3
2	F	200	TLA	C1-C2-C3-C4
2	F	200	TLA	O2-C2-C3-O3
2	F	200	TLA	O2-C2-C3-C4
2	F	201	TLA	C1-C2-C3-O3
2	F	201	TLA	C1-C2-C3-C4
2	F	201	TLA	O2-C2-C3-O3
2	F	201	TLA	O2-C2-C3-C4
2	G	200	TLA	C1-C2-C3-O3
2	G	200	TLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	G	200	TLA	O2-C2-C3-O3
2	G	200	TLA	O2-C2-C3-C4
2	G	201	TLA	C1-C2-C3-O3
2	G	201	TLA	C1-C2-C3-C4
2	G	201	TLA	O2-C2-C3-O3
2	G	201	TLA	O2-C2-C3-C4
2	G	201	TLA	O3-C3-C4-O4
2	G	201	TLA	O3-C3-C4-O41
2	H	201	TLA	C1-C2-C3-C4
2	I	200	TLA	C1-C2-C3-O3
2	I	200	TLA	C1-C2-C3-C4
2	I	200	TLA	O2-C2-C3-O3
2	I	200	TLA	O2-C2-C3-C4
2	J	201	TLA	C1-C2-C3-O3
2	J	201	TLA	C1-C2-C3-C4
2	J	201	TLA	O2-C2-C3-O3
2	J	201	TLA	O2-C2-C3-C4
2	K	201	TLA	C1-C2-C3-C4
2	K	201	TLA	O2-C2-C3-O3
2	L	200	TLA	C1-C2-C3-O3
2	L	200	TLA	C1-C2-C3-C4
2	L	200	TLA	O2-C2-C3-O3
2	L	200	TLA	O2-C2-C3-C4
2	L	201	TLA	C1-C2-C3-O3
2	L	201	TLA	C1-C2-C3-C4
2	L	201	TLA	O2-C2-C3-O3
2	L	201	TLA	O2-C2-C3-C4
3	A	202	TAR	O1-C1-C2-O2
3	A	202	TAR	O11-C1-C2-O2
3	E	202	TAR	O1-C1-C2-O2
3	E	202	TAR	O11-C1-C2-O2
3	E	202	TAR	O3-C3-C4-O4
3	E	202	TAR	O3-C3-C4-O41
3	G	202	TAR	O1-C1-C2-O2
3	G	202	TAR	O11-C1-C2-O2
3	G	202	TAR	O3-C3-C4-O4
3	G	202	TAR	O3-C3-C4-O41
3	H	202	TAR	O1-C1-C2-O2
3	H	202	TAR	O11-C1-C2-O2
3	H	202	TAR	O3-C3-C4-O4
3	H	202	TAR	O3-C3-C4-O41
3	I	202	TAR	O3-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
3	I	202	TAR	O3-C3-C4-O41
3	J	202	TAR	O1-C1-C2-O2
3	J	202	TAR	O11-C1-C2-O2
3	J	202	TAR	C2-C3-C4-O41
2	C	201	TLA	C1-C2-C3-O3
2	K	201	TLA	C1-C2-C3-O3
2	K	201	TLA	O2-C2-C3-C4
2	B	202	TLA	O2-C2-C3-O3
2	I	201	TLA	O2-C2-C3-O3
2	I	201	TLA	C1-C2-C3-C4
2	H	201	TLA	C1-C2-C3-O3
2	H	201	TLA	O2-C2-C3-C4
2	B	202	TLA	O1-C1-C2-O2
2	B	202	TLA	O3-C3-C4-O4
2	B	202	TLA	O3-C3-C4-O41
2	C	201	TLA	O3-C3-C4-O4
2	E	201	TLA	O3-C3-C4-O4
2	E	201	TLA	O3-C3-C4-O41
2	F	201	TLA	O1-C1-C2-O2
2	F	201	TLA	O3-C3-C4-O4
2	F	201	TLA	O3-C3-C4-O41
2	G	201	TLA	O1-C1-C2-O2
2	H	201	TLA	O3-C3-C4-O4
2	H	201	TLA	O3-C3-C4-O41
2	I	201	TLA	O3-C3-C4-O4
2	I	201	TLA	O3-C3-C4-O41
2	J	201	TLA	O3-C3-C4-O4
2	J	201	TLA	O3-C3-C4-O41
2	K	200	TLA	O1-C1-C2-O2
2	K	200	TLA	O11-C1-C2-O2
3	A	202	TAR	O3-C3-C4-O4
3	A	202	TAR	O3-C3-C4-O41
3	B	203	TAR	O1-C1-C2-O2
3	B	203	TAR	O11-C1-C2-O2
3	B	203	TAR	O3-C3-C4-O4
3	B	203	TAR	O3-C3-C4-O41
3	C	202	TAR	O1-C1-C2-O2
3	C	202	TAR	O11-C1-C2-O2
3	C	202	TAR	O3-C3-C4-O4
3	C	202	TAR	O3-C3-C4-O41
3	D	202	TAR	O1-C1-C2-O2
3	D	202	TAR	O11-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	D	202	TAR	O3-C3-C4-O4
3	D	202	TAR	O3-C3-C4-O41
3	F	202	TAR	O1-C1-C2-O2
3	F	202	TAR	O11-C1-C2-O2
3	F	202	TAR	O3-C3-C4-O4
3	F	202	TAR	O3-C3-C4-O41
3	I	202	TAR	O1-C1-C2-O2
3	I	202	TAR	O11-C1-C2-O2
3	K	202	TAR	O1-C1-C2-O2
3	K	202	TAR	O11-C1-C2-O2
3	K	202	TAR	O3-C3-C4-O4
3	K	202	TAR	O3-C3-C4-O41
3	L	202	TAR	O1-C1-C2-O2
3	L	202	TAR	O11-C1-C2-O2
3	L	202	TAR	O3-C3-C4-O4
3	L	202	TAR	O3-C3-C4-O41
2	C	201	TLA	C2-C3-C4-O4
2	D	201	TLA	O11-C1-C2-C3
2	K	200	TLA	O1-C1-C2-C3
2	K	200	TLA	O11-C1-C2-C3
3	A	202	TAR	O1-C1-C2-C3
3	A	202	TAR	O11-C1-C2-C3
3	A	202	TAR	C2-C3-C4-O4
3	A	202	TAR	C2-C3-C4-O41
3	E	202	TAR	C2-C3-C4-O4
3	E	202	TAR	C2-C3-C4-O41
3	F	202	TAR	O1-C1-C2-C3
3	F	202	TAR	O11-C1-C2-C3
3	H	202	TAR	C2-C3-C4-O4
3	H	202	TAR	C2-C3-C4-O41
3	I	202	TAR	C2-C3-C4-O4
3	I	202	TAR	C2-C3-C4-O41
3	J	202	TAR	C2-C3-C4-O4
3	K	202	TAR	C2-C3-C4-O41
2	C	201	TLA	O2-C2-C3-C4
2	B	202	TLA	O11-C1-C2-O2
2	C	201	TLA	O3-C3-C4-O41
2	K	201	TLA	O1-C1-C2-O2
2	K	201	TLA	O11-C1-C2-O2
2	L	201	TLA	O3-C3-C4-O4
2	L	201	TLA	O3-C3-C4-O41
3	J	202	TAR	O3-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	L	200	TLA	C2-C3-C4-O4
3	G	202	TAR	C2-C3-C4-O41
3	K	202	TAR	C2-C3-C4-O4
2	D	201	TLA	C1-C2-C3-O3
2	J	200	TLA	C1-C2-C3-O3
2	J	200	TLA	O2-C2-C3-C4
2	D	201	TLA	O1-C1-C2-O2
2	D	201	TLA	O11-C1-C2-O2
2	F	201	TLA	O11-C1-C2-O2
2	H	201	TLA	O1-C1-C2-O2
2	H	201	TLA	O11-C1-C2-O2
3	J	202	TAR	O3-C3-C4-O41
2	G	200	TLA	C2-C3-C4-O41
3	B	203	TAR	O11-C1-C2-C3
3	C	202	TAR	O11-C1-C2-C3
3	L	202	TAR	C2-C3-C4-O41
2	I	201	TLA	C1-C2-C3-O3
3	J	202	TAR	C1-C2-C3-O3
3	J	202	TAR	O2-C2-C3-C4
2	A	200	TLA	C2-C3-C4-O4
2	D	200	TLA	C2-C3-C4-O41
2	E	200	TLA	C2-C3-C4-O4
2	F	200	TLA	C2-C3-C4-O41
2	L	200	TLA	C2-C3-C4-O41
3	G	202	TAR	C2-C3-C4-O4
2	J	200	TLA	O2-C2-C3-O3
2	L	201	TLA	O1-C1-C2-O2
2	C	200	TLA	C2-C3-C4-O41
2	E	200	TLA	C2-C3-C4-O41
2	H	200	TLA	C2-C3-C4-O41
2	J	200	TLA	C2-C3-C4-O41
3	B	203	TAR	O1-C1-C2-C3
3	C	202	TAR	O1-C1-C2-C3
3	D	202	TAR	O1-C1-C2-C3
3	G	202	TAR	O1-C1-C2-C3
3	H	202	TAR	O1-C1-C2-C3
3	H	202	TAR	O11-C1-C2-C3
3	L	202	TAR	C2-C3-C4-O4
2	G	201	TLA	O11-C1-C2-O2
2	L	200	TLA	O3-C3-C4-O4
2	A	200	TLA	C2-C3-C4-O41
2	I	200	TLA	C2-C3-C4-O41

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Mol	Chain	Res	Type	Atoms
3	D	202	TAR	O11-C1-C2-C3
3	D	202	TAR	C2-C3-C4-O4
3	D	202	TAR	C2-C3-C4-O41
3	F	202	TAR	C2-C3-C4-O4
3	G	202	TAR	O11-C1-C2-C3
3	L	202	TAR	O1-C1-C2-C3
3	J	202	TAR	O2-C2-C3-O3
2	I	201	TLA	O2-C2-C3-C4
2	L	201	TLA	O11-C1-C2-O2
2	C	200	TLA	C2-C3-C4-O4
2	F	200	TLA	C2-C3-C4-O4
2	G	200	TLA	C2-C3-C4-O4
2	H	200	TLA	C2-C3-C4-O4
2	J	200	TLA	C2-C3-C4-O4
3	F	202	TAR	C2-C3-C4-O41
3	L	202	TAR	O11-C1-C2-C3
2	G	200	TLA	O3-C3-C4-O41
2	D	200	TLA	C2-C3-C4-O4
3	B	203	TAR	C2-C3-C4-O4
3	B	203	TAR	C2-C3-C4-O41
2	L	200	TLA	O3-C3-C4-O41
2	J	200	TLA	C1-C2-C3-C4
2	H	200	TLA	O3-C3-C4-O41
2	K	200	TLA	O3-C3-C4-O41
3	I	202	TAR	O11-C1-C2-C3
3	J	202	TAR	C1-C2-C3-C4
2	D	201	TLA	O3-C3-C4-O41
2	I	200	TLA	C2-C3-C4-O4
3	K	202	TAR	O1-C1-C2-C3
2	K	200	TLA	O3-C3-C4-O4
3	K	202	TAR	O11-C1-C2-C3
2	E	201	TLA	O11-C1-C2-O2
2	F	200	TLA	O3-C3-C4-O41
3	I	202	TAR	O1-C1-C2-C3
2	A	200	TLA	O3-C3-C4-O4
2	E	200	TLA	O3-C3-C4-O4
2	G	200	TLA	O3-C3-C4-O4
2	J	201	TLA	O1-C1-C2-C3
2	K	200	TLA	C2-C3-C4-O4
2	K	200	TLA	C2-C3-C4-O41
2	J	200	TLA	O3-C3-C4-O41
2	L	201	TLA	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	H	200	TLA	O3-C3-C4-O4
2	J	201	TLA	O1-C1-C2-O2
2	H	201	TLA	O2-C2-C3-O3
2	D	201	TLA	C2-C3-C4-O41
2	D	200	TLA	O3-C3-C4-O41
2	E	201	TLA	O1-C1-C2-O2
2	D	201	TLA	C2-C3-C4-O4
2	J	201	TLA	O11-C1-C2-C3
2	L	201	TLA	O1-C1-C2-C3
2	E	201	TLA	O1-C1-C2-C3
2	E	201	TLA	O11-C1-C2-C3
3	C	202	TAR	C2-C3-C4-O4
2	I	200	TLA	O3-C3-C4-O41
2	C	200	TLA	O3-C3-C4-O41
2	F	200	TLA	O3-C3-C4-O4
3	C	202	TAR	C2-C3-C4-O41
2	D	201	TLA	O3-C3-C4-O4
2	J	200	TLA	O3-C3-C4-O4
2	F	201	TLA	O11-C1-C2-C3
2	G	201	TLA	O11-C1-C2-C3
2	D	200	TLA	O3-C3-C4-O4
2	J	201	TLA	O11-C1-C2-O2
2	E	200	TLA	O3-C3-C4-O41
2	H	201	TLA	C2-C3-C4-O4
2	A	200	TLA	O3-C3-C4-O41
2	I	201	TLA	O1-C1-C2-O2
2	F	201	TLA	O1-C1-C2-C3
2	E	201	TLA	C2-C3-C4-O41
2	G	201	TLA	O1-C1-C2-C3
2	F	201	TLA	C2-C3-C4-O41
2	H	201	TLA	C2-C3-C4-O41
2	I	201	TLA	C2-C3-C4-O41

There are no ring outliers.

20 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	TLA	3	0
2	C	201	TLA	1	0
3	H	202	TAR	2	0
3	D	202	TAR	1	0
2	F	201	TLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	202	TAR	1	0
2	E	201	TLA	2	0
2	G	201	TLA	1	0
3	L	202	TAR	1	0
2	H	200	TLA	1	0
3	B	203	TAR	1	0
3	J	202	TAR	3	0
2	I	201	TLA	1	0
2	B	201	TLA	2	0
3	F	202	TAR	2	0
2	B	202	TLA	2	0
2	D	201	TLA	1	0
3	E	202	TAR	2	0
3	G	202	TAR	3	0
2	J	201	TLA	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	145/166 (87%)	-0.75	0 100 100	18, 27, 54, 90	0
1	B	145/166 (87%)	-0.73	0 100 100	16, 24, 54, 80	0
1	C	145/166 (87%)	-0.80	1 (0%) 87 86	17, 26, 49, 85	0
1	D	144/166 (86%)	-0.86	0 100 100	17, 28, 49, 69	0
1	E	145/166 (87%)	-0.61	2 (1%) 75 71	17, 31, 55, 83	0
1	F	145/166 (87%)	-0.84	1 (0%) 87 86	18, 29, 63, 92	0
1	G	145/166 (87%)	-0.72	2 (1%) 75 71	25, 32, 54, 131	0
1	H	145/166 (87%)	-0.63	1 (0%) 87 86	30, 42, 60, 122	0
1	I	146/166 (87%)	-0.67	1 (0%) 87 86	32, 46, 78, 99	0
1	J	144/166 (86%)	-0.08	4 (2%) 53 46	45, 61, 84, 98	0
1	K	144/166 (86%)	0.30	15 (10%) 6 4	58, 69, 87, 99	0
1	L	144/166 (86%)	-0.06	1 (0%) 87 86	44, 59, 80, 94	0
All	All	1737/1992 (87%)	-0.54	28 (1%) 72 68	16, 39, 77, 131	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	145	GLY	7.0
1	G	144	SER	4.7
1	K	38	LEU	4.5
1	K	144	SER	4.3
1	K	134	LEU	4.1
1	K	40	ALA	3.5
1	G	145	GLY	3.4
1	K	35	LEU	3.2
1	K	143	GLN	3.1
1	J	20	PRO	3.1
1	K	141	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	25	THR	3.1
1	K	138	ARG	3.0
1	F	21	VAL	2.8
1	J	19	ASP	2.6
1	K	42	LEU	2.5
1	K	24	GLY	2.4
1	K	46	VAL	2.2
1	E	20	PRO	2.2
1	E	21	VAL	2.2
1	K	37	ALA	2.2
1	J	26	ILE	2.1
1	I	145	GLY	2.1
1	K	4	VAL	2.1
1	J	25	THR	2.1
1	K	1	MET	2.1
1	C	144	SER	2.0
1	K	137	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	B-factors(Å^2)	Q<0.9
3	TAR	J	202	10/10	0.64	0.47	163,164,165,166	10
3	TAR	H	202	10/10	0.68	0.48	163,164,165,166	10
3	TAR	G	202	10/10	0.68	0.43	148,149,151,151	10
3	TAR	A	202	10/10	0.69	0.47	121,123,124,124	10
3	TAR	C	202	10/10	0.70	0.43	121,123,124,124	10
3	TAR	B	203	10/10	0.76	0.47	144,145,146,147	10

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TLA	K	201	10/10	0.77	0.21	68,85,96,98	0
3	TAR	F	202	10/10	0.82	0.42	157,158,159,159	10
3	TAR	D	202	10/10	0.82	0.39	124,125,127,128	10
3	TAR	L	202	10/10	0.82	0.25	109,111,113,113	10
2	TLA	G	200	10/10	0.83	0.30	92,99,102,109	0
3	TAR	K	202	10/10	0.83	0.56	149,150,150,151	10
3	TAR	I	202	10/10	0.83	0.23	105,110,112,113	10
3	TAR	E	202	10/10	0.84	0.39	156,158,159,160	10
2	TLA	J	201	10/10	0.84	0.21	67,85,92,94	0
2	TLA	D	200	10/10	0.85	0.25	62,66,71,76	0
2	TLA	I	201	10/10	0.87	0.19	55,70,76,76	0
2	TLA	L	201	10/10	0.87	0.18	48,66,70,71	0
2	TLA	J	200	10/10	0.88	0.23	77,82,86,88	0
2	TLA	L	200	10/10	0.88	0.30	71,84,89,92	0
2	TLA	K	200	10/10	0.88	0.22	80,90,94,98	0
2	TLA	C	200	10/10	0.89	0.24	48,53,63,67	0
2	TLA	E	200	10/10	0.89	0.21	54,63,69,69	0
2	TLA	B	201	10/10	0.90	0.20	59,63,68,69	0
2	TLA	H	201	10/10	0.90	0.17	39,61,74,74	0
2	TLA	E	201	10/10	0.90	0.14	31,50,59,61	0
2	TLA	B	202	10/10	0.91	0.14	31,41,56,60	0
2	TLA	A	201	10/10	0.91	0.13	32,54,60,63	0
2	TLA	A	200	10/10	0.91	0.20	43,47,52,60	0
2	TLA	G	201	10/10	0.91	0.14	39,58,76,80	0
2	TLA	F	201	10/10	0.92	0.14	29,51,62,63	0
2	TLA	I	200	10/10	0.93	0.16	64,66,73,78	0
2	TLA	C	201	10/10	0.93	0.15	33,46,56,57	0
2	TLA	F	200	10/10	0.94	0.22	46,53,65,77	0
2	TLA	D	201	10/10	0.94	0.16	31,38,49,53	0
2	TLA	H	200	10/10	0.94	0.17	47,56,66,67	0
4	CL	B	204	1/1	0.94	0.35	76,76,76,76	1

6.5 Other polymers (i)

There are no such residues in this entry.