Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 06:44 AM EDT

PDB ID	:	7C0D
Title	:	Crystal structure of Azospirillum brasilense L-2-keto-3-deoxyarabonate dehydratase (Hydroxypyruvate-bound form)
Authors	:	Watanabe, Y.; Watanabe, S.
Deposited on	:	2020-05-01
Resolution	:	1.60 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:

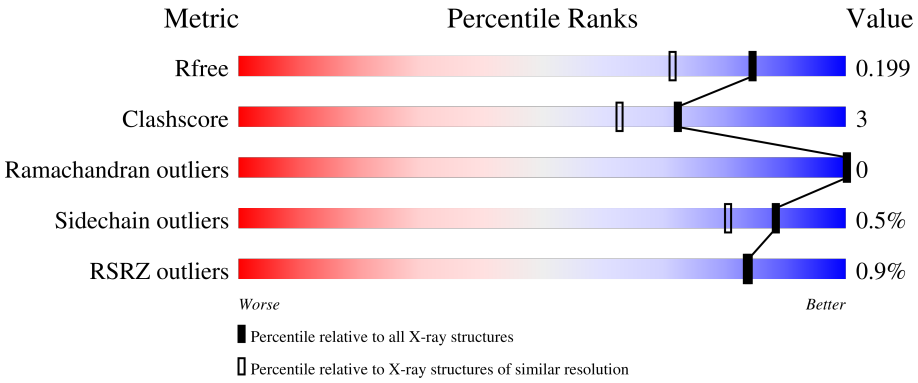
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	320	88% 7% 5%
1	B	320	88% 7% 5%
1	C	320	88% 7% 5%
1	D	320	91% 5%
1	E	320	88% 7% 5%

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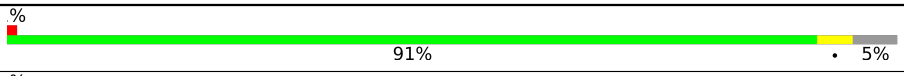
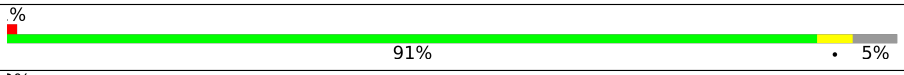
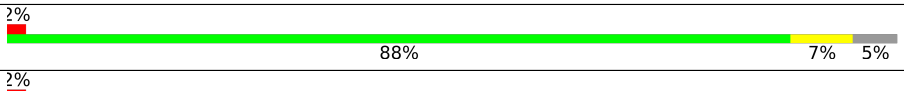
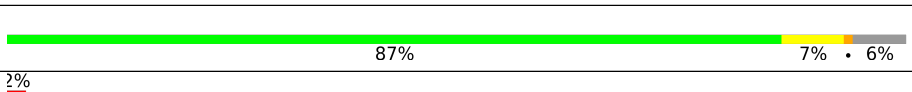
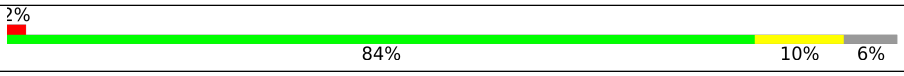
Mol	Chain	Length	Quality of chain
1	F	320	
1	G	320	
1	H	320	
1	I	320	
1	J	320	
1	K	320	
1	L	320	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 32122 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 L-2-keto-3-deoxyarabonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2342	1477	424	430	11			
1	B	304	Total	C	N	O	S	0	0	0
			2348	1480	424	433	11			
1	C	303	Total	C	N	O	S	0	0	0
			2337	1474	421	431	11			
1	D	303	Total	C	N	O	S	0	0	0
			2331	1471	421	428	11			
1	E	303	Total	C	N	O	S	0	0	0
			2331	1471	421	428	11			
1	F	303	Total	C	N	O	S	0	0	0
			2331	1471	421	428	11			
1	G	303	Total	C	N	O	S	0	0	0
			2331	1471	421	428	11			
1	H	304	Total	C	N	O	S	0	0	0
			2342	1477	424	430	11			
1	I	302	Total	C	N	O	S	0	0	0
			2326	1468	420	427	11			
1	J	302	Total	C	N	O	S	0	0	0
			2324	1467	420	426	11			
1	K	302	Total	C	N	O	S	0	0	0
			2324	1467	420	426	11			
1	L	302	Total	C	N	O	S	0	0	0
			2326	1468	420	427	11			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q1JUQ0
A	-9	ARG	-	expression tag	UNP Q1JUQ0
A	-8	GLY	-	expression tag	UNP Q1JUQ0
A	-7	SER	-	expression tag	UNP Q1JUQ0
A	-6	HIS	-	expression tag	UNP Q1JUQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q1JUQ0
A	-4	HIS	-	expression tag	UNP Q1JUQ0
A	-3	HIS	-	expression tag	UNP Q1JUQ0
A	-2	HIS	-	expression tag	UNP Q1JUQ0
A	-1	HIS	-	expression tag	UNP Q1JUQ0
A	0	GLY	-	expression tag	UNP Q1JUQ0
A	1	SER	-	expression tag	UNP Q1JUQ0
B	-10	MET	-	expression tag	UNP Q1JUQ0
B	-9	ARG	-	expression tag	UNP Q1JUQ0
B	-8	GLY	-	expression tag	UNP Q1JUQ0
B	-7	SER	-	expression tag	UNP Q1JUQ0
B	-6	HIS	-	expression tag	UNP Q1JUQ0
B	-5	HIS	-	expression tag	UNP Q1JUQ0
B	-4	HIS	-	expression tag	UNP Q1JUQ0
B	-3	HIS	-	expression tag	UNP Q1JUQ0
B	-2	HIS	-	expression tag	UNP Q1JUQ0
B	-1	HIS	-	expression tag	UNP Q1JUQ0
B	0	GLY	-	expression tag	UNP Q1JUQ0
B	1	SER	-	expression tag	UNP Q1JUQ0
C	-10	MET	-	expression tag	UNP Q1JUQ0
C	-9	ARG	-	expression tag	UNP Q1JUQ0
C	-8	GLY	-	expression tag	UNP Q1JUQ0
C	-7	SER	-	expression tag	UNP Q1JUQ0
C	-6	HIS	-	expression tag	UNP Q1JUQ0
C	-5	HIS	-	expression tag	UNP Q1JUQ0
C	-4	HIS	-	expression tag	UNP Q1JUQ0
C	-3	HIS	-	expression tag	UNP Q1JUQ0
C	-2	HIS	-	expression tag	UNP Q1JUQ0
C	-1	HIS	-	expression tag	UNP Q1JUQ0
C	0	GLY	-	expression tag	UNP Q1JUQ0
C	1	SER	-	expression tag	UNP Q1JUQ0
D	-10	MET	-	expression tag	UNP Q1JUQ0
D	-9	ARG	-	expression tag	UNP Q1JUQ0
D	-8	GLY	-	expression tag	UNP Q1JUQ0
D	-7	SER	-	expression tag	UNP Q1JUQ0
D	-6	HIS	-	expression tag	UNP Q1JUQ0
D	-5	HIS	-	expression tag	UNP Q1JUQ0
D	-4	HIS	-	expression tag	UNP Q1JUQ0
D	-3	HIS	-	expression tag	UNP Q1JUQ0
D	-2	HIS	-	expression tag	UNP Q1JUQ0
D	-1	HIS	-	expression tag	UNP Q1JUQ0
D	0	GLY	-	expression tag	UNP Q1JUQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	SER	-	expression tag	UNP Q1JUQ0
E	-10	MET	-	expression tag	UNP Q1JUQ0
E	-9	ARG	-	expression tag	UNP Q1JUQ0
E	-8	GLY	-	expression tag	UNP Q1JUQ0
E	-7	SER	-	expression tag	UNP Q1JUQ0
E	-6	HIS	-	expression tag	UNP Q1JUQ0
E	-5	HIS	-	expression tag	UNP Q1JUQ0
E	-4	HIS	-	expression tag	UNP Q1JUQ0
E	-3	HIS	-	expression tag	UNP Q1JUQ0
E	-2	HIS	-	expression tag	UNP Q1JUQ0
E	-1	HIS	-	expression tag	UNP Q1JUQ0
E	0	GLY	-	expression tag	UNP Q1JUQ0
E	1	SER	-	expression tag	UNP Q1JUQ0
F	-10	MET	-	expression tag	UNP Q1JUQ0
F	-9	ARG	-	expression tag	UNP Q1JUQ0
F	-8	GLY	-	expression tag	UNP Q1JUQ0
F	-7	SER	-	expression tag	UNP Q1JUQ0
F	-6	HIS	-	expression tag	UNP Q1JUQ0
F	-5	HIS	-	expression tag	UNP Q1JUQ0
F	-4	HIS	-	expression tag	UNP Q1JUQ0
F	-3	HIS	-	expression tag	UNP Q1JUQ0
F	-2	HIS	-	expression tag	UNP Q1JUQ0
F	-1	HIS	-	expression tag	UNP Q1JUQ0
F	0	GLY	-	expression tag	UNP Q1JUQ0
F	1	SER	-	expression tag	UNP Q1JUQ0
G	-10	MET	-	expression tag	UNP Q1JUQ0
G	-9	ARG	-	expression tag	UNP Q1JUQ0
G	-8	GLY	-	expression tag	UNP Q1JUQ0
G	-7	SER	-	expression tag	UNP Q1JUQ0
G	-6	HIS	-	expression tag	UNP Q1JUQ0
G	-5	HIS	-	expression tag	UNP Q1JUQ0
G	-4	HIS	-	expression tag	UNP Q1JUQ0
G	-3	HIS	-	expression tag	UNP Q1JUQ0
G	-2	HIS	-	expression tag	UNP Q1JUQ0
G	-1	HIS	-	expression tag	UNP Q1JUQ0
G	0	GLY	-	expression tag	UNP Q1JUQ0
G	1	SER	-	expression tag	UNP Q1JUQ0
H	-10	MET	-	expression tag	UNP Q1JUQ0
H	-9	ARG	-	expression tag	UNP Q1JUQ0
H	-8	GLY	-	expression tag	UNP Q1JUQ0
H	-7	SER	-	expression tag	UNP Q1JUQ0
H	-6	HIS	-	expression tag	UNP Q1JUQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	expression tag	UNP Q1JUQ0
H	-4	HIS	-	expression tag	UNP Q1JUQ0
H	-3	HIS	-	expression tag	UNP Q1JUQ0
H	-2	HIS	-	expression tag	UNP Q1JUQ0
H	-1	HIS	-	expression tag	UNP Q1JUQ0
H	0	GLY	-	expression tag	UNP Q1JUQ0
H	1	SER	-	expression tag	UNP Q1JUQ0
I	-10	MET	-	expression tag	UNP Q1JUQ0
I	-9	ARG	-	expression tag	UNP Q1JUQ0
I	-8	GLY	-	expression tag	UNP Q1JUQ0
I	-7	SER	-	expression tag	UNP Q1JUQ0
I	-6	HIS	-	expression tag	UNP Q1JUQ0
I	-5	HIS	-	expression tag	UNP Q1JUQ0
I	-4	HIS	-	expression tag	UNP Q1JUQ0
I	-3	HIS	-	expression tag	UNP Q1JUQ0
I	-2	HIS	-	expression tag	UNP Q1JUQ0
I	-1	HIS	-	expression tag	UNP Q1JUQ0
I	0	GLY	-	expression tag	UNP Q1JUQ0
I	1	SER	-	expression tag	UNP Q1JUQ0
J	-10	MET	-	expression tag	UNP Q1JUQ0
J	-9	ARG	-	expression tag	UNP Q1JUQ0
J	-8	GLY	-	expression tag	UNP Q1JUQ0
J	-7	SER	-	expression tag	UNP Q1JUQ0
J	-6	HIS	-	expression tag	UNP Q1JUQ0
J	-5	HIS	-	expression tag	UNP Q1JUQ0
J	-4	HIS	-	expression tag	UNP Q1JUQ0
J	-3	HIS	-	expression tag	UNP Q1JUQ0
J	-2	HIS	-	expression tag	UNP Q1JUQ0
J	-1	HIS	-	expression tag	UNP Q1JUQ0
J	0	GLY	-	expression tag	UNP Q1JUQ0
J	1	SER	-	expression tag	UNP Q1JUQ0
K	-10	MET	-	expression tag	UNP Q1JUQ0
K	-9	ARG	-	expression tag	UNP Q1JUQ0
K	-8	GLY	-	expression tag	UNP Q1JUQ0
K	-7	SER	-	expression tag	UNP Q1JUQ0
K	-6	HIS	-	expression tag	UNP Q1JUQ0
K	-5	HIS	-	expression tag	UNP Q1JUQ0
K	-4	HIS	-	expression tag	UNP Q1JUQ0
K	-3	HIS	-	expression tag	UNP Q1JUQ0
K	-2	HIS	-	expression tag	UNP Q1JUQ0
K	-1	HIS	-	expression tag	UNP Q1JUQ0
K	0	GLY	-	expression tag	UNP Q1JUQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1	SER	-	expression tag	UNP Q1JUQ0
L	-10	MET	-	expression tag	UNP Q1JUQ0
L	-9	ARG	-	expression tag	UNP Q1JUQ0
L	-8	GLY	-	expression tag	UNP Q1JUQ0
L	-7	SER	-	expression tag	UNP Q1JUQ0
L	-6	HIS	-	expression tag	UNP Q1JUQ0
L	-5	HIS	-	expression tag	UNP Q1JUQ0
L	-4	HIS	-	expression tag	UNP Q1JUQ0
L	-3	HIS	-	expression tag	UNP Q1JUQ0
L	-2	HIS	-	expression tag	UNP Q1JUQ0
L	-1	HIS	-	expression tag	UNP Q1JUQ0
L	0	GLY	-	expression tag	UNP Q1JUQ0
L	1	SER	-	expression tag	UNP Q1JUQ0

- Molecule 2 is water.

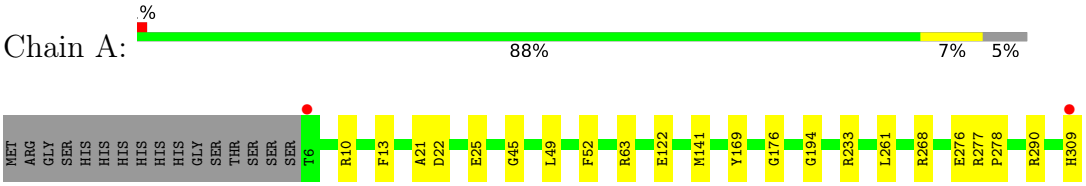
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	444	Total O 444 444	0	0
2	B	391	Total O 391 391	0	0
2	C	405	Total O 405 405	0	0
2	D	418	Total O 418 418	0	0
2	E	331	Total O 331 331	0	0
2	F	334	Total O 334 334	0	0
2	G	389	Total O 389 389	0	0
2	H	289	Total O 289 289	0	0
2	I	233	Total O 233 233	0	0
2	J	350	Total O 350 350	0	0
2	K	310	Total O 310 310	0	0
2	L	235	Total O 235 235	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.

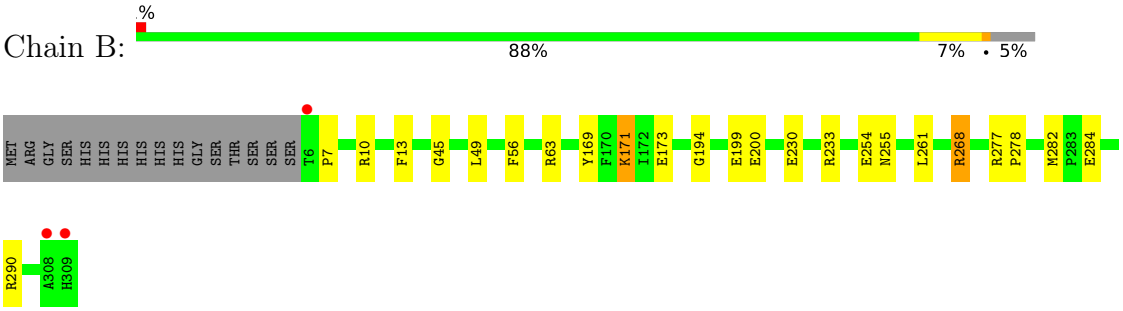
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain A:



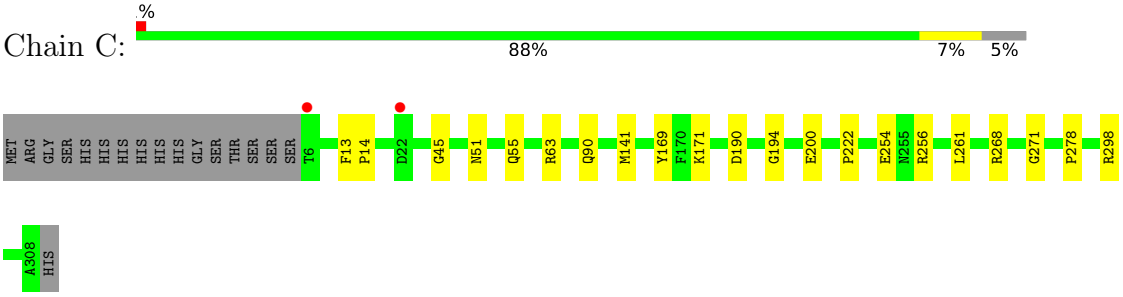
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain B:



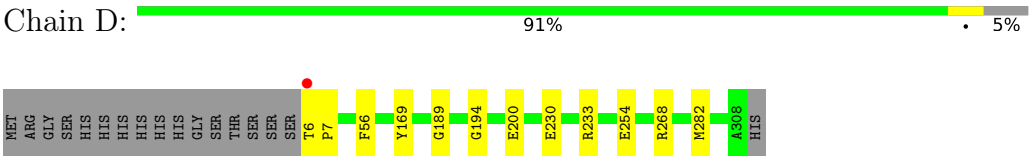
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain C:



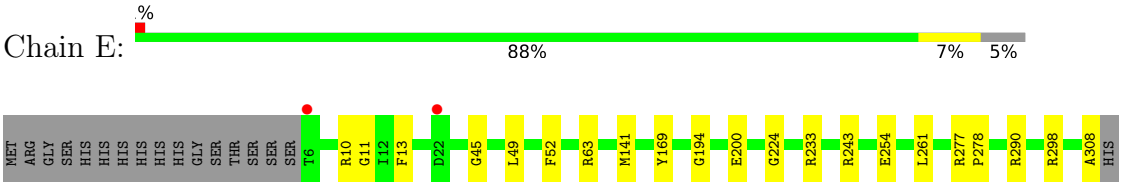
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain D:



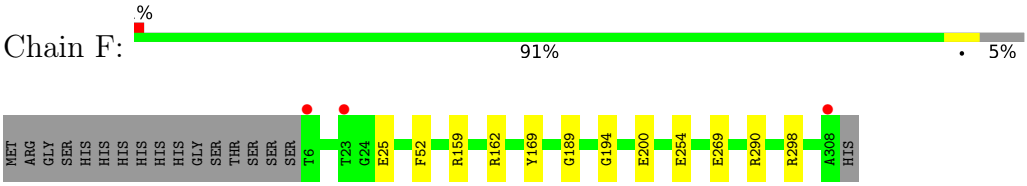
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain E:



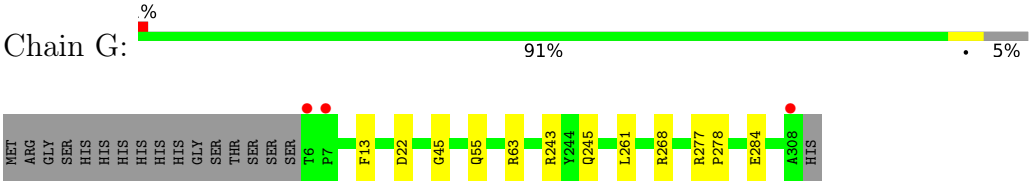
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain F:



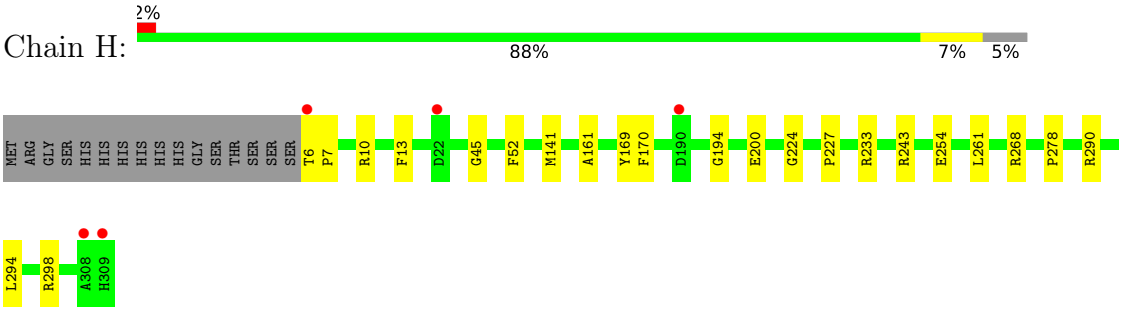
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain G:



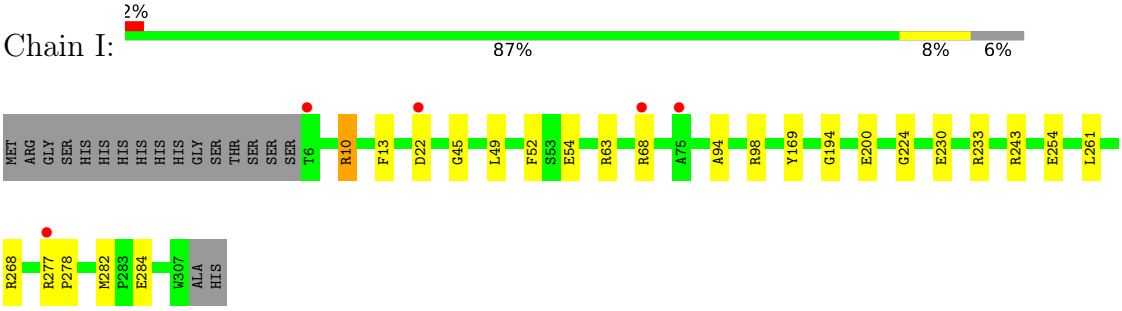
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain H:



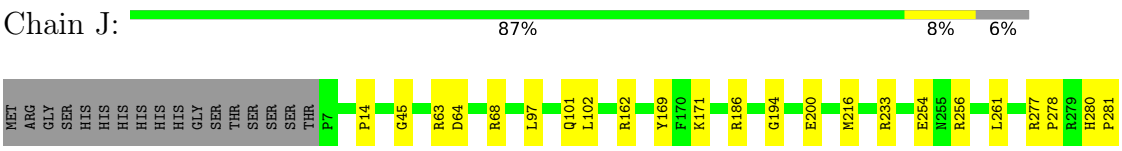
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain I:



• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain J:

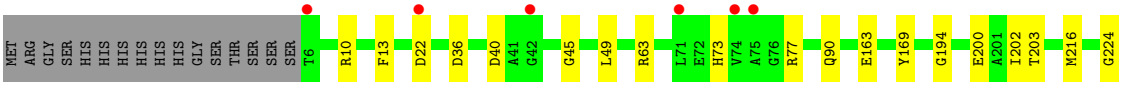


• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain K:

• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.38Å 88.47Å 143.70Å 84.83° 86.00° 73.21°	Depositor
Resolution (Å)	48.81 – 1.60 48.81 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.81-1.60) 95.0 (48.81-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.20 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.170 , 0.199 0.170 , 0.199	Depositor DCC
R_{free} test set	23151 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32122	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: KYQ

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	0.39	0/2386	0.59	0/3244
1	B	0.37	0/2386	0.58	0/3244
1	C	0.34	0/2374	0.55	0/3229
1	D	0.35	0/2374	0.56	0/3229
1	E	0.33	0/2374	0.51	0/3229
1	F	0.34	0/2374	0.52	0/3229
1	G	0.33	0/2374	0.55	0/3229
1	H	0.32	0/2386	0.51	0/3244
1	I	0.31	0/2369	0.49	0/3222
1	J	0.36	0/2367	0.55	0/3218
1	K	0.31	0/2367	0.51	0/3218
1	L	0.31	0/2369	0.50	0/3222
All	All	0.34	0/28500	0.54	0/38757

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	2342	0	2317	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2348	0	2320	18	0
1	C	2337	0	2313	13	0
1	D	2331	0	2310	6	0
1	E	2331	0	2310	17	0
1	F	2331	0	2310	8	0
1	G	2331	0	2310	8	0
1	H	2342	0	2317	18	0
1	I	2326	0	2305	19	0
1	J	2324	0	2304	17	0
1	K	2324	0	2304	15	0
1	L	2326	0	2305	25	0
2	A	444	0	0	11	0
2	B	391	0	0	6	2
2	C	405	0	0	5	0
2	D	418	0	0	2	1
2	E	331	0	0	8	0
2	F	334	0	0	5	0
2	G	389	0	0	3	0
2	H	289	0	0	2	0
2	I	233	0	0	8	0
2	J	350	0	0	6	1
2	K	310	0	0	4	0
2	L	235	0	0	6	0
All	All	32122	0	27725	191	2

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 (191) 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:F:25:GLU:OE1	2:F:401:HOH:O	1.64	1.16
1:E:233:ARG:NH1	2:E:401:HOH:O	1.94	0.99
1:C:268:ARG:NH1	2:C:401:HOH:O	1.95	0.96
1:A:268:ARG:HH21	1:A:276:GLU:H	1.20	0.90
1:L:90:GLN:NE2	2:L:401:HOH:O	2.08	0.87
1:L:10:ARG:HE	1:L:233:ARG:NH2	1.73	0.86
1:I:277:ARG:NH1	2:I:401:HOH:O	2.09	0.85
1:A:25:GLU:OE2	2:A:401:HOH:O	1.94	0.84
1:B:268:ARG:NH2	2:B:402:HOH:O	2.10	0.84
1:A:22:ASP:OD1	2:A:402:HOH:O	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:10:ARG:HD3	1:I:233:ARG:HH11	1.42	0.82
1:E:277:ARG:NH2	2:E:402:HOH:O	2.12	0.81
1:B:173:GLU:OE2	1:B:199:GLU:N	2.13	0.81
1:L:230:GLU:OE2	1:L:233:ARG:NH1	2.15	0.79
1:B:290:ARG:NH2	2:B:403:HOH:O	2.17	0.77
1:A:268:ARG:NH2	1:A:276:GLU:H	1.83	0.76
1:B:10:ARG:NH1	2:B:401:HOH:O	2.02	0.75
1:B:230:GLU:OE2	1:B:233:ARG:NH1	2.19	0.74
1:A:268:ARG:HH21	1:A:276:GLU:N	1.85	0.74
1:H:10:ARG:CZ	1:H:233:ARG:NE	2.51	0.73
1:G:268:ARG:NH1	2:G:401:HOH:O	2.22	0.72
1:A:233:ARG:NH1	2:A:405:HOH:O	2.23	0.71
1:E:233:ARG:NH2	2:E:404:HOH:O	2.23	0.69
1:I:49:LEU:HD13	1:I:63:ARG:HG3	1.74	0.69
1:C:90:GLN:OE1	2:C:403:HOH:O	2.12	0.68
1:A:268:ARG:CZ	1:A:276:GLU:HG2	2.24	0.68
1:J:68:ARG:NH2	2:J:401:HOH:O	2.25	0.68
1:I:268:ARG:NH1	2:I:404:HOH:O	2.26	0.67
1:A:309:HIS:OXT	2:A:403:HOH:O	2.12	0.67
1:I:68:ARG:NH1	2:I:405:HOH:O	2.27	0.67
1:H:10:ARG:NH2	1:H:233:ARG:NE	2.44	0.66
1:K:10:ARG:NH2	2:K:401:HOH:O	2.08	0.66
1:A:122:GLU:OE2	2:A:404:HOH:O	2.13	0.66
1:E:261:LEU:HD21	1:E:278:PRO:HB3	1.77	0.65
1:A:268:ARG:NE	1:A:276:GLU:HG2	2.11	0.65
1:L:10:ARG:HE	1:L:233:ARG:HH22	1.45	0.64
1:F:189:GLY:O	2:F:402:HOH:O	2.15	0.64
1:L:63:ARG:NH2	2:L:409:HOH:O	2.30	0.64
1:A:10:ARG:NH1	2:A:407:HOH:O	2.30	0.64
1:L:163:GLU:OE2	2:L:402:HOH:O	2.15	0.63
1:G:22:ASP:O	1:G:277:ARG:NH2	2.32	0.63
1:K:23:THR:OG1	1:K:25:GLU:HG2	1.98	0.62
1:K:227:PRO:HB2	1:K:243:ARG:HD3	1.81	0.62
1:I:277:ARG:NH2	2:I:408:HOH:O	2.32	0.62
1:E:49:LEU:HD13	1:E:63:ARG:HG3	1.83	0.60
1:L:77:ARG:NH1	2:L:408:HOH:O	2.29	0.60
1:D:230:GLU:OE2	1:D:233:ARG:NH1	2.32	0.59
1:A:141:MET:HE3	1:A:169:TYR:HB3	1.85	0.59
1:J:290:ARG:NH2	2:J:405:HOH:O	2.34	0.59
1:A:63:ARG:HD3	2:A:474:HOH:O	2.02	0.59
1:E:308:ALA:O	2:E:403:HOH:O	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:ARG:NH2	1:H:233:ARG:HE	2.00	0.59
1:C:261:LEU:HD21	1:C:278:PRO:HB3	1.85	0.58
1:I:94:ALA:O	2:I:402:HOH:O	2.17	0.58
1:B:171:KYQ:HEA	1:B:173:GLU:CD	2.24	0.58
1:H:10:ARG:CZ	1:H:233:ARG:CD	2.81	0.58
1:B:10:ARG:NH2	2:B:404:HOH:O	2.31	0.58
1:H:298:ARG:NH1	2:H:403:HOH:O	2.24	0.57
1:A:49:LEU:HD13	1:A:63:ARG:HG3	1.86	0.57
1:A:268:ARG:HE	1:A:276:GLU:H	1.52	0.57
1:I:224:GLY:HA2	1:I:243:ARG:HH11	1.70	0.57
1:J:63:ARG:HD2	2:J:411:HOH:O	2.05	0.57
1:L:10:ARG:NE	1:L:233:ARG:NH2	2.50	0.57
1:A:290:ARG:HD3	2:A:681:HOH:O	2.05	0.56
1:F:162:ARG:NH2	2:F:403:HOH:O	2.33	0.56
1:A:268:ARG:NE	1:A:276:GLU:H	2.05	0.55
1:F:290:ARG:HD3	2:F:640:HOH:O	2.06	0.55
1:H:6:THR:HG23	1:H:7:PRO:HD3	1.89	0.55
1:D:56:PHE:HZ	1:D:282:MET:HE1	1.71	0.55
1:B:277:ARG:HD3	1:B:284:GLU:OE2	2.07	0.54
1:L:40:ASP:OD1	2:L:403:HOH:O	2.18	0.54
1:A:268:ARG:HE	1:A:276:GLU:N	2.06	0.54
1:B:49:LEU:HD13	1:B:63:ARG:HG3	1.89	0.54
1:D:189:GLY:O	2:D:401:HOH:O	2.19	0.54
1:H:290:ARG:NH1	1:H:294:LEU:HD11	2.22	0.54
1:E:10:ARG:HE	1:E:233:ARG:NE	2.06	0.53
1:G:261:LEU:HD21	1:G:278:PRO:HB3	1.91	0.53
1:B:63:ARG:HD3	2:B:432:HOH:O	2.08	0.53
1:I:261:LEU:HD21	1:I:278:PRO:HB3	1.91	0.53
1:C:298:ARG:NH2	2:C:410:HOH:O	2.38	0.52
1:E:290:ARG:HD3	2:E:633:HOH:O	2.09	0.52
1:K:63:ARG:NH2	2:K:405:HOH:O	2.40	0.52
1:K:13:PHE:CE2	1:K:45:GLY:HA3	2.45	0.51
1:A:268:ARG:CZ	1:A:276:GLU:H	2.23	0.51
1:B:10:ARG:HE	1:B:233:ARG:HH21	1.58	0.51
1:K:224:GLY:HA2	1:K:243:ARG:HH21	1.75	0.51
1:F:169:TYR:CD2	1:F:194:GLY:HA3	2.46	0.51
1:K:268:ARG:NH1	2:K:406:HOH:O	2.43	0.51
1:L:169:TYR:CD2	1:L:194:GLY:HA3	2.45	0.51
1:C:55:GLN:OE1	1:C:63:ARG:NH1	2.43	0.51
1:L:202:ILE:HG23	1:L:203:THR:HG23	1.93	0.51
1:I:10:ARG:NH1	2:I:410:HOH:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:ARG:HD2	2:G:668:HOH:O	2.10	0.50
1:I:200:GLU:HG2	1:I:254:GLU:HG2	1.93	0.50
1:A:10:ARG:HD2	1:A:233:ARG:CZ	2.41	0.50
1:G:245:GLN:NE2	2:G:407:HOH:O	2.45	0.49
1:C:14:PRO:HG3	1:C:222:PRO:HB3	1.93	0.49
1:E:169:TYR:CD2	1:E:194:GLY:HA3	2.47	0.49
1:F:269:GLU:OE1	1:F:298:ARG:NH2	2.40	0.49
1:H:10:ARG:NH1	1:H:233:ARG:CD	2.76	0.49
1:L:224:GLY:HA2	1:L:243:ARG:HH11	1.78	0.49
1:I:169:TYR:CD2	1:I:194:GLY:HA3	2.48	0.48
1:D:200:GLU:HG2	1:D:254:GLU:HG2	1.95	0.48
1:E:298:ARG:NH1	2:E:417:HOH:O	2.47	0.48
1:L:49:LEU:HD13	1:L:63:ARG:HG3	1.94	0.48
1:K:49:LEU:HD13	1:K:63:ARG:HG3	1.96	0.48
1:J:200:GLU:HG2	1:J:254:GLU:HG2	1.96	0.48
1:A:268:ARG:NH2	1:A:276:GLU:HG2	2.29	0.48
1:L:10:ARG:NE	1:L:233:ARG:HH21	2.12	0.48
1:J:169:TYR:CD2	1:J:194:GLY:HA3	2.49	0.47
1:J:68:ARG:HG3	1:J:102:LEU:HD13	1.95	0.47
1:H:224:GLY:HA2	1:H:243:ARG:HH21	1.79	0.47
1:L:261:LEU:HD21	1:L:278:PRO:HB3	1.97	0.47
1:B:7:PRO:HG3	2:B:401:HOH:O	2.14	0.47
1:E:13:PHE:CE2	1:E:45:GLY:HA3	2.49	0.47
1:F:200:GLU:HG2	1:F:254:GLU:HG2	1.96	0.47
1:D:169:TYR:CD2	1:D:194:GLY:HA3	2.50	0.47
1:J:277:ARG:NH1	2:J:404:HOH:O	2.31	0.47
1:J:162:ARG:NH1	2:J:410:HOH:O	2.42	0.46
1:I:277:ARG:HD3	1:I:284:GLU:OE1	2.15	0.46
1:E:224:GLY:HA2	1:E:243:ARG:HH11	1.80	0.46
1:L:90:GLN:NE2	2:L:417:HOH:O	2.48	0.46
1:B:255:ASN:OD1	1:C:256:ARG:NH1	2.49	0.46
1:H:10:ARG:NH2	2:H:401:HOH:O	1.91	0.46
1:B:56:PHE:HZ	1:B:282:MET:CE	2.29	0.45
1:B:169:TYR:CD2	1:B:194:GLY:HA3	2.52	0.45
1:J:280:HIS:CG	1:J:281:PRO:HA	2.52	0.45
1:K:159:ARG:NE	2:K:404:HOH:O	2.40	0.45
1:C:271:GLY:HA2	2:C:401:HOH:O	2.16	0.45
1:H:227:PRO:HB2	1:H:243:ARG:HD3	1.97	0.45
1:B:13:PHE:CE2	1:B:45:GLY:HA3	2.51	0.45
1:H:13:PHE:CE2	1:H:45:GLY:HA3	2.52	0.45
1:G:55:GLN:OE1	1:G:63:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:ASP:CG	1:L:73:HIS:HE2	2.20	0.44
1:C:169:TYR:CD2	1:C:194:GLY:HA3	2.51	0.44
1:I:54:GLU:HG2	1:I:282:MET:HE1	1.98	0.44
1:I:98:ARG:HG3	2:I:402:HOH:O	2.18	0.44
1:A:10:ARG:HD2	1:A:233:ARG:NH1	2.33	0.44
1:H:261:LEU:HD21	1:H:278:PRO:HB3	2.00	0.44
1:B:200:GLU:HG2	1:B:254:GLU:HG2	2.01	0.43
1:I:13:PHE:CE2	1:I:45:GLY:HA3	2.53	0.43
1:K:169:TYR:CD2	1:K:194:GLY:HA3	2.53	0.43
1:H:169:TYR:CD2	1:H:194:GLY:HA3	2.54	0.43
1:C:200:GLU:HG2	1:C:254:GLU:HG2	2.00	0.43
1:I:278:PRO:HG2	2:I:401:HOH:O	2.18	0.43
1:K:200:GLU:HG2	1:K:254:GLU:HG2	1.99	0.43
1:L:269:GLU:OE1	1:L:298:ARG:NH2	2.50	0.43
1:A:169:TYR:CD2	1:A:194:GLY:HA3	2.52	0.43
1:H:141:MET:HE3	1:H:169:TYR:HB3	1.99	0.43
1:C:141:MET:HE3	1:C:169:TYR:HB3	2.00	0.43
1:A:176:GLY:HA2	2:D:403:HOH:O	2.19	0.43
1:A:22:ASP:CG	2:A:402:HOH:O	2.46	0.43
1:E:10:ARG:HG3	2:E:401:HOH:O	2.19	0.43
1:B:261:LEU:HD21	1:B:278:PRO:HB3	2.00	0.42
1:A:21:ALA:HB3	2:A:401:HOH:O	2.18	0.42
1:A:277:ARG:NH1	2:A:417:HOH:O	2.52	0.42
1:E:11:GLY:N	2:E:401:HOH:O	2.51	0.42
1:L:13:PHE:O	1:L:216:MET:HG3	2.19	0.42
1:E:200:GLU:HG2	1:E:254:GLU:HG2	2.01	0.42
1:J:64:ASP:O	1:J:68:ARG:HD3	2.19	0.42
1:L:13:PHE:CE2	1:L:45:GLY:HA3	2.53	0.42
1:L:277:ARG:NH1	1:L:284:GLU:CD	2.72	0.42
1:L:10:ARG:HE	1:L:233:ARG:HH21	1.56	0.42
1:E:10:ARG:HE	1:E:233:ARG:HE	1.66	0.42
1:H:200:GLU:HG2	1:H:254:GLU:HG2	2.01	0.42
1:L:297:ALA:O	1:L:302:PRO:HD3	2.20	0.42
1:G:13:PHE:CE2	1:G:45:GLY:HA3	2.54	0.42
1:A:13:PHE:CE2	1:A:45:GLY:HA3	2.55	0.41
1:A:261:LEU:HD21	1:A:278:PRO:HB3	2.01	0.41
1:G:277:ARG:HD2	1:G:284:GLU:OE1	2.20	0.41
1:I:10:ARG:HH11	1:I:233:ARG:HH11	1.68	0.41
1:I:230:GLU:HA	1:I:233:ARG:HH22	1.85	0.41
1:J:261:LEU:HD21	1:J:278:PRO:HB3	2.02	0.41
1:C:13:PHE:CE2	1:C:45:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:171:KYQ:HE	1:J:216:MET:HB3	2.02	0.41
1:J:186:ARG:NH1	2:J:419:HOH:O	2.53	0.41
1:K:280:HIS:CG	1:K:281:PRO:HA	2.56	0.41
1:F:159:ARG:HD2	2:F:525:HOH:O	2.20	0.41
1:K:141:MET:HE3	1:K:169:TYR:HB3	2.03	0.41
1:K:261:LEU:HD21	1:K:278:PRO:HB3	2.02	0.41
1:E:141:MET:HE3	1:E:169:TYR:HB3	2.03	0.41
1:H:10:ARG:NH1	1:H:233:ARG:HD3	2.36	0.41
1:H:161:ALA:HB2	1:H:170:PHE:HZ	1.86	0.41
1:J:97:LEU:O	1:J:101:GLN:HG2	2.20	0.41
1:J:256:ARG:NH1	1:K:255:ASN:OD1	2.54	0.40
1:C:51:ASN:ND2	2:C:402:HOH:O	2.11	0.40
1:L:22:ASP:OD1	1:L:275:SER:HB2	2.21	0.40
1:L:200:GLU:HG2	1:L:254:GLU:HG2	2.04	0.40
1:J:233:ARG:HE	1:J:233:ARG:HB2	1.68	0.40
1:D:6:THR:N	1:D:7:PRO:CD	2.84	0.40
1:J:14:PRO:HD2	1:J:45:GLY:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:629:HOH:O	2:D:608:HOH:O[1_455]	2.12	0.08
2:B:510:HOH:O	2:J:407:HOH:O[1_546]	2.18	0.02

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	301/320 (94%)	294 (98%)	7 (2%)	0	100	100
1	B	301/320 (94%)	293 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	300/320 (94%)	293 (98%)	7 (2%)	0	100	100
1	D	300/320 (94%)	293 (98%)	7 (2%)	0	100	100
1	E	300/320 (94%)	295 (98%)	5 (2%)	0	100	100
1	F	300/320 (94%)	294 (98%)	6 (2%)	0	100	100
1	G	300/320 (94%)	293 (98%)	7 (2%)	0	100	100
1	H	301/320 (94%)	294 (98%)	7 (2%)	0	100	100
1	I	299/320 (93%)	293 (98%)	6 (2%)	0	100	100
1	J	299/320 (93%)	295 (99%)	4 (1%)	0	100	100
1	K	299/320 (93%)	292 (98%)	7 (2%)	0	100	100
1	L	299/320 (93%)	293 (98%)	6 (2%)	0	100	100
All	All	3599/3840 (94%)	3522 (98%)	77 (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	236/250 (94%)	235 (100%)	1 (0%)	91	84
1	B	236/250 (94%)	235 (100%)	1 (0%)	91	84
1	C	235/250 (94%)	234 (100%)	1 (0%)	91	84
1	D	235/250 (94%)	234 (100%)	1 (0%)	91	84
1	E	235/250 (94%)	234 (100%)	1 (0%)	91	84
1	F	235/250 (94%)	234 (100%)	1 (0%)	91	84
1	G	235/250 (94%)	235 (100%)	0	100	100
1	H	236/250 (94%)	234 (99%)	2 (1%)	81	70
1	I	235/250 (94%)	232 (99%)	3 (1%)	69	50
1	J	234/250 (94%)	234 (100%)	0	100	100
1	K	234/250 (94%)	231 (99%)	3 (1%)	69	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	235/250 (94%)	234 (100%)	1 (0%)	91 84
All	All	2821/3000 (94%)	2806 (100%)	15 (0%)	88 80

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	PHE
1	B	268	ARG
1	C	190	ASP
1	D	268	ARG
1	E	52	PHE
1	F	52	PHE
1	H	52	PHE
1	H	268	ARG
1	I	10	ARG
1	I	22	ASP
1	I	52	PHE
1	K	10	ARG
1	K	22	ASP
1	K	268	ARG
1	L	268	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	179	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)

12 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	KYQ	A	171	1	7,8,15	0.64	0	3,8,18	0.72	0
1	KYQ	G	171	1	7,8,15	0.54	0	3,8,18	0.64	0
1	KYQ	L	171	1	7,8,15	0.57	0	3,8,18	0.73	0
1	KYQ	D	171	1	7,8,15	0.50	0	3,8,18	0.63	0
1	KYQ	E	171	1	7,8,15	0.58	0	3,8,18	0.49	0
1	KYQ	I	171	1	7,8,15	0.56	0	3,8,18	0.64	0
1	KYQ	K	171	1	7,8,15	0.55	0	3,8,18	0.56	0
1	KYQ	F	171	1	7,8,15	0.53	0	3,8,18	0.56	0
1	KYQ	B	171	1	11,14,15	0.85	0	6,16,18	1.68	2 (33%)
1	KYQ	J	171	1	7,8,15	0.54	0	3,8,18	0.82	0
1	KYQ	H	171	1	7,8,15	0.54	0	3,8,18	0.58	0
1	KYQ	C	171	1	11,14,15	1.00	0	6,16,18	1.65	1 (16%)

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
1	KYQ	A	171	1	-	1/6/7/18	-
1	KYQ	G	171	1	-	1/6/7/18	-
1	KYQ	L	171	1	-	1/6/7/18	-
1	KYQ	D	171	1	-	1/6/7/18	-
1	KYQ	E	171	1	-	1/6/7/18	-
1	KYQ	I	171	1	-	1/6/7/18	-
1	KYQ	K	171	1	-	1/6/7/18	-
1	KYQ	F	171	1	-	1/6/7/18	-
1	KYQ	B	171	1	-	4/11/16/18	-
1	KYQ	J	171	1	-	1/6/7/18	-
1	KYQ	H	171	1	-	1/6/7/18	-
1	KYQ	C	171	1	-	3/11/16/18	-

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	C	171	KYQ	CE-NZ-C11	3.53	131.25	121.67
1	B	171	KYQ	CE-NZ-C11	3.12	130.14	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	171	KYQ	O16-C12-O15	-2.04	118.94	123.61

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	171	KYQ	O-C-CA-CB
1	B	171	KYQ	O-C-CA-CB
1	B	171	KYQ	NZ-C11-C12-O16
1	B	171	KYQ	NZ-C11-C12-O15
1	B	171	KYQ	C12-C11-C13-O14
1	C	171	KYQ	O-C-CA-CB
1	C	171	KYQ	NZ-C11-C12-O16
1	C	171	KYQ	C12-C11-C13-O14
1	D	171	KYQ	O-C-CA-CB
1	E	171	KYQ	O-C-CA-CB
1	F	171	KYQ	O-C-CA-CB
1	G	171	KYQ	O-C-CA-CB
1	H	171	KYQ	O-C-CA-CB
1	I	171	KYQ	O-C-CA-CB
1	J	171	KYQ	O-C-CA-CB
1	K	171	KYQ	O-C-CA-CB
1	L	171	KYQ	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	171	KYQ	1	0
1	J	171	KYQ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	303/320 (94%)	-0.40	2 (0%)	87	87	9, 14, 23, 43	0
1	B	303/320 (94%)	-0.35	3 (0%)	82	82	8, 12, 22, 42	0
1	C	302/320 (94%)	-0.42	2 (0%)	87	87	8, 14, 23, 46	0
1	D	302/320 (94%)	-0.34	1 (0%)	94	93	9, 13, 21, 38	0
1	E	302/320 (94%)	-0.32	2 (0%)	87	87	12, 19, 29, 45	0
1	F	302/320 (94%)	-0.30	3 (0%)	82	82	11, 18, 27, 46	0
1	G	302/320 (94%)	-0.40	3 (0%)	82	82	10, 15, 24, 46	0
1	H	303/320 (94%)	-0.22	5 (1%)	70	69	12, 20, 31, 56	0
1	I	301/320 (94%)	0.15	5 (1%)	70	69	14, 24, 36, 49	0
1	J	301/320 (94%)	-0.37	0	100	100	11, 15, 26, 38	0
1	K	301/320 (94%)	-0.31	1 (0%)	94	93	11, 20, 31, 38	0
1	L	301/320 (94%)	0.24	7 (2%)	60	59	17, 26, 37, 52	0
All	All	3623/3840 (94%)	-0.25	34 (0%)	84	84	8, 17, 31, 56	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	308	ALA	7.8
1	G	6	THR	7.0
1	F	6	THR	6.2
1	C	6	THR	5.6
1	A	6	THR	5.4
1	E	6	THR	4.8
1	H	6	THR	4.7
1	H	309	HIS	4.4
1	I	6	THR	4.2
1	B	308	ALA	4.0
1	B	309	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	6	THR	3.8
1	A	309	HIS	3.5
1	L	6	THR	3.5
1	G	308	ALA	3.5
1	B	6	THR	3.5
1	I	22	ASP	3.3
1	L	22	ASP	3.2
1	H	22	ASP	3.2
1	L	71	LEU	2.7
1	F	308	ALA	2.7
1	I	68	ARG	2.6
1	I	75	ALA	2.5
1	H	190	ASP	2.5
1	E	22	ASP	2.4
1	K	22	ASP	2.4
1	G	7	PRO	2.3
1	L	74	VAL	2.3
1	C	22	ASP	2.3
1	L	42	GLY	2.1
1	L	233	ARG	2.1
1	L	75	ALA	2.1
1	I	277	ARG	2.1
1	F	23	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	KYQ	I	171	9/16	0.89	0.10	17,21,26,27	0
1	KYQ	L	171	9/16	0.90	0.10	20,22,28,29	0
1	KYQ	C	171	15/16	0.93	0.12	8,14,25,25	6
1	KYQ	F	171	9/16	0.94	0.09	14,14,21,23	0
1	KYQ	H	171	9/16	0.94	0.08	15,16,22,23	0
1	KYQ	B	171	15/16	0.94	0.11	8,13,24,26	6
1	KYQ	E	171	9/16	0.94	0.08	14,14,21,22	0
1	KYQ	D	171	9/16	0.95	0.12	14,14,17,20	0
1	KYQ	J	171	9/16	0.96	0.09	11,12,21,23	0
1	KYQ	K	171	9/16	0.96	0.07	14,16,23,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KYQ	A	171	9/16	0.96	0.11	14,14,17,22	0
1	KYQ	G	171	9/16	0.97	0.10	14,14,18,23	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.