



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 10:14 PM JST

PDB ID : 7C0C  
Title : Crystal structure of Azospirillum brasilense L-2-keto-3-deoxyarabonate dehydratase (apo form)  
Authors : Watanabe, Y.; Nobuchi, R.; Watanabe, S.  
Deposited on : 2020-05-01  
Resolution : 1.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

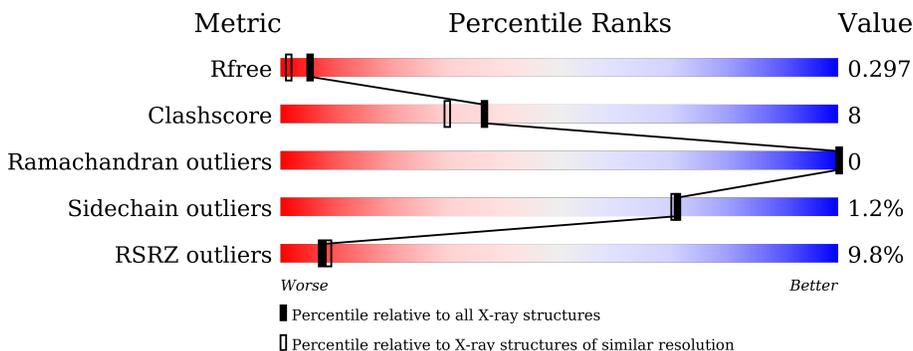
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	320	
1	B	320	
1	C	320	
1	D	320	
1	E	320	
1	F	320	

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Mol	Chain	Length	Quality of chain
1	G	320	<p>% 84% 10% 5%</p>
1	H	320	<p>% 85% 9% 5%</p>
1	I	320	<p>14% 78% 17% 5%</p>
1	J	320	<p>18% 72% 23% 5%</p>
1	K	320	<p>44% 57% 36% 5%</p>
1	L	320	<p>26% 62% 31% 5%</p>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29770 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
			Total	C	N	O	S			
1	A	302	2326	1468	420	427	11	0	0	0
1	B	304	2342	1477	424	430	11	0	0	0
1	C	303	2331	1471	421	428	11	0	0	0
1	D	303	2331	1471	421	428	11	0	0	0
1	E	304	2342	1477	424	430	11	0	0	0
1	F	304	2342	1477	424	430	11	0	0	0
1	G	303	2331	1471	421	428	11	0	0	0
1	H	303	2331	1471	421	428	11	0	0	0
1	I	304	2330	1471	418	430	11	0	0	0
1	J	304	2342	1477	424	430	11	0	0	0
1	K	303	2327	1469	420	427	11	0	0	0
1	L	303	2331	1471	421	428	11	0	0	0

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.

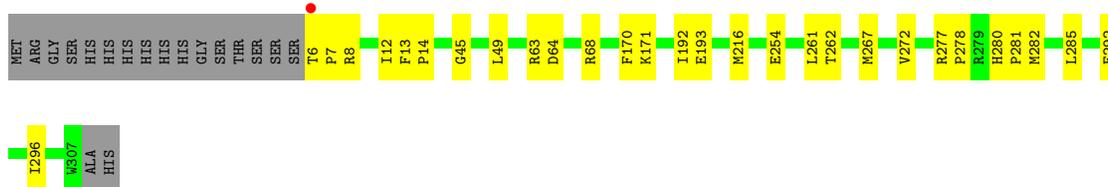
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	178	Total O 178 178	0	0
2	B	112	Total O 112 112	0	0
2	C	123	Total O 123 123	0	0
2	D	140	Total O 140 140	0	0
2	E	228	Total O 228 228	0	0
2	F	199	Total O 199 199	0	0
2	G	192	Total O 192 192	0	0
2	H	238	Total O 238 238	0	0
2	I	116	Total O 116 116	0	0
2	J	83	Total O 83 83	0	0
2	K	93	Total O 93 93	0	0
2	L	62	Total O 62 62	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.

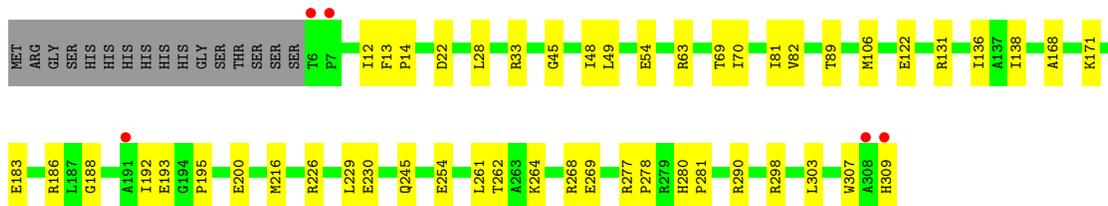
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain A: 



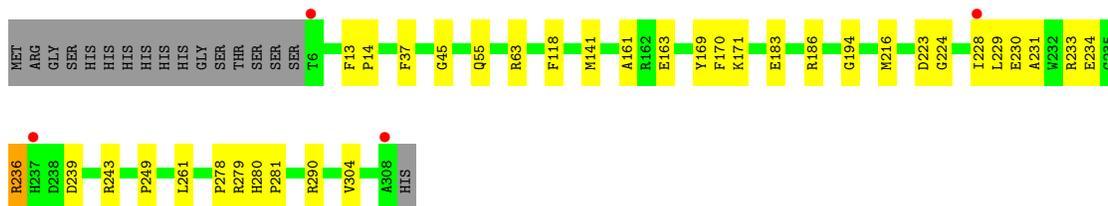
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain B: 



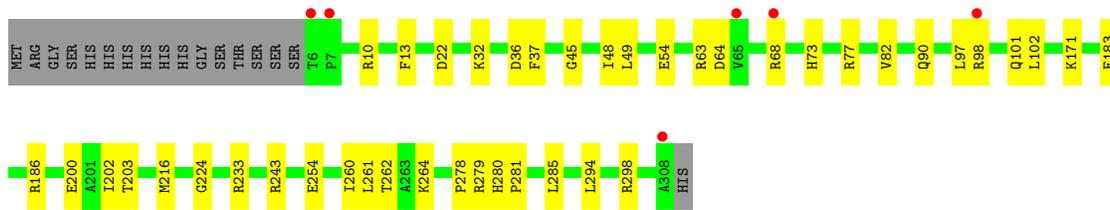
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain C: 

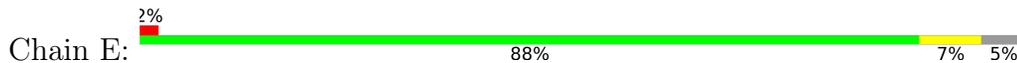


- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

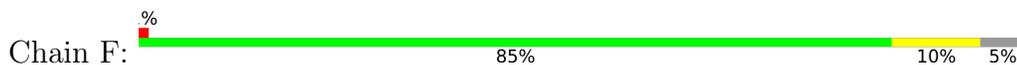
Chain D: 



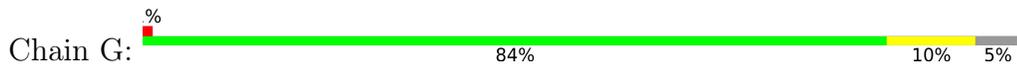
● Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



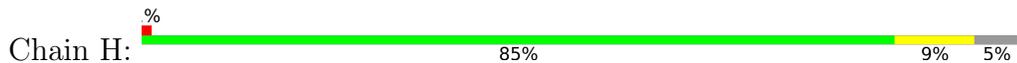
● Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



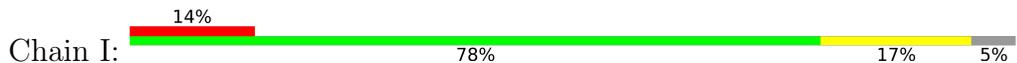
● Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

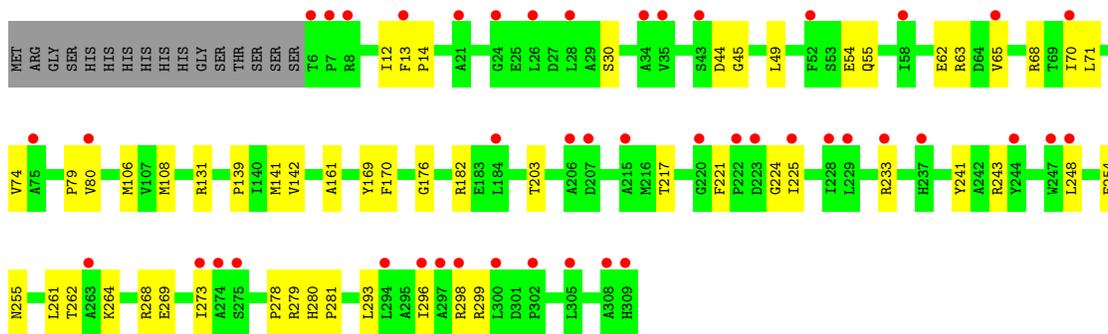


● Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

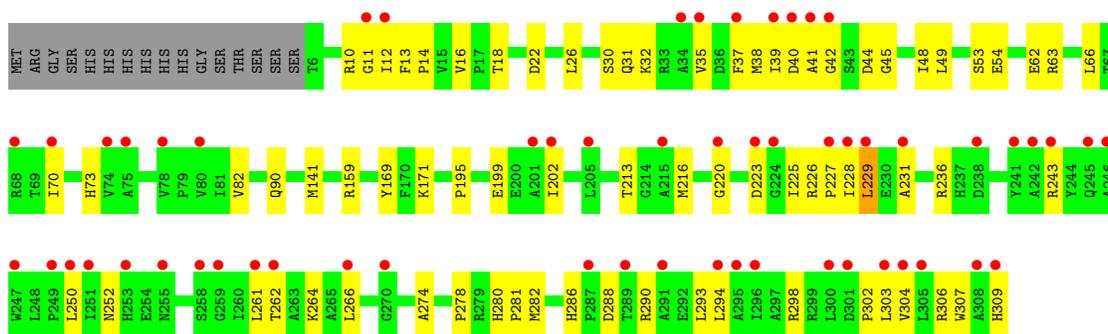


● Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

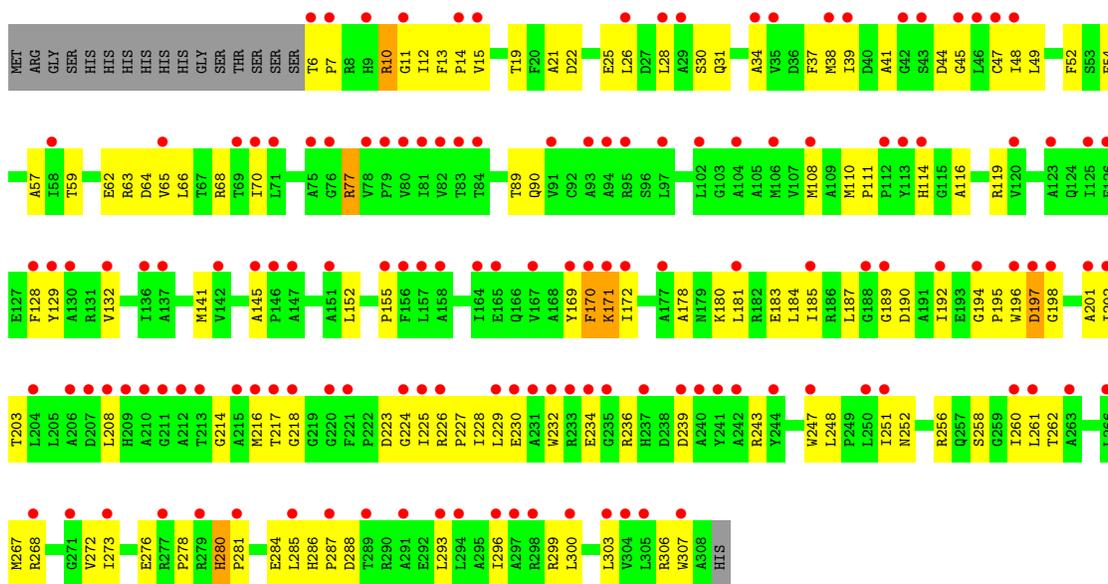




- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

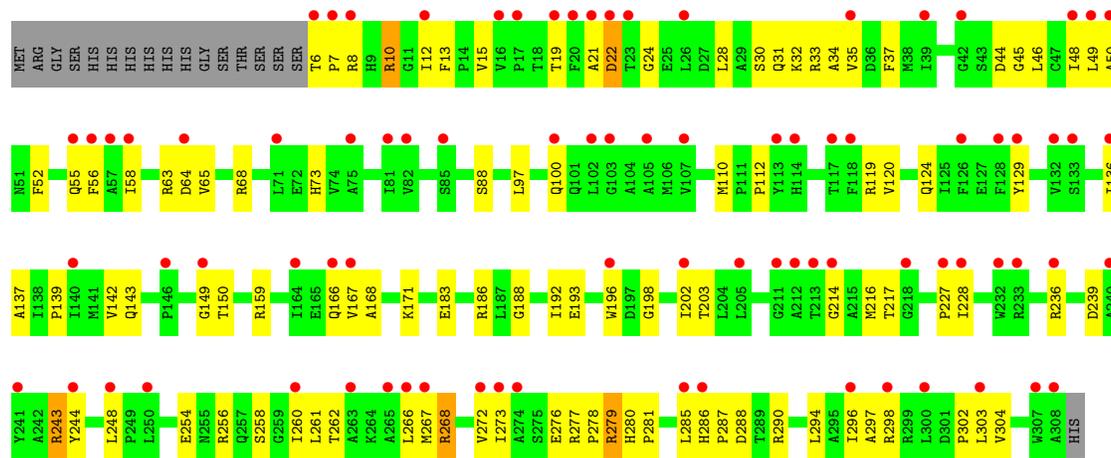


- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.39Å 81.81Å 144.42Å 85.47° 87.86° 75.62°	Depositor
Resolution (Å)	40.44 – 1.90 40.44 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.1 (40.44-1.90) 96.1 (40.44-1.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 1.89Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.252 , 0.297 0.252 , 0.297	Depositor DCC
$R_{free}$ test set	12870 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtrriage
Anisotropy	0.426	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	29770	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.25	0/2379	0.43	0/3236
1	B	0.25	0/2396	0.42	0/3258
1	C	0.25	0/2384	0.43	0/3243
1	D	0.25	0/2384	0.44	0/3243
1	E	0.26	0/2396	0.44	0/3258
1	F	0.26	0/2396	0.44	0/3258
1	G	0.25	0/2384	0.43	0/3243
1	H	0.26	0/2384	0.43	0/3243
1	I	0.25	0/2384	0.44	0/3244
1	J	0.27	0/2396	0.46	0/3258
1	K	0.28	0/2380	0.48	0/3238
1	L	0.26	0/2384	0.44	0/3243
All	All	0.26	0/28647	0.44	0/38965

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	K	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	190	ASP	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	2326	0	2309	17	0
1	B	2342	0	2321	30	0
1	C	2331	0	2314	25	0
1	D	2331	0	2314	26	0
1	E	2342	0	2321	15	0
1	F	2342	0	2321	18	0
1	G	2331	0	2314	21	0
1	H	2331	0	2314	18	0
1	I	2330	0	2299	38	0
1	J	2342	0	2321	57	0
1	K	2327	0	2308	107	0
1	L	2331	0	2314	84	0
2	A	178	0	0	2	0
2	B	112	0	0	2	0
2	C	123	0	0	1	0
2	D	140	0	0	2	0
2	E	228	0	0	4	0
2	F	199	0	0	2	0
2	G	192	0	0	3	0
2	H	238	0	0	4	0
2	I	116	0	0	10	0
2	J	83	0	0	7	0
2	K	93	0	0	11	0
2	L	62	0	0	11	0
All	All	29770	0	27770	442	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 8.

All (442) 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:J:31:GLN:NE2	2:J:401:HOH:O	2.04	0.90
1:J:228:ILE:N	1:J:243:ARG:HH22	1.69	0.89
1:K:226:ARG:HE	1:K:230:GLU:HG3	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:110:MET:SD	1:L:143:GLN:NE2	2.48	0.85
1:I:248:LEU:HD12	1:L:248:LEU:HG	1.57	0.84
1:K:224:GLY:HA2	1:K:243:ARG:HH21	1.43	0.82
1:L:100:GLN:HE22	1:L:136:ILE:HA	1.44	0.82
1:K:89:THR:HG22	1:K:128:PHE:HD2	1.45	0.80
1:J:266:LEU:HD13	1:J:304:VAL:HG11	1.62	0.80
1:K:31:GLN:NE2	2:K:401:HOH:O	2.14	0.78
1:K:192:ILE:HG13	1:K:192:ILE:O	1.81	0.78
1:J:227:PRO:HB2	1:J:243:ARG:NH2	2.00	0.76
1:K:189:GLY:O	1:K:192:ILE:HG12	1.85	0.76
1:E:68:ARG:NH2	2:E:401:HOH:O	2.20	0.75
1:H:55:GLN:OE1	1:H:63:ARG:NH1	2.20	0.75
1:C:224:GLY:HA2	1:C:243:ARG:HH21	1.53	0.73
1:D:224:GLY:HA2	1:D:243:ARG:HH21	1.54	0.72
1:J:228:ILE:H	1:J:243:ARG:HH22	1.36	0.72
1:K:226:ARG:NE	1:K:230:GLU:HG3	2.06	0.71
1:A:261:LEU:HD21	1:A:278:PRO:HB3	1.73	0.69
1:K:22:ASP:OD1	1:K:22:ASP:N	2.25	0.69
1:E:261:LEU:HD21	1:E:278:PRO:HB3	1.74	0.69
1:J:252:ASN:ND2	2:J:403:HOH:O	2.26	0.69
1:K:44:ASP:OD2	1:K:226:ARG:NH1	2.25	0.69
1:C:186:ARG:O	1:L:186:ARG:NH1	2.26	0.68
1:H:269:GLU:OE1	1:H:298:ARG:NH2	2.26	0.68
1:L:285:LEU:HD22	1:L:290:ARG:HB2	1.74	0.68
1:A:282:MET:SD	2:A:570:HOH:O	2.52	0.67
1:I:261:LEU:HD21	1:I:278:PRO:HB3	1.75	0.67
1:J:54:GLU:OE2	1:J:264:LYS:NZ	2.26	0.67
1:K:12:ILE:HD12	1:K:225:ILE:CG2	2.25	0.67
1:K:201:ALA:CB	1:K:225:ILE:HD11	2.25	0.66
1:K:170:PHE:CE1	1:K:184:LEU:HD21	2.31	0.66
1:L:261:LEU:HD11	1:L:278:PRO:HB3	1.78	0.66
1:L:268:ARG:NH1	2:L:403:HOH:O	2.27	0.65
1:C:163:GLU:OE2	1:J:159:ARG:NH1	2.29	0.65
1:C:234:GLU:HB2	1:C:236:ARG:HE	1.62	0.65
1:F:230:GLU:OE2	1:F:233:ARG:NH1	2.29	0.65
1:L:183:GLU:OE2	1:L:186:ARG:NH2	2.30	0.64
1:K:303:LEU:HD23	1:K:307:TRP:HB2	1.80	0.64
1:J:220:GLY:HA2	1:J:266:LEU:HD11	1.78	0.64
1:K:261:LEU:HD21	1:K:278:PRO:HB3	1.80	0.64
1:K:171:LYS:HE2	1:K:216:MET:HB3	1.78	0.64
1:K:178:ALA:HA	1:K:181:LEU:HD12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:280:HIS:CG	1:K:281:PRO:HA	2.33	0.63
1:B:183:GLU:OE1	1:B:186:ARG:NH2	2.30	0.63
1:I:54:GLU:OE2	1:I:264:LYS:NZ	2.30	0.63
1:C:231:ALA:HA	1:C:236:ARG:NH1	2.14	0.63
1:K:12:ILE:HD11	1:K:217:THR:HG21	1.80	0.63
1:H:269:GLU:OE2	2:H:401:HOH:O	2.16	0.63
1:K:284:GLU:OE2	2:K:402:HOH:O	2.15	0.62
1:K:10:ARG:HH22	1:K:229:LEU:HB3	1.64	0.62
1:L:298:ARG:NH1	2:L:406:HOH:O	2.30	0.62
1:G:261:LEU:HD21	1:G:278:PRO:HB3	1.82	0.62
1:C:261:LEU:HD21	1:C:278:PRO:HB3	1.81	0.61
1:B:12:ILE:HG12	1:B:14:PRO:HD3	1.83	0.61
1:K:48:ILE:HG21	1:K:70:ILE:HG21	1.81	0.61
1:I:182:ARG:NH2	2:I:413:HOH:O	2.34	0.61
1:J:227:PRO:HB2	1:J:243:ARG:CZ	2.31	0.61
1:K:114:HIS:CD2	1:L:56:PHE:HB3	2.36	0.61
1:K:172:ILE:HD11	1:K:184:LEU:HD13	1.83	0.61
1:J:90:GLN:NE2	2:J:408:HOH:O	2.34	0.60
1:L:236:ARG:HB3	1:L:239:ASP:HB2	1.83	0.60
1:J:298:ARG:NH1	2:J:407:HOH:O	2.33	0.60
1:B:261:LEU:HD21	1:B:278:PRO:HB3	1.84	0.60
1:F:234:GLU:OE1	1:F:236:ARG:NH1	2.29	0.60
1:J:39:ILE:O	1:J:42:GLY:N	2.34	0.60
1:B:303:LEU:HD21	1:B:307:TRP:HD1	1.67	0.60
1:K:261:LEU:HD11	1:K:278:PRO:HG3	1.84	0.60
1:B:298:ARG:NH1	2:B:402:HOH:O	2.27	0.59
1:J:171:LYS:HE3	1:J:216:MET:HB3	1.83	0.59
1:L:119:ARG:HH21	1:L:149:GLY:HA3	1.67	0.59
1:I:106:MET:HG3	1:I:139:PRO:HG2	1.85	0.59
1:B:226:ARG:NH1	1:B:230:GLU:OE2	2.36	0.58
1:J:32:LYS:HB3	1:J:73:HIS:CE1	2.37	0.58
1:K:12:ILE:HD11	1:K:217:THR:CG2	2.33	0.58
1:K:185:ILE:HA	1:K:192:ILE:HD13	1.85	0.58
1:L:10:ARG:HA	1:L:196:TRP:CZ2	2.38	0.58
1:I:108:MET:SD	2:I:510:HOH:O	2.57	0.58
1:K:228:ILE:HG13	1:K:243:ARG:HG2	1.84	0.57
1:L:168:ALA:HB1	1:L:193:GLU:HB2	1.85	0.57
1:A:49:LEU:HD13	1:A:63:ARG:HG3	1.86	0.57
1:F:268:ARG:NH2	2:F:406:HOH:O	2.37	0.57
1:D:97:LEU:O	1:D:101:GLN:HG2	2.04	0.57
1:A:171:LYS:HE3	1:A:216:MET:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:293:LEU:HD13	2:K:403:HOH:O	2.05	0.57
1:B:303:LEU:HD21	1:B:307:TRP:CD1	2.40	0.56
1:B:48:ILE:HD11	1:B:82:VAL:HG22	1.86	0.56
1:F:261:LEU:HD21	1:F:278:PRO:HB3	1.86	0.56
1:J:12:ILE:HG12	1:J:14:PRO:HD3	1.87	0.56
1:K:234:GLU:OE1	1:K:236:ARG:NH1	2.38	0.56
1:G:243:ARG:NH1	2:G:405:HOH:O	2.39	0.56
1:K:31:GLN:HE21	1:K:66:LEU:HD22	1.71	0.56
1:K:202:ILE:HG23	1:K:203:THR:HG23	1.88	0.56
1:H:54:GLU:OE2	1:H:264:LYS:NZ	2.38	0.55
1:I:30:SER:HB3	1:I:273:ILE:HG22	1.88	0.55
1:K:243:ARG:HG2	2:K:436:HOH:O	2.06	0.55
1:D:36:ASP:OD1	1:D:77:ARG:NH2	2.36	0.55
1:I:221:PHE:CE2	1:I:225:ILE:HD11	2.42	0.55
1:K:224:GLY:HA2	1:K:243:ARG:NH2	2.19	0.55
1:L:33:ARG:NH1	2:L:412:HOH:O	2.39	0.55
1:A:170:PHE:CE1	1:A:192:ILE:HD12	2.42	0.55
1:L:171:LYS:HE2	1:L:216:MET:HB3	1.88	0.54
1:I:182:ARG:NH2	2:I:414:HOH:O	2.39	0.54
1:A:277:ARG:NH2	2:A:410:HOH:O	2.41	0.54
1:D:54:GLU:OE2	1:D:264:LYS:NZ	2.36	0.54
1:K:38:MET:HG2	2:K:411:HOH:O	2.07	0.54
1:L:167:VAL:N	2:L:415:HOH:O	2.40	0.54
1:E:186:ARG:NH1	2:E:407:HOH:O	2.34	0.54
1:G:8:ARG:NE	1:G:193:GLU:OE1	2.39	0.53
1:L:48:ILE:HG13	1:L:49:LEU:HG	1.90	0.53
1:L:167:VAL:HG23	2:L:415:HOH:O	2.09	0.53
2:I:417:HOH:O	1:J:282:MET:SD	2.59	0.53
1:J:11:GLY:HA2	1:J:229:LEU:HD21	1.90	0.53
1:L:49:LEU:HB3	1:L:63:ARG:CZ	2.39	0.53
1:L:64:ASP:O	1:L:68:ARG:HG2	2.08	0.53
1:L:290:ARG:O	1:L:294:LEU:HG	2.07	0.53
1:K:12:ILE:HD12	1:K:225:ILE:HG23	1.90	0.53
1:D:183:GLU:OE1	1:D:186:ARG:NH2	2.35	0.53
1:E:202:ILE:HG23	1:E:203:THR:HG23	1.89	0.53
1:J:306:ARG:NH1	2:J:402:HOH:O	2.26	0.53
1:J:38:MET:O	1:J:41:ALA:HB3	2.09	0.53
1:K:54:GLU:N	2:K:404:HOH:O	2.20	0.53
1:E:243:ARG:NE	2:E:417:HOH:O	2.41	0.52
1:J:32:LYS:HA	1:J:35:VAL:HG22	1.91	0.52
1:K:12:ILE:HG12	1:K:14:PRO:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:261:LEU:HB2	1:K:285:LEU:HD21	1.91	0.52
1:K:171:LYS:NZ	1:K:198:GLY:HA3	2.24	0.52
1:D:32:LYS:HB3	1:D:73:HIS:CE1	2.44	0.52
1:G:185:ILE:HG12	1:G:192:ILE:HD13	1.90	0.52
1:K:247:TRP:CD2	1:K:300:LEU:HD13	2.45	0.52
1:L:10:ARG:HA	1:L:196:TRP:HZ2	1.75	0.52
1:L:55:GLN:NE2	2:L:413:HOH:O	2.40	0.52
1:J:141:MET:HE2	1:J:169:TYR:HB3	1.91	0.52
1:K:89:THR:HG21	1:L:280:HIS:ND1	2.25	0.52
1:L:280:HIS:CD2	1:L:281:PRO:HA	2.45	0.52
1:K:30:SER:HB3	1:K:273:ILE:HB	1.92	0.52
1:L:286:HIS:ND1	1:L:287:PRO:HD2	2.25	0.52
1:B:200:GLU:HG2	1:B:254:GLU:HG2	1.91	0.52
1:L:15:VAL:HG12	1:L:217:THR:O	2.10	0.51
1:B:168:ALA:HB1	1:B:193:GLU:HB2	1.91	0.51
1:C:171:LYS:HE3	1:C:216:MET:HB3	1.91	0.51
1:I:62:GLU:HA	1:I:65:VAL:HG12	1.92	0.51
1:K:256:ARG:NH2	2:K:414:HOH:O	2.32	0.51
1:G:202:ILE:HG23	1:G:203:THR:HG23	1.93	0.51
1:H:277:ARG:HD3	1:H:284:GLU:OE2	2.10	0.51
1:K:169:TYR:CD2	1:K:194:GLY:HA3	2.45	0.51
1:L:12:ILE:N	1:L:44:ASP:OD2	2.35	0.51
1:L:100:GLN:OE1	1:L:137:ALA:N	2.28	0.51
1:J:303:LEU:HA	1:J:306:ARG:HG3	1.93	0.51
1:C:280:HIS:CG	1:C:281:PRO:HA	2.46	0.51
1:J:266:LEU:CD1	1:J:304:VAL:HG11	2.39	0.51
1:K:181:LEU:O	1:K:185:ILE:HG23	2.10	0.51
1:H:261:LEU:HD21	1:H:278:PRO:HB3	1.91	0.51
1:K:13:PHE:CE2	1:K:45:GLY:HA3	2.45	0.51
1:G:236:ARG:HB3	1:G:239:ASP:HB2	1.93	0.51
1:K:12:ILE:CD1	1:K:225:ILE:CG2	2.89	0.51
1:A:12:ILE:HG12	1:A:14:PRO:HD3	1.93	0.50
1:G:236:ARG:HG3	2:G:421:HOH:O	2.11	0.50
1:G:68:ARG:NH1	2:G:412:HOH:O	2.44	0.50
1:J:199:GLU:O	1:J:202:ILE:HG22	2.11	0.50
1:K:208:LEU:HD23	1:K:232:TRP:CB	2.41	0.50
1:K:227:PRO:HB2	1:K:243:ARG:HD3	1.94	0.50
1:L:171:LYS:NZ	1:L:198:GLY:HA3	2.26	0.50
1:B:28:LEU:HD22	1:B:69:THR:HG21	1.92	0.50
1:K:12:ILE:HG21	1:K:226:ARG:HB2	1.94	0.50
1:K:28:LEU:HA	1:K:31:GLN:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:108:MET:SD	1:K:216:MET:HE1	2.51	0.50
1:H:48:ILE:HG21	1:H:70:ILE:HG21	1.93	0.50
1:J:231:ALA:O	1:J:236:ARG:N	2.44	0.50
1:J:22:ASP:OD2	1:J:22:ASP:N	2.44	0.50
1:F:49:LEU:HD13	1:F:63:ARG:HG3	1.94	0.49
1:K:201:ALA:HB1	1:K:225:ILE:HD11	1.93	0.49
1:B:245:GLN:HG3	1:C:249:PRO:HG2	1.95	0.49
1:B:269:GLU:OE1	1:B:298:ARG:NH2	2.44	0.49
1:J:262:THR:O	1:J:266:LEU:HG	2.12	0.49
1:H:72:GLU:OE2	2:H:402:HOH:O	2.20	0.49
1:H:202:ILE:HG23	1:H:203:THR:HG23	1.95	0.49
1:L:97:LEU:HD12	1:L:100:GLN:HE21	1.76	0.49
1:B:254:GLU:HB2	1:B:262:THR:HG21	1.95	0.49
1:D:98:ARG:O	1:D:102:LEU:HD23	2.11	0.49
1:I:255:ASN:OD1	1:L:256:ARG:NH1	2.45	0.49
1:F:133:SER:OG	1:F:166:GLN:HG2	2.13	0.49
1:F:183:GLU:OE1	1:F:186:ARG:NH2	2.38	0.49
1:K:90:GLN:NE2	2:K:433:HOH:O	2.45	0.49
1:I:70:ILE:O	1:I:74:VAL:HG13	2.13	0.49
1:C:236:ARG:HB3	1:C:239:ASP:HB2	1.94	0.49
1:I:221:PHE:O	1:I:225:ILE:HD13	2.12	0.49
1:B:171:LYS:HE3	1:B:216:MET:HB3	1.95	0.48
1:J:37:PHE:CE1	1:J:303:LEU:HD23	2.48	0.48
1:K:110:MET:CE	1:K:145:ALA:HB3	2.43	0.48
1:L:258:SER:HB2	1:L:262:THR:OG1	2.13	0.48
1:K:64:ASP:O	1:K:68:ARG:HG3	2.12	0.48
1:L:276:GLU:OE2	1:L:290:ARG:NH1	2.43	0.48
1:G:55:GLN:OE1	1:G:63:ARG:NH1	2.47	0.48
1:L:65:VAL:O	1:L:68:ARG:HG3	2.14	0.48
1:F:277:ARG:NE	2:F:412:HOH:O	2.46	0.48
1:J:26:LEU:HD11	1:J:62:GLU:HG2	1.95	0.48
1:C:55:GLN:OE1	1:C:63:ARG:NH1	2.47	0.48
1:J:303:LEU:HA	1:J:306:ARG:CZ	2.43	0.48
1:G:67:THR:O	1:G:71:LEU:HD23	2.13	0.48
1:A:280:HIS:CG	1:A:281:PRO:HA	2.49	0.48
1:K:111:PRO:HG3	1:K:152:LEU:HD11	1.96	0.48
1:J:250:LEU:N	2:J:420:HOH:O	2.47	0.48
1:L:236:ARG:NH1	2:L:417:HOH:O	2.47	0.47
1:J:261:LEU:HD21	1:J:278:PRO:HB3	1.96	0.47
1:L:13:PHE:HB3	2:L:427:HOH:O	2.14	0.47
1:L:55:GLN:HG3	1:L:56:PHE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:MET:HE3	1:C:169:TYR:HB3	1.97	0.47
1:D:261:LEU:HD21	1:D:278:PRO:HB3	1.97	0.47
1:H:64:ASP:O	1:H:68:ARG:HG3	2.14	0.47
1:J:307:TRP:CH2	1:J:309:HIS:HB2	2.48	0.47
1:D:13:PHE:CE2	1:D:45:GLY:HA3	2.49	0.47
1:L:30:SER:HB3	1:L:273:ILE:HG22	1.97	0.47
1:E:13:PHE:CE2	1:E:45:GLY:HA3	2.49	0.47
1:I:71:LEU:HD21	1:I:80:VAL:HB	1.97	0.47
1:H:290:ARG:NH1	2:H:401:HOH:O	2.39	0.47
1:I:254:GLU:HB2	1:I:262:THR:HG21	1.96	0.47
1:J:303:LEU:O	1:J:307:TRP:N	2.47	0.47
1:L:58:ILE:HG22	1:L:279:ARG:NH1	2.30	0.47
1:L:124:GLN:OE1	1:L:124:GLN:N	2.47	0.47
1:L:267:MET:HB3	1:L:272:VAL:HB	1.96	0.47
1:A:6:THR:N	1:A:7:PRO:HD2	2.29	0.47
1:B:280:HIS:CG	1:B:281:PRO:HA	2.50	0.47
1:I:49:LEU:HD13	1:I:63:ARG:HG2	1.96	0.47
1:I:264:LYS:HA	2:I:504:HOH:O	2.15	0.47
1:K:89:THR:HG22	1:K:128:PHE:CD2	2.36	0.47
1:K:116:ALA:HA	1:K:119:ARG:HH12	1.78	0.47
1:K:226:ARG:O	1:K:229:LEU:N	2.48	0.47
1:K:21:ALA:N	1:K:25:GLU:O	2.48	0.47
1:D:171:LYS:HE3	1:D:216:MET:HB3	1.96	0.46
1:D:48:ILE:HD11	1:D:82:VAL:HG22	1.97	0.46
1:J:26:LEU:HD13	1:J:66:LEU:HD21	1.96	0.46
1:F:171:LYS:HE3	1:F:216:MET:HB3	1.96	0.46
1:K:31:GLN:NE2	1:K:66:LEU:HD22	2.30	0.46
1:K:286:HIS:CD2	1:K:287:PRO:HD2	2.50	0.46
1:I:131:ARG:NH2	2:I:410:HOH:O	2.33	0.46
1:L:227:PRO:HB2	1:L:243:ARG:HD3	1.97	0.46
1:A:13:PHE:CE2	1:A:45:GLY:HA3	2.50	0.46
1:F:23:THR:HG23	1:F:25:GLU:H	1.79	0.46
1:J:12:ILE:HG22	1:J:44:ASP:OD1	2.15	0.46
1:L:50:ALA:O	1:L:55:GLN:HB3	2.16	0.46
1:K:6:THR:N	1:K:7:PRO:HD2	2.31	0.46
1:B:49:LEU:HD13	1:B:63:ARG:HG3	1.98	0.46
1:K:155:PRO:HA	1:K:187:LEU:HD23	1.97	0.46
1:D:202:ILE:HG23	1:D:203:THR:HG23	1.98	0.46
1:K:57:ALA:HB1	1:L:88:SER:HB2	1.96	0.46
1:L:254:GLU:HB2	1:L:262:THR:HG21	1.97	0.46
1:I:55:GLN:OE1	1:I:63:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ILE:HG21	1:B:70:ILE:HG21	1.97	0.46
1:J:14:PRO:HD2	1:J:45:GLY:O	2.16	0.46
1:L:32:LYS:HB3	1:L:73:HIS:CD2	2.51	0.46
1:B:192:ILE:HG22	1:B:195:PRO:HD3	1.97	0.45
1:I:161:ALA:O	2:I:401:HOH:O	2.21	0.45
1:K:171:LYS:HD3	1:K:197:ASP:C	2.36	0.45
1:L:49:LEU:HD22	1:L:63:ARG:HD2	1.97	0.45
1:B:54:GLU:OE2	1:B:264:LYS:NZ	2.43	0.45
2:I:413:HOH:O	1:L:288:ASP:HB2	2.15	0.45
1:J:13:PHE:CE2	1:J:45:GLY:HA3	2.51	0.45
1:D:68:ARG:HD3	1:D:98:ARG:HH21	1.81	0.45
1:F:12:ILE:HG12	1:F:14:PRO:HD3	1.98	0.45
1:I:269:GLU:OE1	1:I:298:ARG:NH1	2.49	0.45
1:K:248:LEU:O	1:K:252:ASN:N	2.40	0.45
1:L:8:ARG:NH2	1:L:193:GLU:OE2	2.49	0.45
1:E:48:ILE:HD11	1:E:82:VAL:HG22	1.97	0.45
1:J:290:ARG:O	1:J:293:LEU:HB3	2.16	0.45
1:L:34:ALA:CB	1:L:267:MET:HE1	2.46	0.45
1:L:280:HIS:CG	1:L:281:PRO:HA	2.51	0.45
1:F:81:ILE:HG12	1:F:106:MET:HB3	1.98	0.45
1:F:280:HIS:CG	1:F:281:PRO:HA	2.51	0.45
1:K:258:SER:OG	2:K:403:HOH:O	2.19	0.45
1:L:21:ALA:O	1:L:277:ARG:HD3	2.17	0.45
1:L:49:LEU:HB3	1:L:63:ARG:NH2	2.30	0.45
1:C:290:ARG:NH1	2:C:412:HOH:O	2.50	0.45
1:G:227:PRO:HB2	1:G:243:ARG:HG2	1.99	0.45
1:K:236:ARG:HG2	1:K:239:ASP:HB2	1.98	0.45
1:L:22:ASP:N	2:L:414:HOH:O	2.40	0.45
1:L:31:GLN:O	1:L:35:VAL:HG23	2.17	0.45
1:J:30:SER:OG	1:J:274:ALA:N	2.38	0.45
1:L:37:PHE:HE1	1:L:303:LEU:HG	1.81	0.45
1:L:297:ALA:O	1:L:302:PRO:HD3	2.17	0.45
1:J:18:THR:OG1	1:J:53:SER:O	2.20	0.45
1:L:32:LYS:HB3	1:L:73:HIS:CG	2.52	0.45
1:L:129:TYR:CE1	1:L:142:VAL:HG22	2.52	0.45
1:A:8:ARG:NH2	1:A:193:GLU:OE2	2.47	0.44
1:G:192:ILE:O	1:G:192:ILE:HG13	2.17	0.44
1:G:280:HIS:CG	1:G:281:PRO:HA	2.52	0.44
1:K:52:PHE:CD1	1:K:260:ILE:HG12	2.52	0.44
1:K:296:ILE:HA	1:K:299:ARG:NE	2.32	0.44
1:I:241:TYR:CE1	1:L:296:ILE:HD12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:19:THR:OG1	1:K:31:GLN:HG2	2.17	0.44
1:G:199:GLU:HG2	1:G:255:ASN:ND2	2.33	0.44
1:I:142:VAL:HB	1:I:170:PHE:CD2	2.52	0.44
1:J:220:GLY:CA	1:J:266:LEU:HD11	2.46	0.44
1:K:114:HIS:HD2	1:L:56:PHE:HB3	1.82	0.44
1:L:139:PRO:HA	1:L:166:GLN:HB3	1.98	0.44
1:F:202:ILE:HG23	1:F:203:THR:HG23	1.99	0.44
1:H:254:GLU:HB2	1:H:262:THR:HG21	2.00	0.44
1:K:223:ASP:OD1	1:K:223:ASP:N	2.44	0.44
1:K:286:HIS:CE1	1:K:288:ASP:HB2	2.53	0.44
1:A:64:ASP:OD1	1:A:68:ARG:HD2	2.17	0.44
1:K:26:LEU:HD11	1:K:62:GLU:HB3	1.97	0.44
1:K:65:VAL:HG22	1:K:68:ARG:NH1	2.33	0.44
1:L:244:TYR:CE2	1:L:248:LEU:HD22	2.52	0.44
1:G:12:ILE:HG12	1:G:14:PRO:HD3	2.00	0.44
1:L:22:ASP:HA	1:L:277:ARG:HD3	1.99	0.44
1:J:37:PHE:CZ	1:J:304:VAL:HB	2.51	0.44
1:K:34:ALA:O	1:K:38:MET:HG3	2.17	0.44
1:L:6:THR:N	1:L:7:PRO:HD3	2.32	0.44
1:C:223:ASP:OD1	1:C:223:ASP:N	2.45	0.44
1:E:23:THR:OG1	1:E:25:GLU:OE2	2.29	0.44
1:G:223:ASP:OD1	1:G:223:ASP:N	2.50	0.44
1:L:266:LEU:HB3	1:L:304:VAL:HG21	2.00	0.44
1:C:118:PHE:HE1	1:D:260:ILE:HD11	1.83	0.44
1:L:202:ILE:HG23	1:L:203:THR:HG23	1.99	0.44
1:A:292:GLU:O	1:A:296:ILE:HG13	2.18	0.43
1:K:90:GLN:NE2	2:K:441:HOH:O	2.51	0.43
1:B:13:PHE:CE2	1:B:45:GLY:HA3	2.53	0.43
1:F:52:PHE:CD1	1:F:260:ILE:HG12	2.52	0.43
1:K:15:VAL:HA	1:K:47:CYS:HB3	1.99	0.43
1:B:33:ARG:NH1	1:B:309:HIS:O	2.51	0.43
1:B:136:ILE:HD12	1:B:138:ILE:HG13	2.00	0.43
1:D:200:GLU:HG2	1:D:254:GLU:HG2	1.99	0.43
1:K:258:SER:HB2	1:K:262:THR:HB	2.00	0.43
1:E:261:LEU:HD11	1:E:278:PRO:HG3	2.00	0.43
1:E:280:HIS:CG	1:E:281:PRO:HA	2.52	0.43
1:J:195:PRO:HG2	1:J:213:THR:HG23	2.01	0.43
1:K:217:THR:OG1	1:K:218:GLY:N	2.52	0.43
1:L:46:LEU:N	2:L:410:HOH:O	2.36	0.43
1:G:183:GLU:HG3	1:G:186:ARG:NH2	2.33	0.43
1:I:221:PHE:CD2	1:I:225:ILE:CD1	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:49:LEU:HD13	1:J:63:ARG:HG2	2.00	0.43
1:K:141:MET:HA	1:K:169:TYR:O	2.19	0.43
1:A:267:MET:HB3	1:A:272:VAL:HB	2.01	0.43
1:C:228:ILE:HG12	1:C:243:ARG:HB3	2.01	0.43
1:I:296:ILE:O	1:I:299:ARG:HB2	2.18	0.43
1:C:13:PHE:CE2	1:C:45:GLY:HA3	2.52	0.43
1:D:280:HIS:CG	1:D:281:PRO:HA	2.54	0.43
1:F:36:ASP:CG	1:F:73:HIS:HE2	2.21	0.43
1:H:179:ASN:ND2	2:H:403:HOH:O	2.21	0.43
1:H:280:HIS:CG	1:H:281:PRO:HA	2.53	0.43
1:I:224:GLY:HA2	1:I:243:ARG:HH21	1.83	0.43
1:J:48:ILE:HG21	1:J:70:ILE:HG21	2.01	0.43
1:L:112:PRO:HB2	1:L:120:VAL:HG21	2.01	0.43
1:I:141:MET:HA	1:I:169:TYR:O	2.19	0.43
1:J:225:ILE:O	1:J:228:ILE:HB	2.19	0.43
1:K:152:LEU:O	1:K:180:LYS:NZ	2.39	0.43
1:C:14:PRO:HD2	1:C:45:GLY:O	2.18	0.43
1:H:261:LEU:HB2	1:H:285:LEU:HD13	2.00	0.43
1:I:13:PHE:CE2	1:I:45:GLY:HA3	2.53	0.43
1:K:90:GLN:HE22	1:L:24:GLY:HA3	1.84	0.43
1:L:119:ARG:HD2	1:L:150:THR:HG22	1.99	0.43
1:A:254:GLU:HB2	1:A:262:THR:HG21	2.01	0.42
1:K:59:THR:O	1:K:63:ARG:HG3	2.18	0.42
1:B:229:LEU:HD12	1:B:229:LEU:H	1.84	0.42
1:D:90:GLN:NE2	2:D:816:HOH:O	2.51	0.42
1:I:44:ASP:O	1:I:79:PRO:HD2	2.18	0.42
1:I:203:THR:HB	2:I:402:HOH:O	2.19	0.42
1:K:306:ARG:NE	2:K:409:HOH:O	2.52	0.42
1:D:261:LEU:HD11	1:D:278:PRO:HG3	2.01	0.42
1:I:233:ARG:HD3	1:I:233:ARG:HA	1.78	0.42
1:J:40:ASP:OD2	1:J:40:ASP:N	2.51	0.42
2:J:403:HOH:O	1:K:203:THR:HA	2.18	0.42
1:A:170:PHE:HE1	1:A:192:ILE:HD12	1.84	0.42
1:C:161:ALA:HB2	1:C:170:PHE:HZ	1.84	0.42
1:D:64:ASP:OD1	2:D:801:HOH:O	2.21	0.42
1:J:16:VAL:HG11	1:J:70:ILE:HD12	2.02	0.42
1:J:286:HIS:CE1	1:J:288:ASP:HB2	2.54	0.42
1:K:192:ILE:HD12	1:K:195:PRO:HG3	2.01	0.42
1:B:81:ILE:HG12	1:B:106:MET:HB3	2.01	0.42
1:G:65:VAL:HG22	1:G:68:ARG:HH12	1.85	0.42
1:L:268:ARG:HD2	1:L:276:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:THR:HG21	1:B:131:ARG:HD2	2.01	0.42
1:C:169:TYR:CD2	1:C:194:GLY:HA3	2.54	0.42
1:L:28:LEU:O	1:L:32:LYS:HG3	2.20	0.42
1:I:176:GLY:N	2:I:434:HOH:O	2.53	0.42
1:D:49:LEU:HD13	1:D:63:ARG:HG3	2.01	0.42
1:I:62:GLU:OE2	1:I:279:ARG:NH2	2.28	0.42
1:I:217:THR:HG21	1:I:225:ILE:HG21	2.02	0.42
1:D:10:ARG:NH1	1:D:233:ARG:HD2	2.35	0.42
1:E:290:ARG:NH1	2:E:432:HOH:O	2.52	0.42
1:H:169:TYR:CD2	1:H:194:GLY:HA3	2.55	0.42
1:K:236:ARG:CG	1:K:239:ASP:HB2	2.50	0.42
1:L:58:ILE:HG22	1:L:279:ARG:HH12	1.85	0.42
1:C:230:GLU:OE1	1:C:233:ARG:NH2	2.53	0.41
1:J:226:ARG:O	1:J:229:LEU:HB3	2.19	0.41
1:K:171:LYS:HD3	1:K:198:GLY:N	2.35	0.41
1:D:294:LEU:O	1:D:298:ARG:HG3	2.21	0.41
1:H:183:GLU:OE1	1:H:186:ARG:NH2	2.31	0.41
1:J:48:ILE:HD11	1:J:82:VAL:HG22	2.01	0.41
1:K:37:PHE:CE1	1:K:303:LEU:HD22	2.55	0.41
1:B:183:GLU:CD	1:B:186:ARG:HH21	2.19	0.41
1:B:188:GLY:HA3	1:B:192:ILE:HD11	2.02	0.41
1:B:303:LEU:HD23	1:B:303:LEU:O	2.20	0.41
1:C:230:GLU:CD	1:C:233:ARG:HH22	2.24	0.41
1:G:6:THR:N	1:G:7:PRO:HD2	2.35	0.41
1:I:262:THR:HG23	1:I:293:LEU:HD11	2.02	0.41
1:G:90:GLN:NE2	1:H:25:GLU:OE1	2.53	0.41
1:I:71:LEU:HA	1:I:74:VAL:HG22	2.03	0.41
1:J:278:PRO:HB2	1:J:282:MET:HB3	2.03	0.41
1:K:224:GLY:CA	1:K:243:ARG:HH21	2.22	0.41
1:L:32:LYS:HB3	1:L:73:HIS:CE1	2.55	0.41
1:E:294:LEU:O	1:E:298:ARG:HG3	2.21	0.41
1:K:10:ARG:HH22	1:K:229:LEU:CB	2.31	0.41
1:L:52:PHE:CD1	1:L:260:ILE:HG12	2.56	0.41
1:B:122:GLU:OE1	2:B:401:HOH:O	2.22	0.41
1:D:285:LEU:HD23	1:D:285:LEU:HA	1.94	0.41
1:D:294:LEU:HB3	1:D:298:ARG:NH1	2.35	0.41
1:E:269:GLU:OE1	1:E:298:ARG:NH1	2.47	0.41
1:G:64:ASP:OD2	1:G:68:ARG:NH2	2.54	0.41
1:K:248:LEU:HA	1:K:251:ILE:HB	2.02	0.41
1:D:254:GLU:HB2	1:D:262:THR:HG21	2.03	0.41
1:J:286:HIS:ND1	1:J:288:ASP:HB2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:302:PRO:O	1:J:306:ARG:HG2	2.20	0.41
1:K:10:ARG:NH1	1:K:11:GLY:HA2	2.35	0.41
1:K:37:PHE:O	1:K:41:ALA:N	2.51	0.41
1:K:268:ARG:CB	1:K:276:GLU:HB3	2.51	0.41
1:L:196:TRP:CE2	1:L:214:GLY:HA3	2.56	0.41
1:L:228:ILE:HG13	1:L:243:ARG:HG2	2.03	0.41
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.93	0.41
1:J:280:HIS:CG	1:J:281:PRO:HA	2.56	0.41
1:L:188:GLY:HA3	1:L:192:ILE:HG12	2.03	0.41
1:K:37:PHE:CD1	1:K:303:LEU:HD22	2.55	0.40
1:K:172:ILE:HD12	1:K:181:LEU:HD23	2.03	0.40
1:L:13:PHE:CE2	1:L:45:GLY:HA3	2.56	0.40
1:L:19:THR:HG21	1:L:273:ILE:HG21	2.03	0.40
1:C:280:HIS:CD2	1:C:281:PRO:HA	2.56	0.40
1:D:68:ARG:H	1:D:68:ARG:HG2	1.77	0.40
1:F:20:PHE:CZ	1:F:279:ARG:HG3	2.57	0.40
1:I:280:HIS:CG	1:I:281:PRO:HA	2.56	0.40
1:K:171:LYS:HA	1:K:196:TRP:O	2.21	0.40
1:K:196:TRP:CD2	1:K:214:GLY:HA3	2.56	0.40
1:E:24:GLY:HA3	1:F:90:GLN:HE22	1.86	0.40
1:I:12:ILE:HG12	1:I:14:PRO:HD3	2.03	0.40
1:K:48:ILE:HG13	1:K:49:LEU:HD12	2.03	0.40
1:C:37:PHE:CZ	1:C:304:VAL:HB	2.57	0.40
1:C:183:GLU:OE1	1:C:186:ARG:NH2	2.54	0.40
1:E:227:PRO:HB2	1:E:243:ARG:HE	1.86	0.40
1:K:39:ILE:HD13	1:K:77:ARG:HG3	2.03	0.40
1:K:129:TYR:HA	1:K:132:VAL:HG22	2.02	0.40
1:K:267:MET:HB3	1:K:272:VAL:HB	2.04	0.40
1:L:120:VAL:N	2:L:402:HOH:O	2.39	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	300/320 (94%)	294 (98%)	6 (2%)	0	100	100
1	B	302/320 (94%)	292 (97%)	10 (3%)	0	100	100
1	C	301/320 (94%)	294 (98%)	7 (2%)	0	100	100
1	D	301/320 (94%)	294 (98%)	7 (2%)	0	100	100
1	E	302/320 (94%)	295 (98%)	7 (2%)	0	100	100
1	F	302/320 (94%)	295 (98%)	7 (2%)	0	100	100
1	G	301/320 (94%)	293 (97%)	8 (3%)	0	100	100
1	H	301/320 (94%)	292 (97%)	9 (3%)	0	100	100
1	I	302/320 (94%)	293 (97%)	9 (3%)	0	100	100
1	J	302/320 (94%)	291 (96%)	11 (4%)	0	100	100
1	K	301/320 (94%)	288 (96%)	13 (4%)	0	100	100
1	L	301/320 (94%)	285 (95%)	16 (5%)	0	100	100
All	All	3616/3840 (94%)	3506 (97%)	110 (3%)	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	236/251 (94%)	236 (100%)	0	100	100
1	B	237/251 (94%)	233 (98%)	4 (2%)	60	57
1	C	236/251 (94%)	233 (99%)	3 (1%)	69	68
1	D	236/251 (94%)	233 (99%)	3 (1%)	69	68
1	E	237/251 (94%)	236 (100%)	1 (0%)	91	91
1	F	237/251 (94%)	236 (100%)	1 (0%)	91	91
1	G	236/251 (94%)	234 (99%)	2 (1%)	81	82
1	H	236/251 (94%)	235 (100%)	1 (0%)	91	91
1	I	235/251 (94%)	233 (99%)	2 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	237/251 (94%)	233 (98%)	4 (2%)	60	57
1	K	235/251 (94%)	228 (97%)	7 (3%)	41	33
1	L	236/251 (94%)	230 (98%)	6 (2%)	47	41
All	All	2834/3012 (94%)	2800 (99%)	34 (1%)	71	70

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	ASP
1	B	268	ARG
1	B	277	ARG
1	B	290	ARG
1	C	229	LEU
1	C	236	ARG
1	C	279	ARG
1	D	22	ASP
1	D	37	PHE
1	D	279	ARG
1	E	277	ARG
1	F	268	ARG
1	G	10	ARG
1	G	279	ARG
1	H	268	ARG
1	I	68	ARG
1	I	268	ARG
1	J	10	ARG
1	J	223	ASP
1	J	229	LEU
1	J	294	LEU
1	K	10	ARG
1	K	77	ARG
1	K	170	PHE
1	K	171	LYS
1	K	183	GLU
1	K	197	ASP
1	K	280	HIS
1	L	10	ARG
1	L	22	ASP
1	L	159	ARG
1	L	243	ARG
1	L	268	ARG

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Mol	Chain	Res	Type
1	L	279	ARG

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

Mol	Chain	Res	Type
1	K	90	GLN
1	K	114	HIS
1	L	55	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	302/320 (94%)	0.12	1 (0%) 94 94	16, 25, 34, 52	0
1	B	304/320 (95%)	0.31	5 (1%) 72 74	19, 31, 44, 59	0
1	C	303/320 (94%)	0.23	4 (1%) 77 79	17, 29, 41, 55	0
1	D	303/320 (94%)	0.25	6 (1%) 65 68	18, 29, 42, 62	0
1	E	304/320 (95%)	-0.07	5 (1%) 72 74	13, 20, 32, 53	0
1	F	304/320 (95%)	-0.07	3 (0%) 82 84	14, 21, 31, 48	0
1	G	303/320 (94%)	0.02	4 (1%) 77 79	17, 24, 35, 55	0
1	H	303/320 (94%)	-0.04	2 (0%) 87 88	14, 21, 30, 50	0
1	I	304/320 (95%)	1.02	45 (14%) 2 2	17, 38, 52, 71	0
1	J	304/320 (95%)	1.04	57 (18%) 1 1	17, 41, 58, 69	0
1	K	303/320 (94%)	2.08	141 (46%) 0 0	38, 48, 56, 67	0
1	L	303/320 (94%)	1.47	83 (27%) 0 0	30, 45, 55, 73	0
All	All	3640/3840 (94%)	0.53	356 (9%) 7 8	13, 28, 51, 73	0

All (356) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	308	ALA	9.3
1	K	251	ILE	7.4
1	K	181	LEU	7.3
1	D	308	ALA	6.4
1	K	46	LEU	6.3
1	L	81	ILE	6.2
1	I	309	HIS	6.2
1	I	294	LEU	6.1
1	K	208	LEU	6.0
1	B	308	ALA	6.0
1	I	6	THR	5.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	K	303	LEU	5.8
1	I	298	ARG	5.7
1	K	293	LEU	5.7
1	J	305	LEU	5.5
1	K	261	LEU	5.4
1	H	308	ALA	5.4
1	E	308	ALA	5.3
1	I	297	ALA	5.2
1	I	21	ALA	5.2
1	E	309	HIS	5.2
1	K	196	TRP	5.1
1	F	308	ALA	5.1
1	J	42	GLY	4.8
1	L	58	ILE	4.8
1	J	231	ALA	4.8
1	K	128	PHE	4.7
1	K	91	VAL	4.7
1	K	132	VAL	4.7
1	I	35	VAL	4.6
1	L	42	GLY	4.6
1	J	296	ILE	4.5
1	I	24	GLY	4.5
1	J	291	ALA	4.5
1	J	308	ALA	4.5
1	K	97	LEU	4.4
1	K	136	ILE	4.4
1	L	266	LEU	4.4
1	K	287	PRO	4.4
1	J	229	LEU	4.4
1	K	220	GLY	4.3
1	J	78	VAL	4.3
1	L	6	THR	4.3
1	I	229	LEU	4.3
1	A	6	THR	4.3
1	I	275	SER	4.2
1	G	308	ALA	4.2
1	I	308	ALA	4.2
1	K	142	VAL	4.2
1	B	7	PRO	4.1
1	J	249	PRO	4.1
1	K	247	TRP	4.1
1	K	285	LEU	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	6	THR	4.1
1	J	242	ALA	4.1
1	K	298	ARG	4.0
1	L	21	ALA	4.0
1	K	242	ALA	4.0
1	L	274	ALA	4.0
1	J	309	HIS	4.0
1	L	300	LEU	4.0
1	K	232	TRP	3.9
1	L	71	LEU	3.9
1	K	156	PHE	3.9
1	K	263	ALA	3.9
1	J	304	VAL	3.9
1	K	291	ALA	3.8
1	K	304	VAL	3.8
1	J	251	ILE	3.8
1	K	164	ILE	3.8
1	J	202	ILE	3.7
1	K	204	LEU	3.7
1	K	237	HIS	3.7
1	K	170	PHE	3.7
1	K	197	ASP	3.7
1	K	80	VAL	3.6
1	J	253	HIS	3.6
1	J	289	THR	3.6
1	K	112	PRO	3.6
1	L	20	PHE	3.6
1	K	213	THR	3.6
1	K	167	VAL	3.6
1	L	114	HIS	3.6
1	J	270	GLY	3.5
1	K	102	LEU	3.5
1	L	244	TYR	3.5
1	J	295	ALA	3.5
1	K	218	GLY	3.5
1	K	296	ILE	3.5
1	K	305	LEU	3.5
1	J	75	ALA	3.5
1	D	6	THR	3.4
1	K	185	ILE	3.4
1	J	266	LEU	3.4
1	K	250	LEU	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	K	151	ALA	3.4
1	G	6	THR	3.4
1	K	125	ILE	3.4
1	K	129	TYR	3.4
1	K	239	ASP	3.3
1	K	225	ILE	3.3
1	J	227	PRO	3.3
1	K	26	LEU	3.3
1	L	75	ALA	3.3
1	K	35	VAL	3.3
1	K	210	ALA	3.3
1	K	198	GLY	3.2
1	L	100	GLN	3.2
1	K	76	GLY	3.2
1	I	273	ILE	3.2
1	K	172	ILE	3.2
1	K	6	THR	3.2
1	K	289	THR	3.2
1	J	205	LEU	3.2
1	L	26	LEU	3.2
1	K	241	TYR	3.2
1	L	213	THR	3.2
1	L	212	ALA	3.2
1	K	188	GLY	3.1
1	K	39	ILE	3.1
1	K	78	VAL	3.1
1	J	247	TRP	3.1
1	K	120	VAL	3.1
1	K	9	HIS	3.1
1	L	241	TYR	3.1
1	K	307	TRP	3.0
1	K	75	ALA	3.0
1	L	17	PRO	3.0
1	J	241	TYR	3.0
1	K	47	CYS	3.0
1	K	244	TYR	3.0
1	L	102	LEU	3.0
1	K	94	ALA	3.0
1	I	225	ILE	3.0
1	J	228	ILE	3.0
1	L	56	PHE	3.0
1	L	16	VAL	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	296	ILE	2.9
1	G	190	ASP	2.9
1	L	19	THR	2.9
1	K	169	TYR	2.9
1	L	296	ILE	2.9
1	K	201	ALA	2.9
1	K	84	THR	2.9
1	F	309	HIS	2.9
1	J	300	LEU	2.9
1	L	49	LEU	2.9
1	L	126	PHE	2.9
1	L	248	LEU	2.9
1	K	194	GLY	2.9
1	K	297	ALA	2.9
1	K	273	ILE	2.8
1	L	7	PRO	2.8
1	K	211	GLY	2.8
1	K	277	ARG	2.8
1	L	205	LEU	2.8
1	K	123	ALA	2.8
1	E	6	THR	2.8
1	L	196	TRP	2.8
1	K	58	ILE	2.8
1	K	79	PRO	2.8
1	L	227	PRO	2.8
1	L	107	VAL	2.8
1	E	7	PRO	2.8
1	J	303	LEU	2.7
1	L	260	ILE	2.7
1	K	221	PHE	2.7
1	J	35	VAL	2.7
1	I	26	LEU	2.7
1	L	285	LEU	2.7
1	L	48	ILE	2.7
1	C	6	THR	2.7
1	K	65	VAL	2.7
1	K	82	VAL	2.7
1	L	22	ASP	2.7
1	L	303	LEU	2.7
1	K	11	GLY	2.7
1	J	243	ARG	2.7
1	K	137	ALA	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	220	GLY	2.7
1	K	229	LEU	2.7
1	K	294	LEU	2.7
1	K	300	LEU	2.7
1	J	258	SER	2.7
1	K	231	ALA	2.6
1	L	240	ALA	2.6
1	C	228	ILE	2.6
1	I	228	ILE	2.6
1	K	202	ILE	2.6
1	I	215	ALA	2.6
1	J	201	ALA	2.6
1	K	235	GLY	2.6
1	K	81	ILE	2.6
1	I	65	VAL	2.6
1	K	230	GLU	2.6
1	L	82	VAL	2.6
1	J	41	ALA	2.6
1	K	233	ARG	2.6
1	L	149	GLY	2.6
1	K	28	LEU	2.6
1	I	237	HIS	2.6
1	J	215	ALA	2.6
1	L	232	TRP	2.6
1	L	8	ARG	2.6
1	K	260	ILE	2.6
1	J	74	VAL	2.6
1	K	15	VAL	2.6
1	K	271	GLY	2.6
1	K	34	ALA	2.5
1	K	104	ALA	2.5
1	K	192	ILE	2.5
1	K	69	THR	2.5
1	L	132	VAL	2.5
1	L	167	VAL	2.5
1	L	211	GLY	2.5
1	J	40	ASP	2.5
1	L	307	TRP	2.5
1	I	222	PRO	2.5
1	I	274	ALA	2.5
1	J	287	PRO	2.5
1	K	147	ALA	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	35	VAL	2.5
1	L	233	ARG	2.5
1	J	259	GLY	2.5
1	K	126	PHE	2.5
1	L	118	PHE	2.5
1	I	300	LEU	2.5
1	K	177	ALA	2.5
1	I	80	VAL	2.5
1	I	244	TYR	2.5
1	L	128	PHE	2.5
1	L	166	GLN	2.4
1	K	215	ALA	2.4
1	L	39	ILE	2.4
1	F	6	THR	2.4
1	I	302	PRO	2.4
1	J	11	GLY	2.4
1	J	238	ASP	2.4
1	K	93	ALA	2.4
1	I	13	PHE	2.4
1	K	114	HIS	2.4
1	J	255	ASN	2.4
1	K	279	ARG	2.4
1	C	308	ALA	2.4
1	K	29	ALA	2.4
1	L	57	ALA	2.4
1	K	83	THR	2.4
1	J	223	ASP	2.4
1	K	146	PRO	2.4
1	K	268	ARG	2.4
1	K	206	ALA	2.4
1	I	43	SER	2.4
1	K	113	TYR	2.4
1	J	34	ALA	2.4
1	J	246	ALA	2.4
1	L	265	ALA	2.4
1	J	220	GLY	2.4
1	K	42	GLY	2.4
1	K	48	ILE	2.4
1	K	43	SER	2.3
1	K	266	LEU	2.3
1	L	113	TYR	2.3
1	I	207	ASP	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	298	ARG	2.3
1	I	263	ALA	2.3
1	L	103	GLY	2.3
1	I	223	ASP	2.3
1	J	68	ARG	2.3
1	K	226	ARG	2.3
1	B	309	HIS	2.3
1	J	294	LEU	2.3
1	J	12	ILE	2.3
1	K	70	ILE	2.3
1	L	267	MET	2.3
1	B	191	ALA	2.3
1	K	71	LEU	2.3
1	L	214	GLY	2.3
1	H	6	THR	2.3
1	I	75	ALA	2.3
1	K	155	PRO	2.3
1	K	217	THR	2.3
1	L	236	ARG	2.3
1	K	108	MET	2.2
1	K	145	ALA	2.2
1	I	247	TRP	2.2
1	J	250	LEU	2.2
1	L	23	THR	2.2
1	L	117	THR	2.2
1	I	206	ALA	2.2
1	L	228	ILE	2.2
1	K	157	LEU	2.2
1	L	133	SER	2.2
1	I	34	ALA	2.2
1	K	171	LYS	2.2
1	L	55	GLN	2.2
1	K	189	GLY	2.2
1	L	218	GLY	2.2
1	L	140	ILE	2.2
1	D	98	ARG	2.2
1	I	8	ARG	2.2
1	I	28	LEU	2.2
1	K	14	PRO	2.2
1	L	85	SER	2.2
1	K	240	ALA	2.2
1	J	301	ASP	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	K	165	GLU	2.2
1	D	7	PRO	2.2
1	K	130	ALA	2.2
1	K	207	ASP	2.2
1	J	80	VAL	2.2
1	L	164	ILE	2.1
1	J	261	LEU	2.1
1	K	95	ARG	2.1
1	K	158	ALA	2.1
1	K	212	ALA	2.1
1	L	64	ASP	2.1
1	L	250	LEU	2.1
1	L	105	ALA	2.1
1	I	233	ARG	2.1
1	K	281	PRO	2.1
1	D	65	VAL	2.1
1	L	272	VAL	2.1
1	K	38	MET	2.1
1	G	294	LEU	2.1
1	I	184	LEU	2.1
1	I	248	LEU	2.1
1	I	305	LEU	2.1
1	L	263	ALA	2.1
1	I	52	PHE	2.1
1	J	39	ILE	2.1
1	L	50	ALA	2.1
1	L	202	ILE	2.1
1	L	146	PRO	2.1
1	K	45	GLY	2.1
1	I	58	ILE	2.1
1	K	106	MET	2.0
1	C	237	HIS	2.0
1	I	7	PRO	2.0
1	D	68	ARG	2.0
1	E	186	ARG	2.0
1	K	224	GLY	2.0
1	J	70	ILE	2.0
1	L	12	ILE	2.0
1	L	273	ILE	2.0
1	K	234	GLU	2.0
1	K	209	HIS	2.0
1	L	129	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	37	PHE	2.0
1	J	224	GLY	2.0
1	K	7	PRO	2.0
1	J	245	GLN	2.0
1	I	70	ILE	2.0
1	L	136	ILE	2.0
1	J	262	THR	2.0
1	K	216	MET	2.0
1	L	286	HIS	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.