



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:32 PM UTC

PDB ID : 7C0C / pdb_00007c0c
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

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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

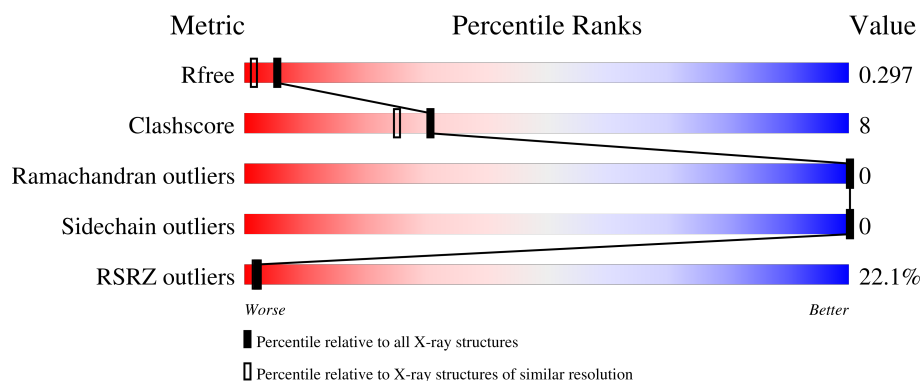
1 Overall quality at a glance

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 ≥ 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	2% 85% 9% 6%
1	B	320	7% 80% 15% 5%
1	C	320	6% 83% 12% 5%
1	D	320	6% 82% 12% 5%
1	E	320	3% 88% 7% 5%

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Mol	Chain	Length	Quality of chain
1	F	320	% 85% 10% 5%
1	G	320	2% 85% 10% 5%
1	H	320	% 85% 10% 5%
1	I	320	35% 76% 19% 5%
1	J	320	46% 72% 22% 5%
1	K	320	78% 57% 38% 5%
1	L	320	63% 63% 32% 5%

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
1	A	302	Total	C	N	O	S	0	0	0
			2326	1468	420	427	11			
1	B	304	Total	C	N	O	S	0	0	0
			2342	1477	424	430	11			
1	C	303	Total	C	N	O	S	0	0	0
			2331	1471	421	428	11			
1	D	303	Total	C	N	O	S	0	0	0
			2331	1471	421	428	11			
1	E	304	Total	C	N	O	S	0	0	0
			2342	1477	424	430	11			
1	F	304	Total	C	N	O	S	0	0	0
			2342	1477	424	430	11			
1	G	303	Total	C	N	O	S	0	0	0
			2331	1471	421	428	11			
1	H	303	Total	C	N	O	S	0	0	0
			2331	1471	421	428	11			
1	I	304	Total	C	N	O	S	0	0	0
			2330	1471	418	430	11			
1	J	304	Total	C	N	O	S	0	0	0
			2342	1477	424	430	11			
1	K	303	Total	C	N	O	S	0	0	0
			2327	1469	420	427	11			
1	L	303	Total	C	N	O	S	0	0	0
			2331	1471	421	428	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

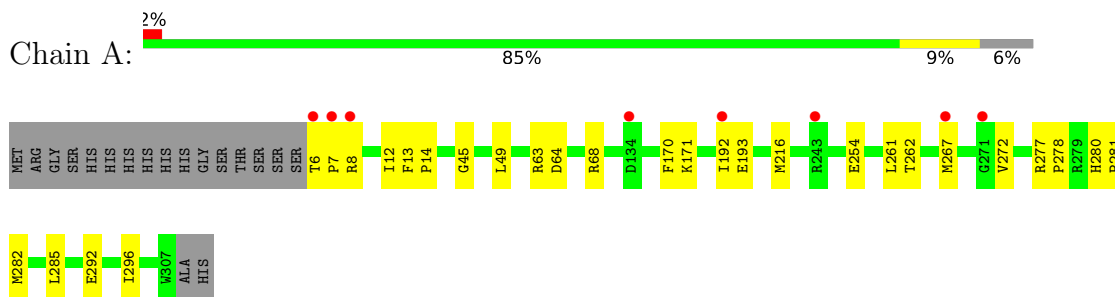
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	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

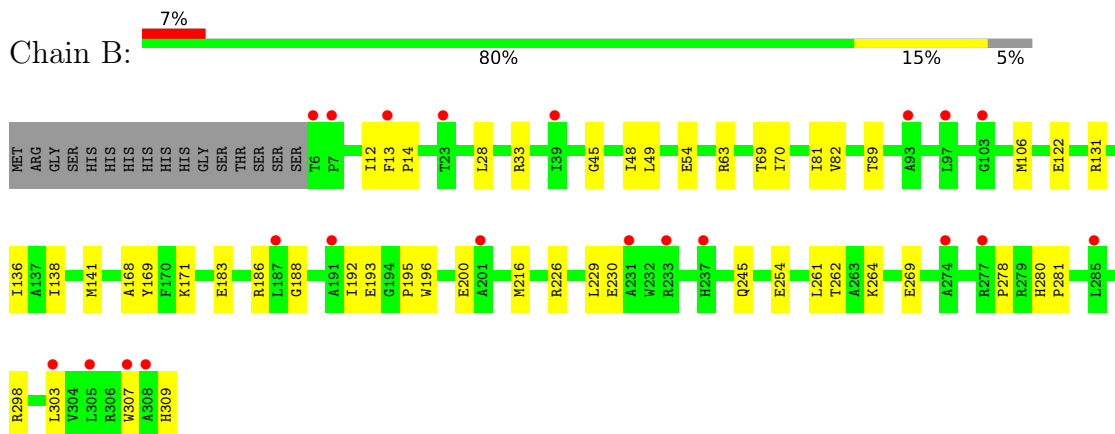
3 Residue-property plots [i](#)

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.

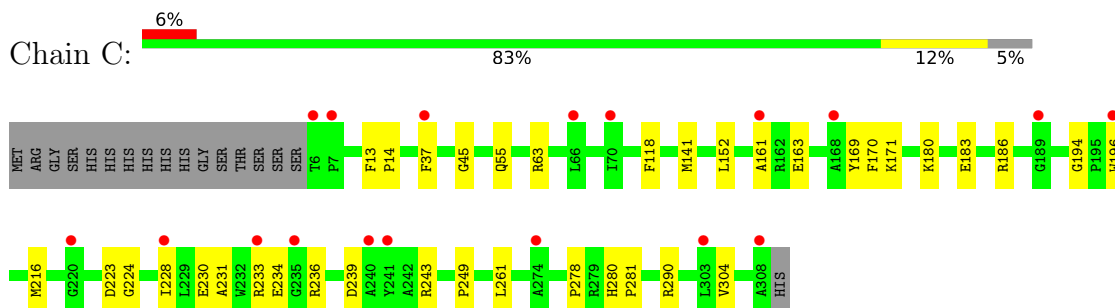
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



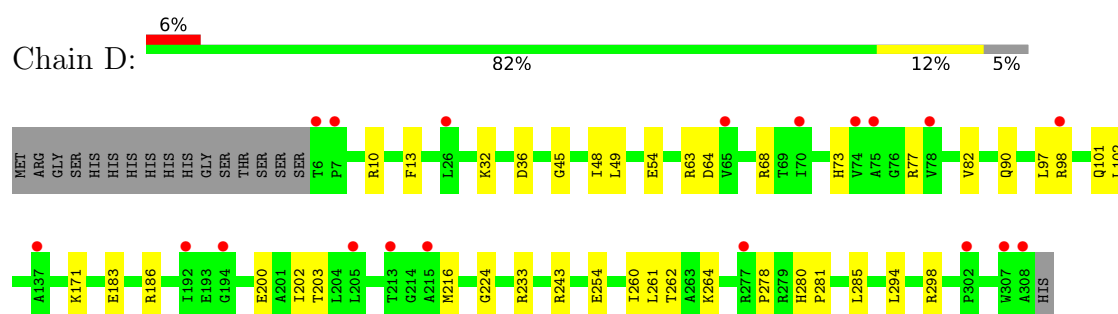
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



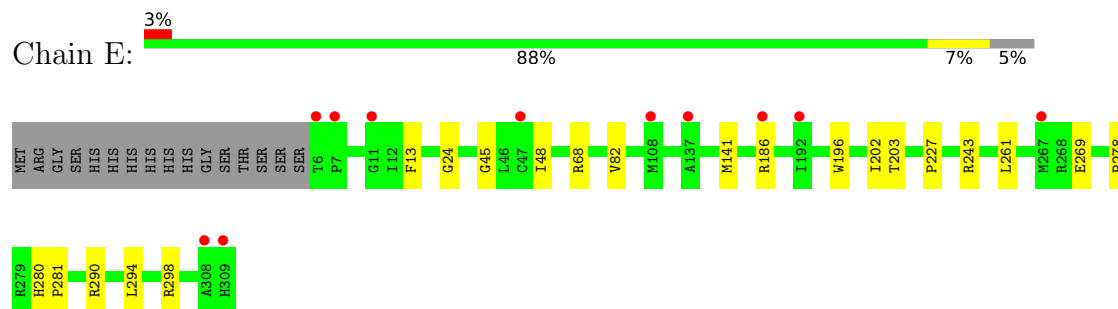
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



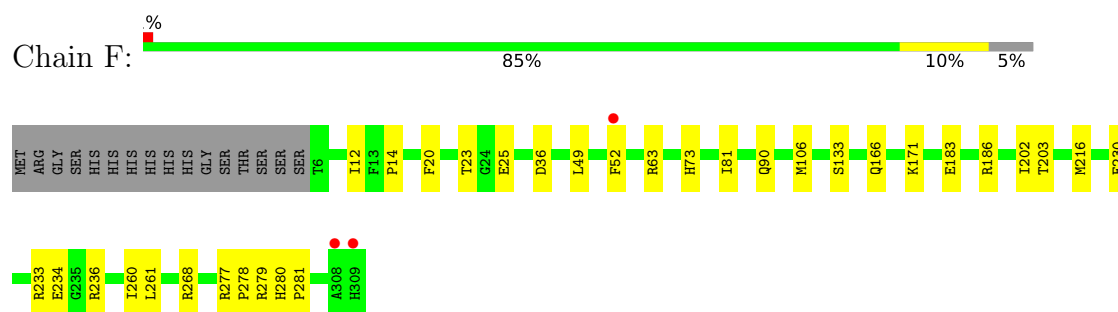
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



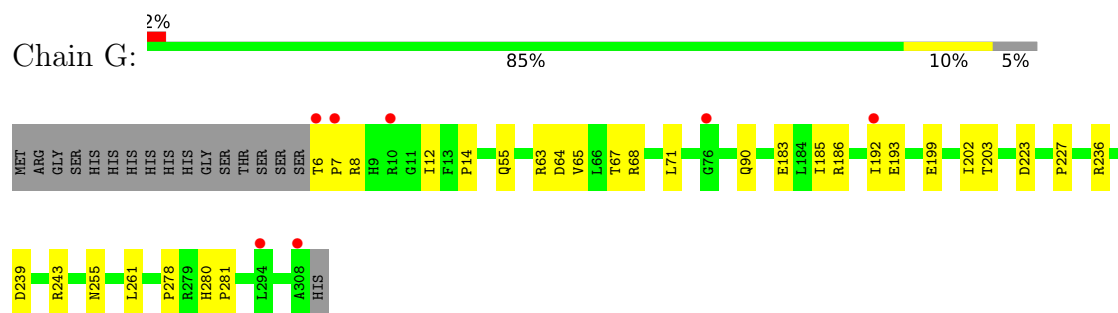
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



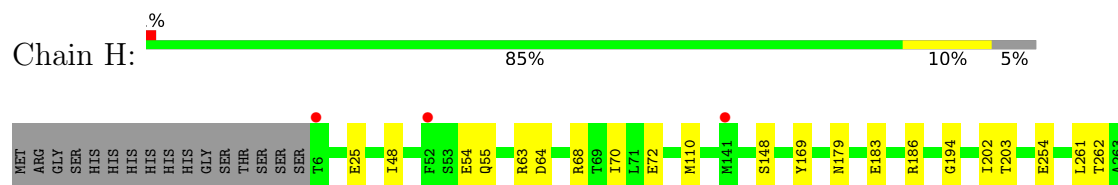
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



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



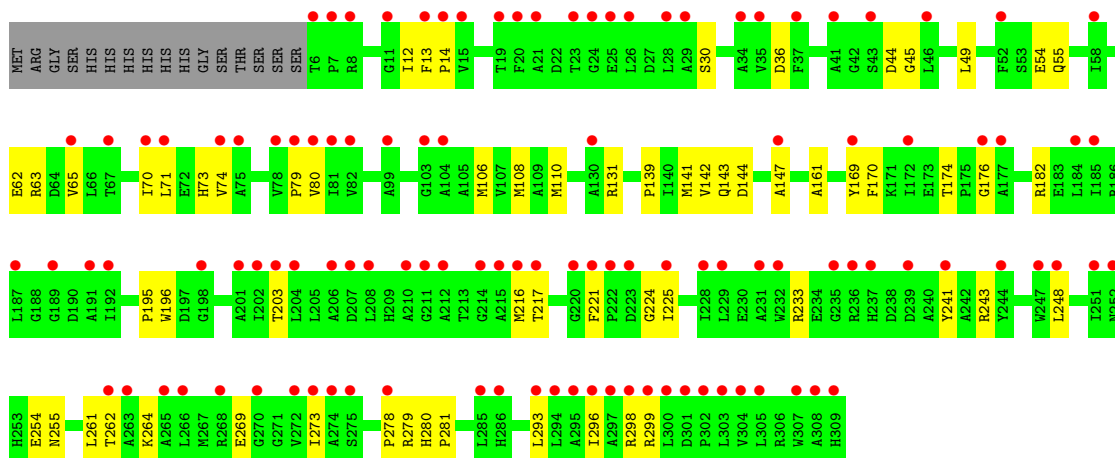
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase





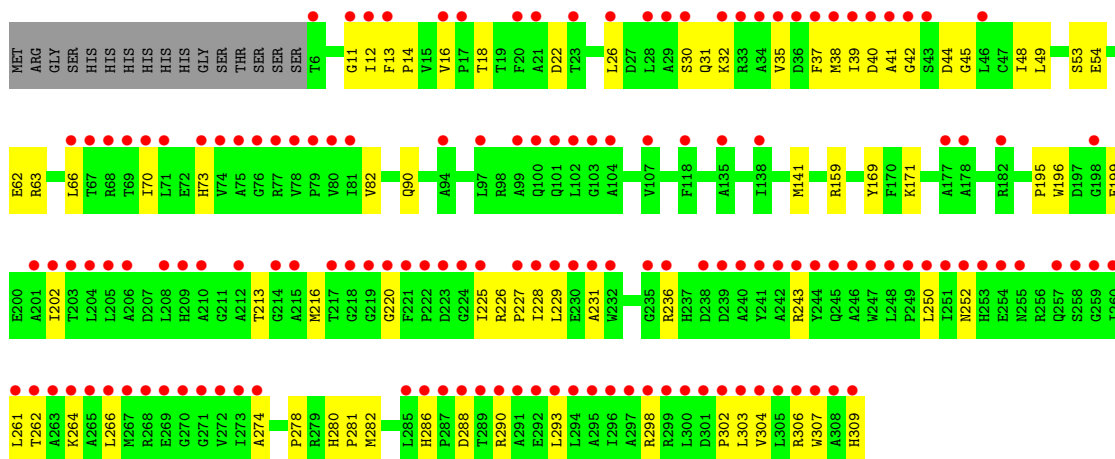
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain I: 35% 76% 19% 5%



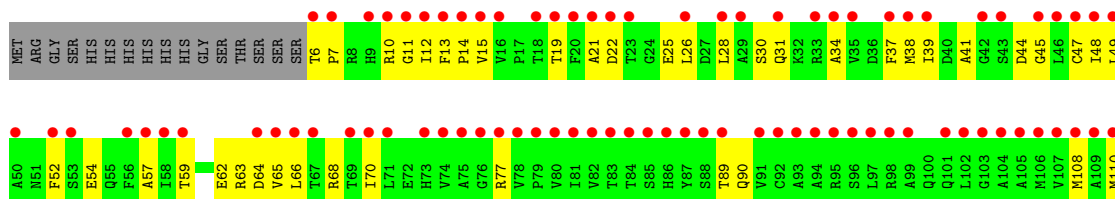
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

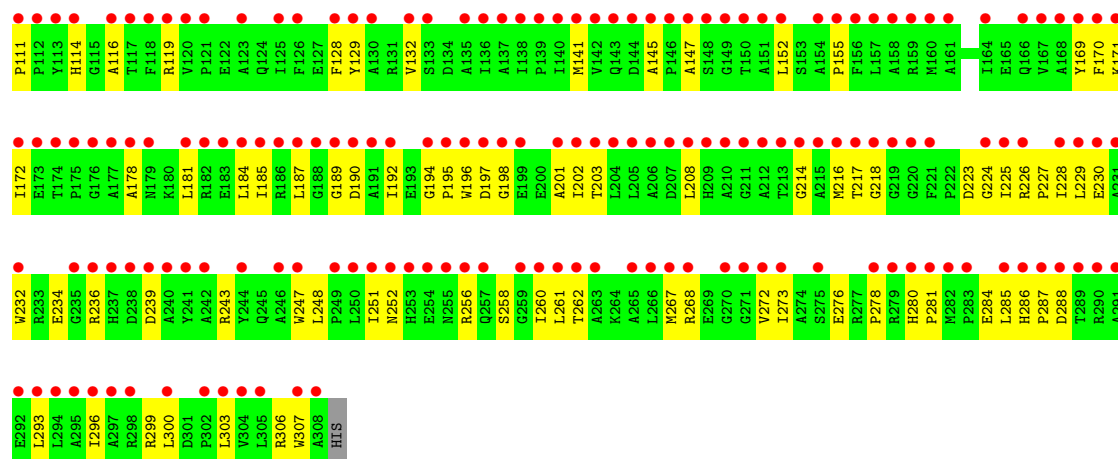
Chain J: 46% 72% 22% 5%



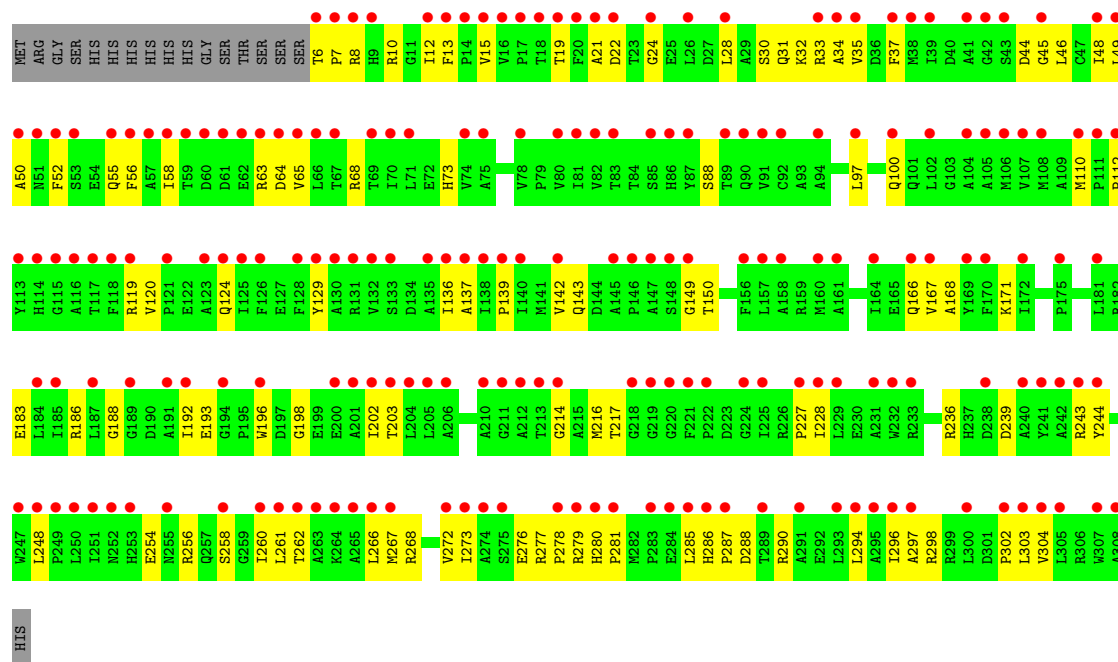
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain K: 78% 57% 38% 5%





• 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, α , β , γ	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) 96.5 (40.44-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.89Å)	Xtriage
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 (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29770	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.14	0/2379	0.35	0/3236
1	B	0.13	0/2396	0.34	0/3258
1	C	0.13	0/2384	0.34	0/3243
1	D	0.13	0/2384	0.35	0/3243
1	E	0.14	0/2396	0.36	0/3258
1	F	0.14	0/2396	0.35	0/3258
1	G	0.14	0/2384	0.35	0/3243
1	H	0.14	0/2384	0.36	0/3243
1	I	0.14	0/2384	0.36	0/3244
1	J	0.18	0/2396	0.38	0/3258
1	K	0.21	0/2380	0.44	0/3238
1	L	0.15	0/2384	0.38	0/3243
All	All	0.15	0/28647	0.36	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 ⓘ

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	32	0
1	C	2331	0	2314	26	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	19	0
1	I	2330	0	2299	44	0
1	J	2342	0	2321	61	0
1	K	2327	0	2308	109	0
1	L	2331	0	2314	86	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	460	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 (460) 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:J:54:GLU:OE2	1:J:264:LYS:NZ	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:H:110:MET:HE3	1:H:148:SER:HB3	1.77	0.67
1:I:261:LEU:HD21	1:I:278:PRO:HB3	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:178:ALA:HA	1:K:181:LEU:HD12	1.78	0.64
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:K:141:MET:HE3	1:K:169:TYR:HB3	1.82	0.61
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:141:MET:HE1	1:J:196:TRP:CE3	2.43	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:K:141:MET:HE1	1:K:196:TRP:CE3	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:110:MET:HE1	1:I:147:ALA:HB3	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: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:K:258:SER:OG	2:K:403:HOH:O	2.19	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:B:183:GLU:CD	1:B:186:ARG:HH21	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:141:MET:HE3	1:J:169:TYR:HB3	1.94	0.50
1:K:171:LYS:HD3	1:K:197:ASP:C	2.36	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:B:141:MET:HE3	1:B:169:TYR:HB3	1.93	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:K:110:MET:HE1	1:K:147:ALA:HB3	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:K:108:MET:SD	1:K:216:MET:HE1	2.53	0.48
1:J:26:LEU:HD11	1:J:62:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:36:ASP:CG	1:F:73:HIS:HE2	2.21	0.47
1:L:236:ARG:NH1	2:L:417:HOH:O	2.47	0.47
1:C:152:LEU:O	1:C:180:LYS:NZ	2.41	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:CE2	1:A:45:GLY:HA3	2.50	0.46
1:B:141:MET:HE1	1:B:196:TRP:CE3	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
1:B:48:ILE:HG21	1:B:70:ILE:HG21	1.97	0.46
1:C:141:MET:HE1	1:C:196:TRP:CE3	2.51	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:L:49:LEU:HD22	1:L:63:ARG:HD2	1.97	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:L:110:MET:HE3	1:L:110:MET:HB3	1.86	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: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: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:230:GLU:CD	1:C:233:ARG:HH22	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:227:PRO:C	1:J:243:ARG:HH22	2.24	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
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:L:171:LYS:HZ3	1:L:198:GLY:HA3	1.83	0.44
1:C:223:ASP:OD1	1:C:223:ASP:N	2.45	0.44
1:G:223:ASP:OD1	1:G:223:ASP:N	2.50	0.44
1:I:195:PRO:C	1:I:196:TRP:HD1	2.26	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:J:278:PRO:HB3	1:J:282:MET:HE2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:108:MET:HE3	1:I:143:GLN:OE1	2.19	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:L:34:ALA:CB	1:L:267:MET:HE1	2.48	0.43
1:B:54:GLU:OE2	1:B:264:LYS:NZ	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:J:40:ASP:OD2	1:J:40:ASP:N	2.51	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:141:MET:HE1	1:E:196:TRP:CE3	2.56	0.40
1:I:36:ASP:CG	1:I:73:HIS:HE2	2.27	0.40
1:I:216:MET:HB2	1:I:216:MET:HE3	1.76	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:144:ASP:OD2	1:I:174:THR:OG1	2.32	0.40
1:J:195:PRO:C	1:J:196:TRP:HD1	2.30	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 ⓘ

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%)	237 (100%)	0	100	100
1	C	236/251 (94%)	236 (100%)	0	100	100
1	D	236/251 (94%)	236 (100%)	0	100	100
1	E	237/251 (94%)	237 (100%)	0	100	100
1	F	237/251 (94%)	237 (100%)	0	100	100
1	G	236/251 (94%)	236 (100%)	0	100	100
1	H	236/251 (94%)	236 (100%)	0	100	100
1	I	235/251 (94%)	235 (100%)	0	100	100
1	J	237/251 (94%)	237 (100%)	0	100	100
1	K	235/251 (94%)	235 (100%)	0	100	100
1	L	236/251 (94%)	236 (100%)	0	100	100
All	All	2834/3012 (94%)	2834 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	245	GLN
1	A	252	ASN
1	B	9	HIS
1	B	166	GLN
1	B	245	GLN
1	C	124	GLN
1	C	166	GLN
1	C	245	GLN
1	C	252	ASN
1	D	124	GLN

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Mol	Chain	Res	Type
1	E	124	GLN
1	E	179	ASN
1	E	257	GLN
1	F	90	GLN
1	G	124	GLN
1	G	166	GLN
1	G	252	ASN
1	H	124	GLN
1	I	124	GLN
1	I	245	GLN
1	J	9	HIS
1	J	252	ASN
1	K	9	HIS
1	K	90	GLN
1	K	114	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	302/320 (94%)	0.50	8 (2%) 57 61	16, 25, 34, 52	0
1	B	304/320 (95%)	0.89	21 (6%) 23 24	19, 31, 44, 59	0
1	C	303/320 (94%)	0.83	18 (5%) 28 30	17, 29, 41, 55	0
1	D	303/320 (94%)	0.80	19 (6%) 26 27	18, 29, 42, 62	0
1	E	304/320 (95%)	0.25	11 (3%) 46 49	13, 20, 32, 53	0
1	F	304/320 (95%)	0.28	3 (0%) 79 82	14, 21, 31, 48	0
1	G	303/320 (94%)	0.49	7 (2%) 61 65	17, 24, 35, 55	0
1	H	303/320 (94%)	0.28	4 (1%) 75 78	14, 21, 30, 50	0
1	I	304/320 (95%)	1.80	113 (37%) 1 0	17, 38, 52, 71	0
1	J	304/320 (95%)	2.03	147 (48%) 0 0	17, 41, 58, 69	0
1	K	303/320 (94%)	3.25	250 (82%) 0 0	38, 48, 56, 67	0
1	L	303/320 (94%)	2.49	202 (66%) 0 0	30, 45, 55, 73	0
All	All	3640/3840 (94%)	1.16	803 (22%) 2 2	13, 28, 51, 73	0

All (803) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	197	ASP	7.1
1	L	81	ILE	7.0
1	K	251	ILE	7.0
1	I	24	GLY	6.7
1	K	192	ILE	6.7
1	K	128	PHE	6.6
1	K	181	LEU	6.5
1	K	293	LEU	6.4
1	I	21	ALA	6.3
1	K	215	ALA	6.3
1	J	289	THR	6.2

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Mol	Chain	Res	Type	RSRZ
1	K	196	TRP	6.2
1	J	220	GLY	6.0
1	J	249	PRO	5.9
1	K	132	VAL	5.8
1	J	305	LEU	5.8
1	K	91	VAL	5.8
1	K	305	LEU	5.7
1	E	308	ALA	5.7
1	K	240	ALA	5.6
1	K	218	GLY	5.6
1	J	205	LEU	5.6
1	J	266	LEU	5.5
1	J	291	ALA	5.5
1	B	308	ALA	5.5
1	K	261	LEU	5.4
1	J	227	PRO	5.4
1	K	263	ALA	5.4
1	J	231	ALA	5.4
1	J	42	GLY	5.3
1	J	295	ALA	5.3
1	K	204	LEU	5.2
1	I	297	ALA	5.2
1	K	46	LEU	5.2
1	K	297	ALA	5.2
1	L	266	LEU	5.2
1	L	308	ALA	5.2
1	K	198	GLY	5.2
1	L	196	TRP	5.1
1	L	240	ALA	5.1
1	J	300	LEU	5.1
1	K	35	VAL	5.1
1	L	260	ILE	5.0
1	K	142	VAL	5.0
1	K	167	VAL	5.0
1	K	172	ILE	5.0
1	I	229	LEU	5.0
1	K	113	TYR	5.0
1	I	220	GLY	5.0
1	K	58	ILE	4.9
1	K	208	LEU	4.9
1	K	285	LEU	4.9
1	K	94	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	J	241	TYR	4.8
1	L	140	ILE	4.8
1	K	82	VAL	4.8
1	K	291	ALA	4.8
1	J	296	ILE	4.8
1	K	81	ILE	4.8
1	L	78	VAL	4.8
1	G	308	ALA	4.8
1	J	308	ALA	4.8
1	K	125	ILE	4.8
1	K	185	ILE	4.8
1	K	217	THR	4.8
1	K	266	LEU	4.7
1	J	202	ILE	4.7
1	K	136	ILE	4.7
1	K	247	TRP	4.7
1	L	248	LEU	4.7
1	L	118	PHE	4.7
1	K	84	THR	4.6
1	K	304	VAL	4.6
1	K	48	ILE	4.6
1	I	225	ILE	4.6
1	K	12	ILE	4.6
1	L	164	ILE	4.6
1	K	156	PHE	4.6
1	J	304	VAL	4.6
1	K	157	LEU	4.6
1	I	215	ALA	4.5
1	K	168	ALA	4.5
1	K	15	VAL	4.5
1	K	80	VAL	4.5
1	I	228	ILE	4.5
1	I	273	ILE	4.5
1	J	228	ILE	4.5
1	K	289	THR	4.5
1	K	57	ALA	4.5
1	J	247	TRP	4.4
1	K	129	TYR	4.4
1	L	241	TYR	4.4
1	J	251	ILE	4.4
1	J	270	GLY	4.4
1	L	48	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	K	34	ALA	4.4
1	J	78	VAL	4.4
1	K	303	LEU	4.4
1	K	79	PRO	4.4
1	K	78	VAL	4.4
1	K	241	TYR	4.4
1	K	194	GLY	4.3
1	I	308	ALA	4.3
1	L	263	ALA	4.3
1	J	35	VAL	4.3
1	J	242	ALA	4.3
1	K	137	ALA	4.3
1	K	206	ALA	4.3
1	K	242	ALA	4.3
1	J	243	ARG	4.3
1	K	149	GLY	4.3
1	J	253	HIS	4.3
1	K	66	LEU	4.3
1	I	35	VAL	4.3
1	D	6	THR	4.2
1	K	205	LEU	4.2
1	K	104	ALA	4.2
1	K	287	PRO	4.2
1	I	6	THR	4.2
1	K	97	LEU	4.2
1	J	221	PHE	4.2
1	D	308	ALA	4.2
1	J	34	ALA	4.2
1	K	99	ALA	4.2
1	K	161	ALA	4.2
1	D	7	PRO	4.2
1	K	86	HIS	4.2
1	K	154	ALA	4.2
1	L	7	PRO	4.2
1	J	232	TRP	4.2
1	K	232	TRP	4.2
1	K	102	LEU	4.2
1	I	275	SER	4.1
1	K	76	GLY	4.1
1	K	126	PHE	4.1
1	I	296	ILE	4.1
1	K	70	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	L	125	ILE	4.1
1	I	26	LEU	4.1
1	J	204	LEU	4.1
1	J	229	LEU	4.1
1	K	45	GLY	4.1
1	C	228	ILE	4.1
1	K	170	PHE	4.1
1	J	222	PRO	4.1
1	J	12	ILE	4.0
1	J	39	ILE	4.0
1	K	225	ILE	4.0
1	L	296	ILE	4.0
1	K	231	ALA	4.0
1	K	239	ASP	4.0
1	L	6	THR	4.0
1	K	211	GLY	4.0
1	L	19	THR	4.0
1	K	189	GLY	4.0
1	K	220	GLY	4.0
1	K	224	GLY	4.0
1	I	294	LEU	4.0
1	H	308	ALA	4.0
1	K	14	PRO	4.0
1	K	21	ALA	4.0
1	K	195	PRO	4.0
1	L	17	PRO	4.0
1	L	35	VAL	4.0
1	L	273	ILE	4.0
1	L	307	TRP	3.9
1	K	187	LEU	3.9
1	K	158	ALA	3.9
1	L	39	ILE	3.9
1	L	56	PHE	3.9
1	J	307	TRP	3.9
1	J	208	LEU	3.9
1	K	250	LEU	3.9
1	K	123	ALA	3.9
1	K	145	ALA	3.9
1	L	212	ALA	3.9
1	I	23	THR	3.9
1	K	83	THR	3.9
1	K	262	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	309	HIS	3.9
1	K	108	MET	3.9
1	L	285	LEU	3.9
1	K	93	ALA	3.9
1	K	210	ALA	3.9
1	K	164	ILE	3.9
1	L	87	TYR	3.8
1	L	303	LEU	3.8
1	K	112	PRO	3.8
1	L	117	THR	3.8
1	K	151	ALA	3.8
1	L	224	GLY	3.8
1	K	39	ILE	3.8
1	J	37	PHE	3.8
1	K	143	GLN	3.8
1	J	43	SER	3.8
1	K	96	SER	3.8
1	I	7	PRO	3.8
1	K	188	GLY	3.8
1	I	177	ALA	3.8
1	K	101	GLN	3.8
1	I	37	PHE	3.8
1	K	169	TYR	3.8
1	K	150	THR	3.8
1	K	107	VAL	3.8
1	L	107	VAL	3.8
1	L	149	GLY	3.7
1	J	75	ALA	3.7
1	L	91	VAL	3.7
1	J	287	PRO	3.7
1	I	266	LEU	3.7
1	K	294	LEU	3.7
1	L	71	LEU	3.7
1	K	228	ILE	3.7
1	K	296	ILE	3.7
1	L	267	MET	3.7
1	J	80	VAL	3.7
1	K	272	VAL	3.7
1	L	272	VAL	3.7
1	K	221	PHE	3.7
1	L	26	LEU	3.7
1	J	215	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	202	ILE	3.7
1	L	132	VAL	3.7
1	K	307	TRP	3.7
1	J	294	LEU	3.6
1	K	229	LEU	3.6
1	K	201	ALA	3.6
1	I	241	TYR	3.6
1	J	225	ILE	3.6
1	K	260	ILE	3.6
1	K	139	PRO	3.6
1	K	146	PRO	3.6
1	L	13	PHE	3.6
1	J	209	HIS	3.6
1	K	212	ALA	3.6
1	L	113	TYR	3.6
1	I	272	VAL	3.6
1	J	309	HIS	3.6
1	K	49	LEU	3.6
1	I	206	ALA	3.6
1	K	50	ALA	3.6
1	I	236	ARG	3.6
1	L	247	TRP	3.6
1	L	114	HIS	3.6
1	J	258	SER	3.6
1	K	52	PHE	3.6
1	L	20	PHE	3.6
1	J	299	ARG	3.6
1	J	246	ALA	3.5
1	K	105	ALA	3.5
1	K	237	HIS	3.5
1	K	182	ARG	3.5
1	L	304	VAL	3.5
1	I	208	LEU	3.5
1	I	263	ALA	3.5
1	K	109	ALA	3.5
1	K	147	ALA	3.5
1	L	49	LEU	3.5
1	L	250	LEU	3.5
1	L	297	ALA	3.5
1	L	305	LEU	3.5
1	L	9	HIS	3.5
1	L	244	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	J	223	ASP	3.5
1	K	283	PRO	3.5
1	K	120	VAL	3.5
1	L	37	PHE	3.5
1	J	201	ALA	3.5
1	J	261	LEU	3.5
1	K	298	ARG	3.5
1	I	207	ASP	3.5
1	J	74	VAL	3.5
1	I	28	LEU	3.5
1	J	303	LEU	3.5
1	K	236	ARG	3.5
1	L	42	GLY	3.5
1	L	133	SER	3.4
1	I	65	VAL	3.4
1	L	15	VAL	3.4
1	K	20	PHE	3.4
1	K	259	GLY	3.4
1	K	130	ALA	3.4
1	B	7	PRO	3.4
1	L	227	PRO	3.4
1	I	244	TYR	3.4
1	K	9	HIS	3.4
1	I	78	VAL	3.4
1	L	82	VAL	3.4
1	J	11	GLY	3.4
1	K	235	GLY	3.4
1	K	47	CYS	3.4
1	I	237	HIS	3.4
1	I	223	ASP	3.4
1	I	11	GLY	3.4
1	J	198	GLY	3.4
1	J	259	GLY	3.4
1	I	231	ALA	3.4
1	J	240	ALA	3.4
1	L	75	ALA	3.4
1	L	104	ALA	3.4
1	L	242	ALA	3.4
1	K	13	PHE	3.4
1	K	89	THR	3.4
1	L	18	THR	3.4
1	I	299	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	50	ALA	3.3
1	K	160	MET	3.3
1	B	6	THR	3.3
1	J	217	THR	3.3
1	K	286	HIS	3.3
1	K	138	ILE	3.3
1	L	136	ILE	3.3
1	I	274	ALA	3.3
1	J	41	ALA	3.3
1	K	178	ALA	3.3
1	K	282	MET	3.3
1	K	28	LEU	3.3
1	I	307	TRP	3.3
1	I	198	GLY	3.3
1	K	87	TYR	3.3
1	K	244	TYR	3.3
1	K	273	ILE	3.3
1	L	274	ALA	3.3
1	L	52	PHE	3.3
1	L	126	PHE	3.3
1	I	247	TRP	3.3
1	J	271	GLY	3.3
1	K	271	GLY	3.3
1	L	138	ILE	3.2
1	L	16	VAL	3.2
1	I	248	LEU	3.2
1	K	111	PRO	3.2
1	K	37	PHE	3.2
1	K	183	GLU	3.2
1	L	255	ASN	3.2
1	I	176	GLY	3.2
1	K	42	GLY	3.2
1	L	85	SER	3.2
1	K	209	HIS	3.2
1	L	86	HIS	3.2
1	K	177	ALA	3.2
1	K	216	MET	3.2
1	K	253	HIS	3.2
1	I	75	ALA	3.2
1	L	12	ILE	3.2
1	A	6	THR	3.2
1	L	83	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	16	VAL	3.2
1	K	219	GLY	3.2
1	L	100	GLN	3.2
1	L	128	PHE	3.2
1	J	288	ASP	3.2
1	L	228	ILE	3.1
1	K	267	MET	3.1
1	B	285	LEU	3.1
1	I	270	GLY	3.1
1	I	305	LEU	3.1
1	K	56	PHE	3.1
1	K	71	LEU	3.1
1	L	97	LEU	3.1
1	L	261	LEU	3.1
1	J	257	GLN	3.1
1	K	110	MET	3.1
1	J	262	THR	3.1
1	F	308	ALA	3.1
1	L	283	PRO	3.1
1	K	288	ASP	3.1
1	L	167	VAL	3.1
1	K	171	LYS	3.1
1	E	108	MET	3.1
1	K	6	THR	3.1
1	K	7	PRO	3.1
1	I	29	ALA	3.1
1	J	21	ALA	3.1
1	K	246	ALA	3.1
1	L	57	ALA	3.1
1	L	218	GLY	3.1
1	I	185	ILE	3.0
1	J	239	ASP	3.0
1	L	202	ILE	3.0
1	B	305	LEU	3.0
1	I	46	LEU	3.0
1	L	142	VAL	3.0
1	B	307	TRP	3.0
1	J	76	GLY	3.0
1	L	158	ALA	3.0
1	J	248	LEU	3.0
1	K	106	MET	3.0
1	L	66	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	130	ALA	3.0
1	L	191	ALA	3.0
1	L	300	LEU	3.0
1	K	65	VAL	3.0
1	K	74	VAL	3.0
1	L	169	TYR	3.0
1	D	307	TRP	3.0
1	L	214	GLY	3.0
1	K	191	ALA	3.0
1	L	21	ALA	3.0
1	J	70	ILE	3.0
1	J	273	ILE	3.0
1	I	300	LEU	2.9
1	J	46	LEU	2.9
1	K	26	LEU	2.9
1	I	74	VAL	2.9
1	J	272	VAL	2.9
1	K	278	PRO	2.9
1	L	222	PRO	2.9
1	I	295	ALA	2.9
1	K	92	CYS	2.9
1	L	92	CYS	2.9
1	L	70	ILE	2.9
1	K	152	LEU	2.9
1	K	19	THR	2.9
1	K	67	THR	2.9
1	L	220	GLY	2.9
1	J	17	PRO	2.9
1	I	309	HIS	2.9
1	K	140	ILE	2.9
1	K	238	ASP	2.9
1	G	294	LEU	2.9
1	K	184	LEU	2.9
1	J	203	THR	2.9
1	L	302	PRO	2.9
1	K	75	ALA	2.9
1	K	265	ALA	2.9
1	K	295	ALA	2.9
1	L	291	ALA	2.9
1	I	232	TRP	2.9
1	J	250	LEU	2.9
1	L	58	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	302	PRO	2.8
1	K	155	PRO	2.8
1	K	280	HIS	2.8
1	I	8	ARG	2.8
1	L	265	ALA	2.8
1	J	36	ASP	2.8
1	L	43	SER	2.8
1	D	26	LEU	2.8
1	L	294	LEU	2.8
1	L	211	GLY	2.8
1	L	219	GLY	2.8
1	L	262	THR	2.8
1	J	73	HIS	2.8
1	K	226	ARG	2.8
1	E	137	ALA	2.8
1	J	38	MET	2.8
1	J	274	ALA	2.8
1	K	148	SER	2.8
1	L	135	ALA	2.8
1	L	161	ALA	2.8
1	K	166	GLN	2.8
1	I	298	ARG	2.8
1	L	172	ILE	2.8
1	L	205	LEU	2.8
1	I	19	THR	2.8
1	K	114	HIS	2.8
1	L	289	THR	2.8
1	K	173	GLU	2.8
1	K	249	PRO	2.8
1	I	43	SER	2.8
1	K	88	SER	2.8
1	J	99	ALA	2.8
1	L	147	ALA	2.8
1	L	221	PHE	2.8
1	K	290	ARG	2.8
1	I	286	HIS	2.8
1	K	213	THR	2.8
1	I	14	PRO	2.8
1	I	80	VAL	2.8
1	I	169	TYR	2.7
1	I	104	ALA	2.7
1	I	212	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	245	GLN	2.7
1	K	29	ALA	2.7
1	K	268	ARG	2.7
1	K	118	PHE	2.7
1	L	170	PHE	2.7
1	J	218	GLY	2.7
1	I	67	THR	2.7
1	J	69	THR	2.7
1	L	213	THR	2.7
1	I	293	LEU	2.7
1	L	184	LEU	2.7
1	I	202	ILE	2.7
1	J	40	ASP	2.7
1	I	302	PRO	2.7
1	L	232	TRP	2.7
1	K	252	ASN	2.7
1	J	206	ALA	2.7
1	J	235	GLY	2.7
1	I	221	PHE	2.7
1	K	23	THR	2.7
1	L	110	MET	2.7
1	L	229	LEU	2.7
1	I	222	PRO	2.7
1	L	278	PRO	2.7
1	F	309	HIS	2.7
1	C	274	ALA	2.7
1	L	116	ALA	2.7
1	L	201	ALA	2.7
1	I	211	GLY	2.7
1	I	214	GLY	2.7
1	G	6	THR	2.7
1	K	203	THR	2.7
1	L	166	GLN	2.7
1	J	71	LEU	2.7
1	J	285	LEU	2.7
1	L	112	PRO	2.7
1	L	121	PRO	2.7
1	G	192	ILE	2.7
1	L	45	GLY	2.6
1	L	231	ALA	2.6
1	E	267	MET	2.6
1	K	133	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	71	LEU	2.6
1	L	28	LEU	2.6
1	L	280	HIS	2.6
1	H	141	MET	2.6
1	J	224	GLY	2.6
1	K	214	GLY	2.6
1	L	115	GLY	2.6
1	L	189	GLY	2.6
1	J	94	ALA	2.6
1	J	135	ALA	2.6
1	K	207	ASP	2.6
1	L	94	ALA	2.6
1	K	230	GLU	2.6
1	I	217	THR	2.6
1	I	13	PHE	2.6
1	K	255	ASN	2.6
1	I	192	ILE	2.6
1	L	108	MET	2.6
1	K	31	GLN	2.6
1	L	55	GLN	2.6
1	J	265	ALA	2.6
1	L	105	ALA	2.6
1	I	262	THR	2.6
1	L	53	SER	2.6
1	B	97	LEU	2.6
1	L	279	ARG	2.6
1	I	58	ILE	2.6
1	I	70	ILE	2.6
1	K	144	ASP	2.6
1	G	76	GLY	2.6
1	J	263	ALA	2.6
1	K	53	SER	2.6
1	K	275	SER	2.6
1	L	275	SER	2.6
1	K	18	THR	2.6
1	K	174	THR	2.6
1	K	121	PRO	2.5
1	J	28	LEU	2.5
1	K	190	ASP	2.5
1	L	22	ASP	2.5
1	I	251	ILE	2.5
1	L	192	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	34	ALA	2.5
1	L	123	ALA	2.5
1	L	145	ALA	2.5
1	L	258	SER	2.5
1	K	73	HIS	2.5
1	L	65	VAL	2.5
1	L	253	HIS	2.5
1	K	117	THR	2.5
1	C	233	ARG	2.5
1	D	277	ARG	2.5
1	J	269	GLU	2.5
1	J	20	PHE	2.5
1	J	97	LEU	2.5
1	J	293	LEU	2.5
1	I	252	ASN	2.5
1	K	10	ARG	2.5
1	I	99	ALA	2.5
1	J	23	THR	2.5
1	L	74	VAL	2.5
1	K	22	ASP	2.5
1	I	303	LEU	2.5
1	J	219	GLY	2.5
1	L	102	LEU	2.5
1	L	157	LEU	2.5
1	L	252	ASN	2.5
1	L	233	ARG	2.5
1	L	286	HIS	2.5
1	D	70	ILE	2.5
1	J	138	ILE	2.5
1	K	257	GLN	2.5
1	J	178	ALA	2.5
1	J	212	ALA	2.5
1	K	308	ALA	2.5
1	H	6	THR	2.5
1	L	89	THR	2.5
1	K	270	GLY	2.4
1	C	241	TYR	2.4
1	J	255	ASN	2.4
1	K	300	LEU	2.4
1	J	101	GLN	2.4
1	J	81	ILE	2.4
1	C	308	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	304	VAL	2.4
1	L	111	PRO	2.4
1	J	290	ARG	2.4
1	D	194	GLY	2.4
1	L	124	GLN	2.4
1	K	38	MET	2.4
1	L	187	LEU	2.4
1	B	39	ILE	2.4
1	I	172	ILE	2.4
1	L	225	ILE	2.4
1	B	274	ALA	2.4
1	K	281	PRO	2.4
1	L	281	PRO	2.4
1	B	237	HIS	2.4
1	J	267	MET	2.4
1	L	148	SER	2.4
1	I	184	LEU	2.4
1	I	52	PHE	2.4
1	J	6	THR	2.4
1	J	268	ARG	2.4
1	K	33	ARG	2.4
1	L	8	ARG	2.4
1	L	59	THR	2.4
1	L	67	THR	2.4
1	I	191	ALA	2.4
1	I	201	ALA	2.4
1	L	206	ALA	2.4
1	L	210	ALA	2.4
1	L	14	PRO	2.4
1	L	139	PRO	2.4
1	J	286	HIS	2.4
1	I	189	GLY	2.4
1	K	176	GLY	2.4
1	K	141	MET	2.4
1	J	30	SER	2.4
1	K	43	SER	2.4
1	L	264	LYS	2.4
1	I	301	ASP	2.3
1	I	204	LEU	2.3
1	L	181	LEU	2.3
1	J	118	PHE	2.3
1	J	67	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	161	ALA	2.3
1	I	34	ALA	2.3
1	I	210	ALA	2.3
1	J	297	ALA	2.3
1	K	179	ASN	2.3
1	E	7	PRO	2.3
1	I	216	MET	2.3
1	I	235	GLY	2.3
1	K	103	GLY	2.3
1	I	15	VAL	2.3
1	J	33	ARG	2.3
1	K	119	ARG	2.3
1	K	279	ARG	2.3
1	J	254	GLU	2.3
1	K	292	GLU	2.3
1	J	244	TYR	2.3
1	K	69	THR	2.3
1	J	252	ASN	2.3
1	K	116	ALA	2.3
1	C	235	GLY	2.3
1	J	264	LYS	2.3
1	J	68	ARG	2.3
1	J	77	ARG	2.3
1	J	236	ARG	2.3
1	K	16	VAL	2.3
1	J	26	LEU	2.3
1	H	52	PHE	2.3
1	I	20	PHE	2.3
1	J	32	LYS	2.3
1	B	93	ALA	2.3
1	D	75	ALA	2.3
1	J	104	ALA	2.3
1	J	210	ALA	2.3
1	K	98	ARG	2.3
1	J	230	GLU	2.3
1	K	199	GLU	2.3
1	L	64	ASP	2.3
1	J	107	VAL	2.3
1	I	203	THR	2.3
1	L	203	THR	2.3
1	A	7	PRO	2.2
1	B	13	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	103	GLY	2.2
1	C	7	PRO	2.2
1	C	37	PHE	2.2
1	K	254	GLU	2.2
1	L	137	ALA	2.2
1	L	156	PHE	2.2
1	L	194	GLY	2.2
1	L	200	GLU	2.2
1	A	192	ILE	2.2
1	E	192	ILE	2.2
1	I	81	ILE	2.2
1	J	260	ILE	2.2
1	A	267	MET	2.2
1	B	23	THR	2.2
1	K	77	ARG	2.2
1	L	63	ARG	2.2
1	L	131	ARG	2.2
1	E	11	GLY	2.2
1	G	7	PRO	2.2
1	I	79	PRO	2.2
1	K	85	SER	2.2
1	L	146	PRO	2.2
1	J	177	ALA	2.2
1	L	238	ASP	2.2
1	L	160	MET	2.2
1	D	98	ARG	2.2
1	K	95	ARG	2.2
1	K	186	ARG	2.2
1	L	119	ARG	2.2
1	I	25	GLU	2.2
1	C	6	THR	2.2
1	D	213	THR	2.2
1	E	47	CYS	2.2
1	B	187	LEU	2.2
1	A	134	ASP	2.2
1	C	189	GLY	2.2
1	L	24	GLY	2.2
1	F	52	PHE	2.2
1	J	306	ARG	2.2
1	K	59	THR	2.2
1	L	69	THR	2.2
1	I	239	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	220	GLY	2.2
1	J	66	LEU	2.2
1	J	102	LEU	2.2
1	J	103	GLY	2.2
1	K	302	PRO	2.2
1	I	41	ALA	2.2
1	J	29	ALA	2.2
1	L	295	ALA	2.2
1	K	256	ARG	2.2
1	C	70	ILE	2.1
1	J	301	ASP	2.1
1	L	61	ASP	2.1
1	D	78	VAL	2.1
1	L	80	VAL	2.1
1	A	271	GLY	2.1
1	J	214	GLY	2.1
1	J	79	PRO	2.1
1	L	175	PRO	2.1
1	L	106	MET	2.1
1	D	137	ALA	2.1
1	K	135	ALA	2.1
1	L	41	ALA	2.1
1	L	51	ASN	2.1
1	J	100	GLN	2.1
1	L	129	TYR	2.1
1	J	238	ASP	2.1
1	C	196	TRP	2.1
1	B	233	ARG	2.1
1	I	82	VAL	2.1
1	J	298	ARG	2.1
1	L	33	ARG	2.1
1	L	38	MET	2.1
1	C	303	LEU	2.1
1	D	302	PRO	2.1
1	I	285	LEU	2.1
1	K	175	PRO	2.1
1	L	204	LEU	2.1
1	C	240	ALA	2.1
1	D	215	ALA	2.1
1	I	130	ALA	2.1
1	I	147	ALA	2.1
1	D	192	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	60	ASP	2.1
1	L	185	ILE	2.1
1	B	277	ARG	2.1
1	K	159	ARG	2.1
1	E	6	THR	2.1
1	L	62	GLU	2.1
1	D	65	VAL	2.1
1	D	74	VAL	2.1
1	B	303	LEU	2.1
1	D	205	LEU	2.1
1	I	187	LEU	2.1
1	B	191	ALA	2.1
1	B	201	ALA	2.1
1	B	231	ALA	2.1
1	C	168	ALA	2.1
1	A	8	ARG	2.1
1	G	10	ARG	2.1
1	I	268	ARG	2.1
1	J	182	ARG	2.1
1	L	243	ARG	2.1
1	L	251	ILE	2.0
1	I	103	GLY	2.0
1	K	11	GLY	2.0
1	L	90	GLN	2.0
1	I	278	PRO	2.0
1	L	249	PRO	2.0
1	L	287	PRO	2.0
1	C	66	LEU	2.0
1	L	293	LEU	2.0
1	E	186	ARG	2.0
1	I	265	ALA	2.0
1	K	64	ASP	2.0
1	J	292	GLU	2.0
1	L	284	GLU	2.0
1	J	13	PHE	2.0
1	A	243	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.