Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:20 AM BST

PDB ID	:	7C0E
Title	:	Crystal structure of Azospirillum brasilense L-2-keto-3-deoxyarabonate dehydratase (2-oxobutyrate-bound form)
Authors	:	Watanabe, Y.; Ono, A.; Watanabe, S.
Deposited on	:	2020-05-01
Resolution	:	2.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

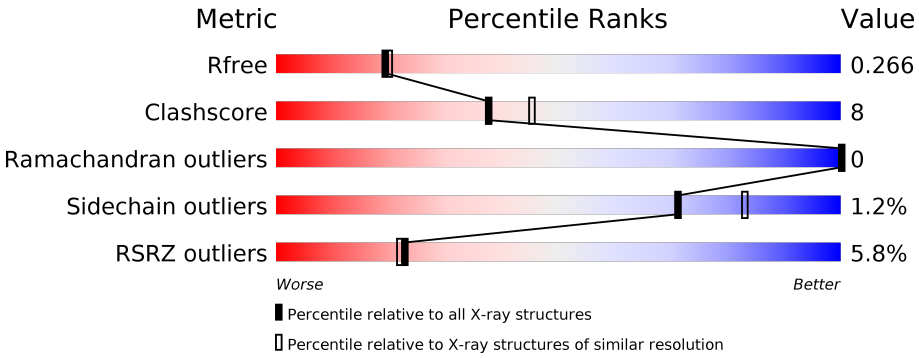
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	320	% 86% 9% 5%
1	B	320	% 83% 12% 6%
1	C	320	% 85% 9% • 5%
1	D	320	% 86% 8% • 5%
1	E	320	% 83% 11% 5%
1	F	320	83% 11% • 6%

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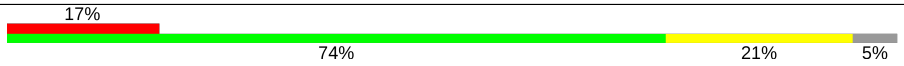
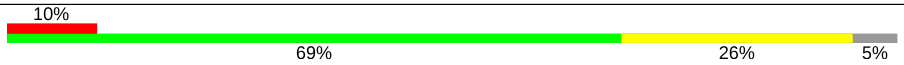
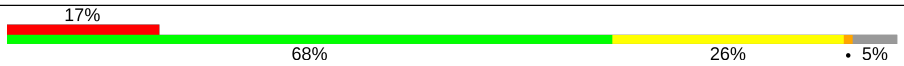
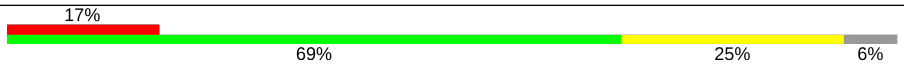
Mol	Chain	Length	Quality of chain
1	G	320	
1	H	320	
1	I	320	
1	J	320	
1	K	320	
1	L	320	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29111 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-2-keto-3-deoxyarabonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2348	1481	424	432	11			
1	B	302	Total	C	N	O	S	0	0	0
			2326	1468	420	427	11			
1	C	304	Total	C	N	O	S	0	0	0
			2342	1477	424	430	11			
1	D	303	Total	C	N	O	S	0	0	0
			2325	1468	418	428	11			
1	E	304	Total	C	N	O	S	0	0	0
			2342	1477	424	430	11			
1	F	302	Total	C	N	O	S	0	0	0
			2326	1468	420	427	11			
1	G	303	Total	C	N	O	S	0	0	0
			2325	1468	418	428	11			
1	H	303	Total	C	N	O	S	0	0	0
			2325	1468	418	428	11			
1	I	304	Total	C	N	O	S	0	0	0
			2336	1474	421	430	11			
1	J	304	Total	C	N	O	S	0	0	0
			2336	1474	421	430	11			
1	K	303	Total	C	N	O	S	0	0	0
			2331	1471	421	428	11			
1	L	301	Total	C	N	O	S	0	0	0
			2317	1462	419	425	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

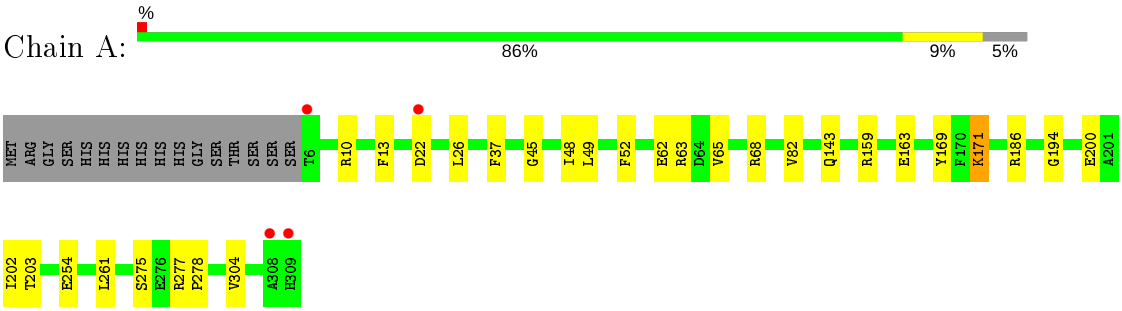
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	105	Total O 105 105	0	0
2	B	92	Total O 92 92	0	0
2	C	107	Total O 107 107	0	0
2	D	111	Total O 111 111	0	0
2	E	112	Total O 112 112	0	0
2	F	105	Total O 105 105	0	0
2	G	116	Total O 116 116	0	0
2	H	97	Total O 97 97	0	0
2	I	65	Total O 65 65	0	0
2	J	71	Total O 71 71	0	0
2	K	89	Total O 89 89	0	0
2	L	62	Total O 62 62	0	0

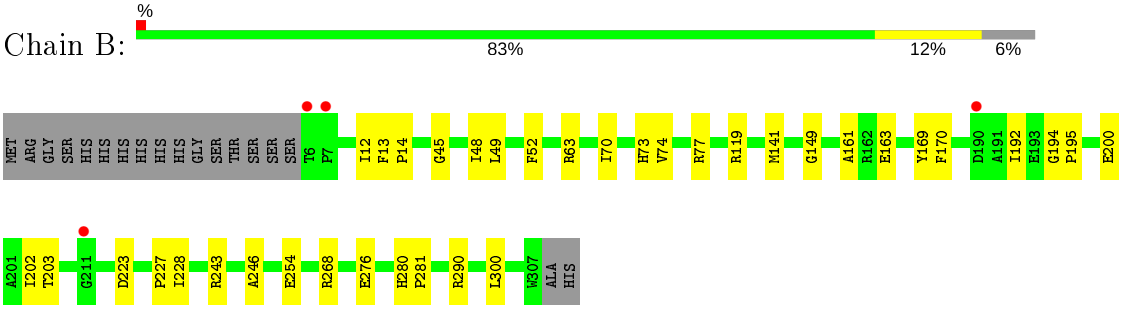
3 Residue-property plots (i)

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.

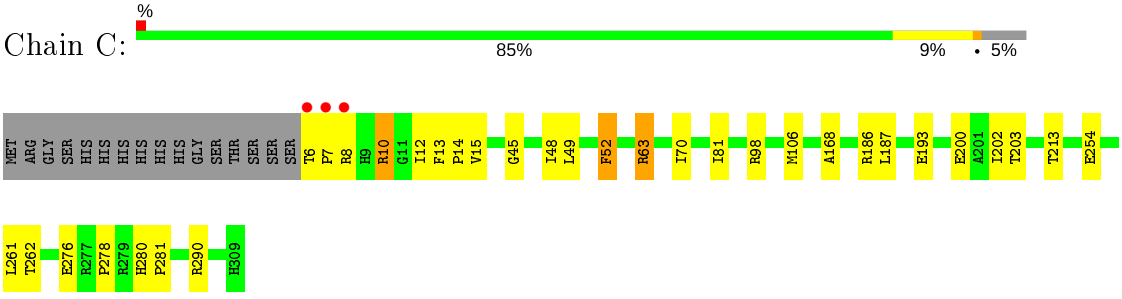
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



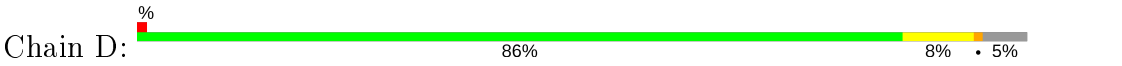
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

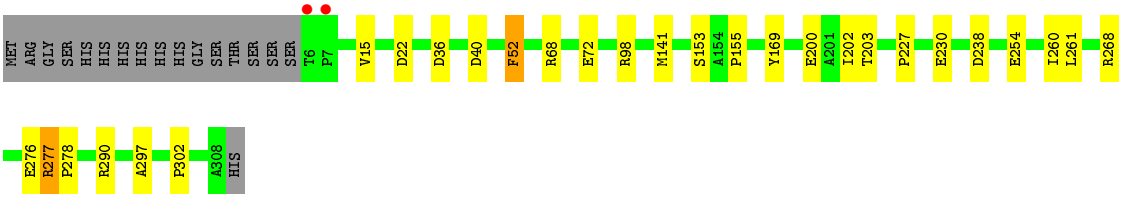


- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



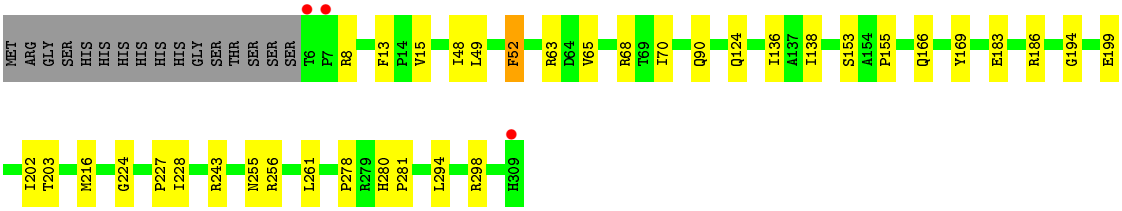
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase





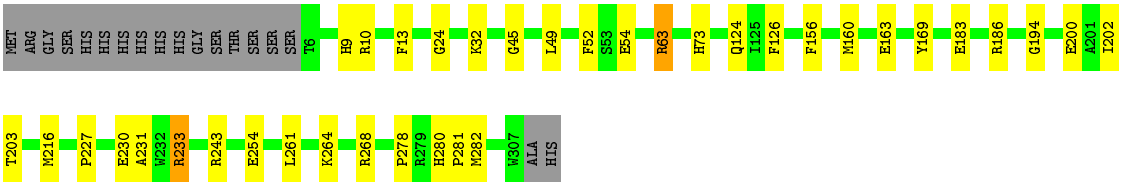
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain E:



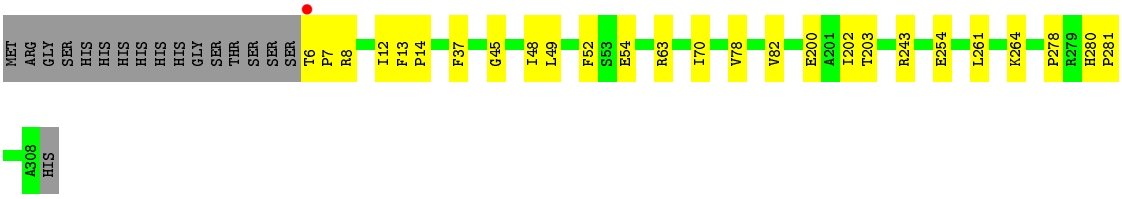
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain F:



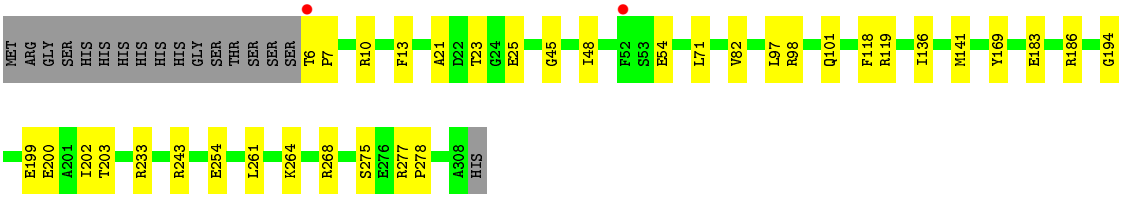
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain G:



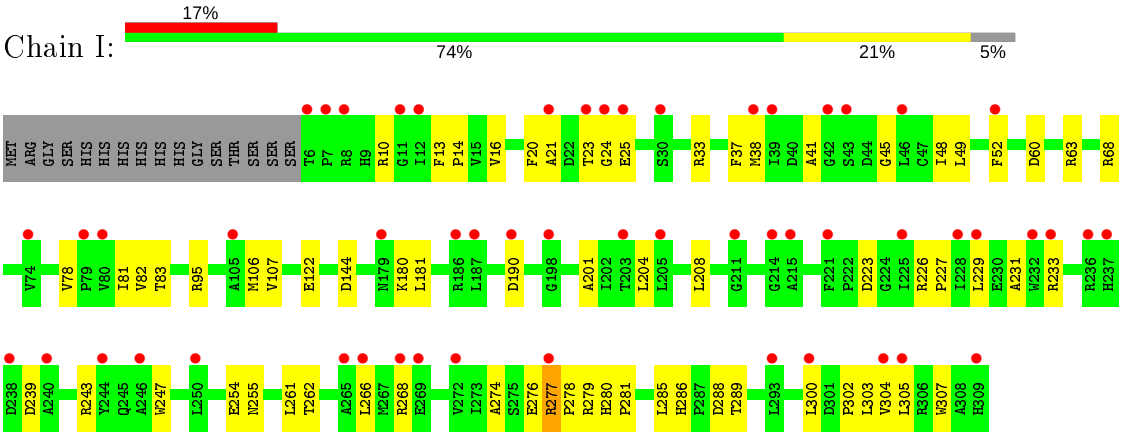
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain H:



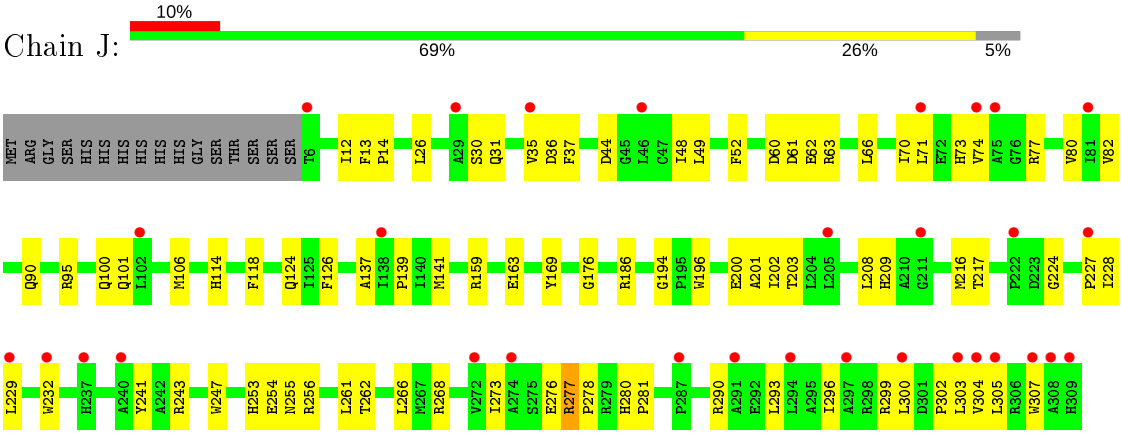
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain I:



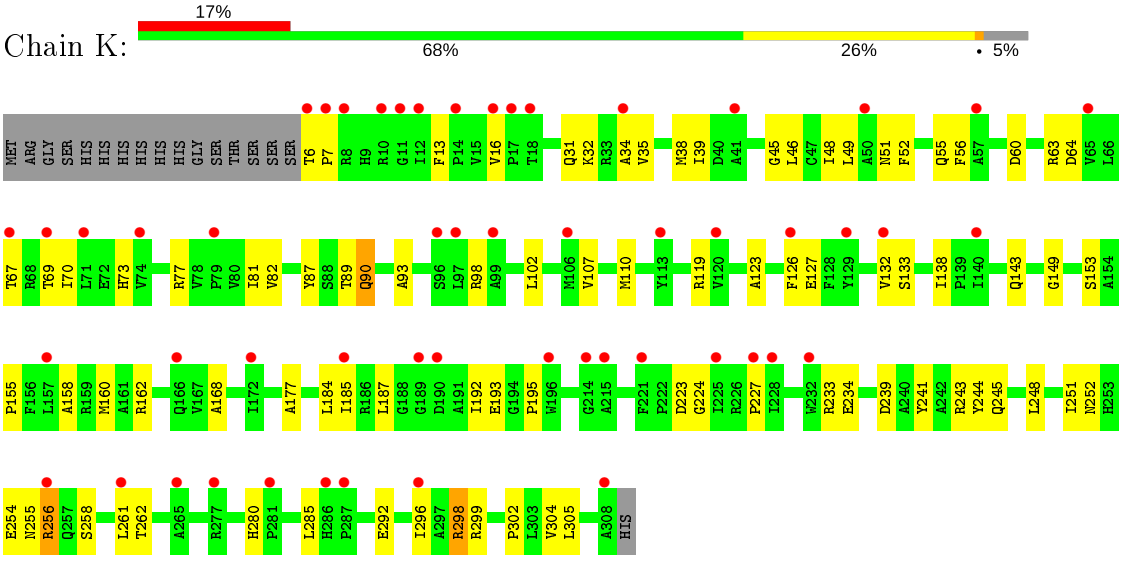
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain J:



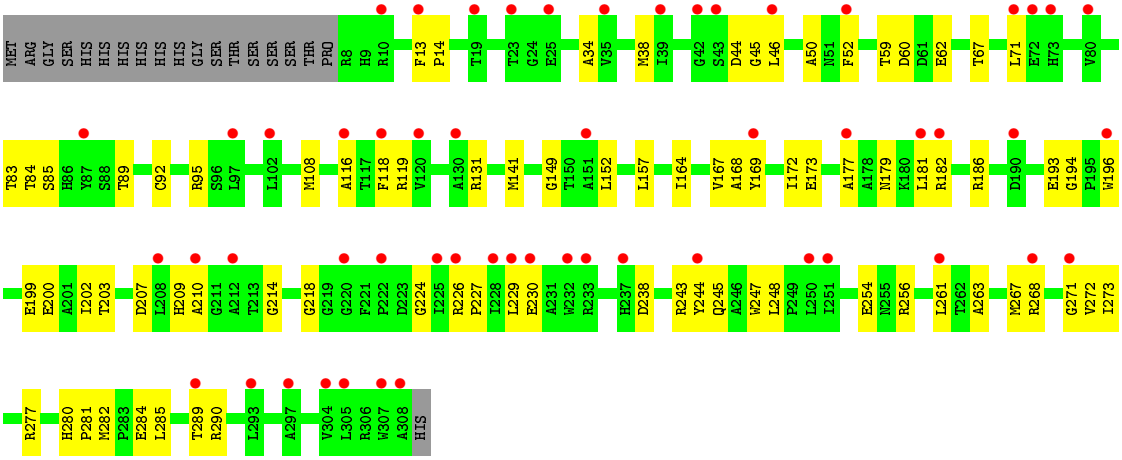
• Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain K:



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

Chain L:


MET ARG GLY SER HIS HIS HIS HIS HIS GLY SER THR SER SER SER THR PRO R8 H9 R10 F13 P14 T19 T23 G24 E25 A34 V35 M38 I39 G42 S43 D44 G45 L46 A50 N51 F52 T59 D60 D61 E62 T67 L71 E72 H73 V80
T83 T84 S85 B86 V87 S88 T89 C92 R95 S96 L97 L102 M108 A116 T117 F118 R119 V120 A130 R131 M141 G149 T150 A151 L152 L157 I164 V167 A168 Y169 I172 E173 A177 A178 N179 K180 L181 R182 R186 D190 E193 G194 P196 W196
E199 E200 A201 I202 T203 D207 L208 H209 A210 G211 A212 T213 G214 G218 G219 G220 F221 P222 D223 G224 I225 R226 P227 I228 L229 E230 A231 W232 R233 H237 D238 R243 Y244 Q245 A246 W247 L248 P249 L250 I251 E254 N255 R256 L261 T262 A263 M267 R268 G271 V272 I273
R277 H280 P281 M282 P283 E284 L285 T289 R290 L293 A297 V304 L305 R306 W307 A308 HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	74.52Å 81.20Å 142.84Å 85.71° 88.43° 75.39°	Depositor
Resolution (Å)	47.95 – 2.20 47.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.95-2.20) 98.3 (47.95-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.221 , 0.269 0.220 , 0.266	Depositor DCC
R_{free} test set	8087 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 38.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	29111	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FF9

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	0.26	0/2386	0.44	0/3244
1	B	0.26	0/2369	0.43	0/3222
1	C	0.26	0/2386	0.43	0/3244
1	D	0.25	0/2368	0.43	0/3222
1	E	0.25	0/2386	0.43	0/3244
1	F	0.26	0/2369	0.44	0/3222
1	G	0.26	0/2368	0.43	0/3222
1	H	0.25	0/2368	0.43	0/3222
1	I	0.26	0/2380	0.44	0/3237
1	J	0.28	0/2380	0.47	0/3237
1	K	0.27	0/2374	0.48	0/3229
1	L	0.28	0/2359	0.45	0/3207
All	All	0.26	0/28493	0.44	0/38752

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2348	0	2308	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2326	0	2296	24	0
1	C	2342	0	2308	18	0
1	D	2325	0	2290	15	0
1	E	2342	0	2308	27	0
1	F	2326	0	2296	27	0
1	G	2325	0	2290	14	0
1	H	2325	0	2290	23	0
1	I	2336	0	2297	54	0
1	J	2336	0	2297	81	0
1	K	2331	0	2301	93	0
1	L	2317	0	2287	60	0
2	A	105	0	0	0	0
2	B	92	0	0	0	0
2	C	107	0	0	1	0
2	D	111	0	0	3	0
2	E	112	0	0	0	0
2	F	105	0	0	3	0
2	G	116	0	0	2	0
2	H	97	0	0	4	0
2	I	65	0	0	6	0
2	J	71	0	0	5	0
2	K	89	0	0	36	0
2	L	62	0	0	9	0
All	All	29111	0	27568	427	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 (427) 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:203:THR:CG2	1:K:256:ARG:HD2	1.87	1.05
1:J:203:THR:HG21	1:K:256:ARG:CD	1.87	1.04
1:J:203:THR:HG21	1:K:256:ARG:HD2	0.98	0.97
1:J:100:GLN:HE22	1:J:137:ALA:H	1.11	0.96
1:K:63:ARG:NH1	2:K:403:HOH:O	2.04	0.90
1:F:227:PRO:HA	1:F:230:GLU:HG2	1.53	0.89
1:K:256:ARG:NH1	2:K:404:HOH:O	2.06	0.88
1:K:90:GLN:OE1	2:K:401:HOH:O	1.90	0.87
1:K:119:ARG:HH11	1:K:149:GLY:HA3	1.41	0.85
1:K:31:GLN:HG3	1:K:70:ILE:HD11	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:84:THR:OG1	2:L:401:HOH:O	1.95	0.84
1:I:45:GLY:HA2	1:I:78:VAL:CG1	2.07	0.84
2:K:401:HOH:O	1:L:280:HIS:O	1.97	0.81
1:I:23:THR:HG23	1:I:25:GLU:H	1.46	0.80
1:A:163:GLU:OE2	1:J:159:ARG:NH1	2.15	0.80
1:K:51:ASN:OD1	2:K:402:HOH:O	1.99	0.80
1:J:303:LEU:HD21	1:J:307:TRP:HD1	1.47	0.79
1:A:159:ARG:NH1	1:J:163:GLU:OE2	2.15	0.79
1:L:89:THR:OG1	2:L:402:HOH:O	2.02	0.78
1:L:224:GLY:HA2	1:L:243:ARG:HH21	1.49	0.78
1:J:253:HIS:HD2	1:J:293:LEU:HD12	1.50	0.77
1:J:277:ARG:NH2	2:J:401:HOH:O	2.18	0.76
1:K:32:LYS:HZ2	1:K:69:THR:HG22	1.49	0.76
1:L:119:ARG:HH21	1:L:149:GLY:HA3	1.50	0.76
1:I:21:ALA:HB3	1:I:23:THR:HG22	1.67	0.76
1:K:185:ILE:HD11	1:K:195:PRO:HB3	1.68	0.75
1:I:243:ARG:NH2	2:I:402:HOH:O	2.19	0.75
1:G:261:LEU:HD21	1:G:278:PRO:HB3	1.69	0.74
1:K:254:GLU:OE2	2:K:405:HOH:O	2.06	0.74
1:J:224:GLY:HA2	1:J:243:ARG:HH21	1.51	0.74
1:L:168:ALA:HB1	1:L:193:GLU:HB2	1.70	0.73
1:I:45:GLY:HA2	1:I:78:VAL:HG13	1.69	0.73
1:K:177:ALA:O	2:K:406:HOH:O	2.07	0.72
1:K:184:LEU:O	2:K:407:HOH:O	2.08	0.72
1:H:243:ARG:NH1	2:H:403:HOH:O	2.23	0.71
1:J:261:LEU:HD21	1:J:278:PRO:HB3	1.74	0.70
1:J:303:LEU:HD21	1:J:307:TRP:CD1	2.27	0.70
1:L:268:ARG:NH1	1:L:273:ILE:O	2.25	0.70
1:I:83:THR:O	2:I:401:HOH:O	2.08	0.69
1:K:49:LEU:O	2:K:403:HOH:O	2.09	0.69
1:J:304:VAL:HG13	1:J:305:LEU:HD22	1.73	0.69
1:I:13:PHE:CE2	1:I:45:GLY:HA3	2.29	0.68
1:I:68:ARG:NH1	2:I:407:HOH:O	2.26	0.68
1:J:262:THR:HG23	1:J:293:LEU:HD11	1.75	0.68
1:K:133:SER:O	2:K:408:HOH:O	2.11	0.68
1:K:32:LYS:NZ	1:K:69:THR:HG22	2.09	0.67
1:J:253:HIS:CD2	1:J:293:LEU:HD12	2.30	0.67
1:F:230:GLU:HG3	1:F:231:ALA:N	2.09	0.67
1:K:299:ARG:NH2	2:K:423:HOH:O	2.27	0.67
1:I:289:THR:HG21	1:L:179:ASN:HD21	1.60	0.67
1:K:35:VAL:HG21	1:K:70:ILE:HD12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:64:ASP:OD2	2:K:410:HOH:O	2.14	0.66
1:A:22:ASP:HB3	1:A:277:ARG:HH11	1.61	0.66
1:J:296:ILE:HA	1:J:299:ARG:HH21	1.60	0.66
1:J:71:LEU:HA	1:J:74:VAL:HG22	1.77	0.66
1:L:226:ARG:NH1	1:L:230:GLU:OE1	2.29	0.66
1:H:98:ARG:NH1	2:H:401:HOH:O	2.27	0.65
1:I:20:PHE:CE1	1:I:279:ARG:HD2	2.31	0.65
1:J:277:ARG:NH1	1:J:278:PRO:O	2.30	0.65
1:K:32:LYS:NZ	1:K:73:HIS:HB2	2.12	0.65
1:B:227:PRO:HB2	1:B:243:ARG:HD3	1.76	0.65
1:L:92:CYS:O	2:L:401:HOH:O	2.14	0.65
1:J:30:SER:HB3	1:J:273:ILE:HA	1.79	0.65
1:F:10:ARG:NH1	2:F:407:HOH:O	2.30	0.64
1:B:202:ILE:HG23	1:B:203:THR:HG23	1.79	0.64
1:I:13:PHE:CZ	1:I:45:GLY:HA3	2.33	0.64
1:J:200:GLU:OE1	1:J:255:ASN:ND2	2.26	0.64
1:C:49:LEU:HD13	1:C:63:ARG:HG3	1.79	0.63
1:K:89:THR:N	2:K:401:HOH:O	2.30	0.63
1:L:164:ILE:HB	1:L:167:VAL:HG12	1.81	0.63
1:I:227:PRO:HB2	1:I:243:ARG:HD3	1.81	0.63
1:K:63:ARG:O	1:K:67:THR:HG23	1.99	0.62
1:B:163:GLU:HG2	1:F:163:GLU:HG2	1.79	0.62
1:K:162:ARG:NH1	2:K:414:HOH:O	2.18	0.62
1:K:55:GLN:NE2	2:K:402:HOH:O	2.32	0.62
1:A:261:LEU:HD21	1:A:278:PRO:HB3	1.80	0.62
1:J:276:GLU:OE2	1:J:290:ARG:NH1	2.23	0.62
1:K:158:ALA:HB2	2:K:407:HOH:O	1.99	0.62
1:L:268:ARG:NE	1:L:268:ARG:O	2.32	0.62
1:H:202:ILE:HG23	1:H:203:THR:HG23	1.81	0.61
1:L:95:ARG:HB2	2:L:401:HOH:O	2.00	0.61
1:A:22:ASP:OD1	1:A:275:SER:OG	2.13	0.61
1:H:101:GLN:NE2	2:H:406:HOH:O	2.34	0.61
1:L:34:ALA:O	1:L:38:MET:HG3	2.01	0.61
1:E:202:ILE:HG23	1:E:203:THR:HG23	1.83	0.60
1:H:101:GLN:OE1	2:H:401:HOH:O	2.16	0.60
1:L:227:PRO:HA	1:L:230:GLU:OE2	2.01	0.60
1:E:136:ILE:HD13	1:E:138:ILE:O	2.01	0.60
1:J:31:GLN:O	1:J:35:VAL:HG23	2.02	0.60
1:K:244:TYR:CE2	1:K:248:LEU:HD22	2.37	0.60
1:B:163:GLU:HA	1:F:163:GLU:HA	1.83	0.60
1:D:261:LEU:HD21	1:D:278:PRO:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:286:HIS:CD2	1:I:288:ASP:HB2	2.37	0.60
1:I:49:LEU:HD13	1:I:63:ARG:HG3	1.83	0.60
1:J:296:ILE:HA	1:J:299:ARG:NH2	2.16	0.60
1:K:254:GLU:HB2	1:K:262:THR:HG21	1.83	0.59
1:K:49:LEU:HD11	1:K:67:THR:HG22	1.84	0.59
1:L:245:GLN:NE2	2:L:404:HOH:O	2.34	0.59
1:F:200:GLU:HG2	1:F:254:GLU:HG2	1.83	0.59
1:K:16:VAL:O	2:K:411:HOH:O	2.15	0.59
1:K:82:VAL:N	2:K:418:HOH:O	2.35	0.59
1:L:164:ILE:HB	1:L:167:VAL:CG1	2.33	0.59
1:H:21:ALA:HB3	1:H:25:GLU:HG3	1.84	0.59
1:K:280:HIS:ND1	2:L:402:HOH:O	2.32	0.58
1:J:247:TRP:CE3	1:J:300:LEU:HD23	2.38	0.58
1:K:64:ASP:OD1	2:K:412:HOH:O	2.17	0.58
1:H:23:THR:OG1	1:H:25:GLU:HG2	2.03	0.58
1:F:261:LEU:HD21	1:F:278:PRO:HB3	1.85	0.58
1:G:8:ARG:NH2	2:G:404:HOH:O	2.36	0.57
1:E:261:LEU:HD21	1:E:278:PRO:HB3	1.86	0.57
1:J:277:ARG:HH22	1:J:280:HIS:H	1.52	0.57
1:A:143:GLN:NE2	1:A:171:FF9:O1	2.35	0.57
1:K:87:TYR:OH	1:L:282:MET:HG3	2.04	0.57
1:L:59:THR:OG1	1:L:62:GLU:HG3	2.05	0.57
1:D:200:GLU:HG2	1:D:254:GLU:HG2	1.86	0.57
1:K:98:ARG:O	1:K:102:LEU:HG	2.05	0.56
1:I:14:PRO:HD2	1:I:45:GLY:O	2.05	0.56
1:J:202:ILE:HG13	2:K:409:HOH:O	2.04	0.56
1:K:119:ARG:HH12	1:L:116:ALA:HB2	1.71	0.56
1:G:48:ILE:HD11	1:G:82:VAL:HG22	1.88	0.56
1:H:268:ARG:HE	1:H:275:SER:HA	1.71	0.56
1:J:12:ILE:HG12	1:J:14:PRO:HD3	1.87	0.56
1:L:200:GLU:HG2	1:L:254:GLU:HG2	1.88	0.56
1:D:277:ARG:HG2	1:D:278:PRO:O	2.06	0.56
1:K:255:ASN:O	2:K:413:HOH:O	2.18	0.56
1:I:268:ARG:HB2	1:I:276:GLU:HB3	1.88	0.55
1:J:227:PRO:HB2	1:J:243:ARG:HD3	1.87	0.55
1:K:299:ARG:NH2	2:K:434:HOH:O	2.39	0.55
1:L:202:ILE:HG23	1:L:203:THR:HG23	1.88	0.55
1:A:22:ASP:HB3	1:A:277:ARG:NH1	2.21	0.55
1:F:233:ARG:NH2	2:F:404:HOH:O	2.26	0.55
1:D:227:PRO:HA	1:D:230:GLU:HB2	1.89	0.55
1:E:281:PRO:HB2	1:F:124:GLN:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:81:ILE:HG12	1:I:106:MET:HB3	1.87	0.55
1:B:49:LEU:HD13	1:B:63:ARG:HG3	1.89	0.55
1:F:202:ILE:HG23	1:F:203:THR:HG23	1.89	0.55
1:J:299:ARG:CZ	1:J:299:ARG:HB2	2.37	0.55
1:F:49:LEU:HD13	1:F:63:ARG:HG3	1.88	0.54
1:K:224:GLY:HA2	1:K:243:ARG:HH21	1.71	0.54
1:A:22:ASP:OD1	1:A:277:ARG:HD2	2.07	0.54
1:K:13:PHE:CE2	1:K:45:GLY:HA3	2.43	0.54
1:J:201:ALA:HB2	1:J:217:THR:HG22	1.89	0.54
1:K:32:LYS:N	1:K:32:LYS:HD2	2.23	0.54
1:I:204:LEU:HD11	1:I:229:LEU:HD11	1.90	0.54
1:J:256:ARG:O	2:J:402:HOH:O	2.18	0.54
1:J:302:PRO:HG2	1:J:305:LEU:HD23	1.90	0.54
1:G:243:ARG:NH1	2:G:408:HOH:O	2.41	0.54
1:L:173:GLU:HB2	1:L:199:GLU:HG3	1.89	0.54
1:I:254:GLU:HB2	1:I:262:THR:HG21	1.90	0.53
1:K:60:ASP:HB2	1:L:60:ASP:HB2	1.89	0.53
1:B:12:ILE:HG12	1:B:14:PRO:HD3	1.90	0.53
1:K:110:MET:SD	1:K:143:GLN:HB3	2.49	0.53
1:K:251:ILE:HA	2:K:405:HOH:O	2.08	0.53
1:J:106:MET:HG3	1:J:139:PRO:HG2	1.90	0.53
1:I:45:GLY:HA2	1:I:78:VAL:HG11	1.87	0.53
1:J:200:GLU:HG2	1:J:254:GLU:HG2	1.90	0.53
1:K:153:SER:HB2	1:K:155:PRO:HD2	1.90	0.53
1:E:199:GLU:HG3	1:E:255:ASN:HD21	1.73	0.53
1:I:255:ASN:OD1	1:L:256:ARG:NH1	2.41	0.53
1:I:33:ARG:HH11	1:I:33:ARG:HG3	1.74	0.53
1:L:285:LEU:HB3	2:L:403:HOH:O	2.08	0.53
1:J:299:ARG:NH2	1:K:241:TYR:CZ	2.78	0.52
1:F:156:PHE:O	1:F:160:MET:HG3	2.09	0.52
1:K:185:ILE:HD11	1:K:195:PRO:CB	2.37	0.52
1:K:227:PRO:HB2	1:K:243:ARG:HD3	1.91	0.52
1:L:182:ARG:HH12	1:L:209:HIS:HB3	1.74	0.52
1:C:10:ARG:HG2	1:C:213:THR:O	2.09	0.52
1:K:298:ARG:HH12	1:K:305:LEU:HD22	1.74	0.52
1:I:227:PRO:HG2	1:I:243:ARG:CZ	2.39	0.52
1:K:56:PHE:HD1	2:K:402:HOH:O	1.93	0.52
1:L:172:ILE:HB	1:L:181:LEU:HD21	1.92	0.52
1:L:268:ARG:HH22	1:L:271:GLY:HA2	1.75	0.52
1:F:227:PRO:HB2	1:F:243:ARG:HD2	1.91	0.52
1:J:100:GLN:HE22	1:J:137:ALA:N	1.94	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:61:ASP:OD1	2:J:403:HOH:O	2.18	0.52
1:K:119:ARG:NH1	1:K:149:GLY:HA3	2.17	0.52
1:C:8:ARG:NH2	2:C:401:HOH:O	2.29	0.52
1:K:55:GLN:OE1	2:K:415:HOH:O	2.19	0.52
1:J:26:LEU:HD11	1:J:62:GLU:HB3	1.92	0.51
1:H:200:GLU:HG2	1:H:254:GLU:HG2	1.91	0.51
1:F:126:PHE:HA	1:F:160:MET:HE3	1.90	0.51
1:E:124:GLN:HB3	1:F:281:PRO:HB2	1.93	0.51
1:C:261:LEU:HD21	1:C:278:PRO:HB3	1.92	0.51
1:E:183:GLU:HA	1:E:186:ARG:HG2	1.93	0.51
1:K:299:ARG:HG3	2:K:434:HOH:O	2.10	0.51
1:J:66:LEU:O	1:J:70:ILE:HG22	2.10	0.51
1:K:292:GLU:O	1:K:296:ILE:HG12	2.10	0.51
1:H:13:PHE:CE2	1:H:45:GLY:HA3	2.46	0.50
1:K:32:LYS:HZ1	1:K:73:HIS:HB2	1.74	0.50
1:B:73:HIS:O	1:B:77:ARG:NH2	2.45	0.50
1:G:202:ILE:HG23	1:G:203:THR:HG23	1.91	0.50
1:K:123:ALA:O	1:K:127:GLU:HG3	2.12	0.50
1:K:239:ASP:OD2	2:K:416:HOH:O	2.19	0.50
1:K:119:ARG:NH1	1:L:116:ALA:HB2	2.27	0.50
1:E:15:VAL:HG11	1:E:52:PHE:HB3	1.93	0.50
1:I:277:ARG:HG3	1:I:278:PRO:O	2.11	0.50
1:F:227:PRO:HA	1:F:230:GLU:CG	2.35	0.49
1:E:228:ILE:HG13	1:E:243:ARG:HG2	1.94	0.49
1:I:281:PRO:HB2	1:J:124:GLN:HB3	1.94	0.49
1:L:169:TYR:CD1	1:L:194:GLY:HA3	2.48	0.49
1:H:10:ARG:HH11	1:H:233:ARG:HH21	1.59	0.49
1:J:44:ASP:N	2:J:410:HOH:O	2.38	0.49
1:K:34:ALA:O	1:K:38:MET:HG3	2.12	0.49
1:F:169:TYR:CD2	1:F:194:GLY:HA3	2.47	0.49
1:I:63:ARG:NH1	2:I:401:HOH:O	2.29	0.49
1:K:184:LEU:HD13	1:K:184:LEU:C	2.32	0.49
1:D:15:VAL:HG11	1:D:52:PHE:HB3	1.95	0.48
1:I:302:PRO:HD2	1:I:305:LEU:HD12	1.93	0.48
1:J:266:LEU:HD21	1:J:293:LEU:CD2	2.42	0.48
1:H:97:LEU:HG	1:H:136:ILE:HG22	1.95	0.48
1:L:289:THR:HB	2:L:403:HOH:O	2.13	0.48
1:A:202:ILE:HG23	1:A:203:THR:HG23	1.94	0.48
1:D:202:ILE:HG23	1:D:203:THR:HG23	1.95	0.48
1:E:294:LEU:O	1:E:298:ARG:HG3	2.13	0.48
1:E:8:ARG:HG3	1:E:8:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:CE2	1:A:45:GLY:HA3	2.48	0.48
1:E:65:VAL:HG22	1:E:68:ARG:HH11	1.79	0.48
1:J:208:LEU:HD21	1:J:229:LEU:CD2	2.43	0.48
1:L:13:PHE:CE2	1:L:45:GLY:HA3	2.49	0.48
1:E:136:ILE:CD1	1:E:166:GLN:HG3	2.43	0.48
1:I:208:LEU:HD21	1:I:229:LEU:HD12	1.95	0.48
1:F:13:PHE:CE2	1:F:45:GLY:HA3	2.49	0.48
1:H:54:GLU:OE2	1:H:264:LYS:NZ	2.44	0.48
1:I:261:LEU:HB2	1:I:285:LEU:HD11	1.94	0.48
1:J:241:TYR:HE2	1:K:296:ILE:HD12	1.79	0.48
1:L:182:ARG:CZ	1:L:210:ALA:HA	2.44	0.48
1:K:261:LEU:HB2	1:K:285:LEU:HD11	1.94	0.47
1:K:38:MET:HE2	1:K:46:LEU:HD22	1.95	0.47
1:A:48:ILE:HD11	1:A:82:VAL:HG22	1.96	0.47
1:C:13:PHE:CE2	1:C:45:GLY:HA3	2.49	0.47
1:D:141:MET:HE3	1:D:169:TYR:HB3	1.95	0.47
1:K:304:VAL:HG13	1:K:305:LEU:HG	1.96	0.47
1:I:286:HIS:HB3	1:I:289:THR:HG23	1.95	0.47
1:I:41:ALA:HA	1:I:303:LEU:HD13	1.94	0.47
1:J:49:LEU:HD13	1:J:63:ARG:HG3	1.95	0.47
1:C:187:LEU:O	1:J:186:ARG:NH1	2.46	0.47
1:K:258:SER:HB2	1:K:262:THR:OG1	2.15	0.47
1:A:200:GLU:HG2	1:A:254:GLU:HG2	1.95	0.47
1:H:169:TYR:CD2	1:H:194:GLY:HA3	2.50	0.47
1:K:93:ALA:HB2	1:K:132:VAL:HG12	1.96	0.47
1:A:37:PHE:CZ	1:A:304:VAL:HB	2.50	0.47
1:J:169:TYR:CD2	1:J:194:GLY:HA3	2.49	0.47
1:L:261:LEU:HD12	1:L:261:LEU:H	1.79	0.47
1:C:15:VAL:HG11	1:C:52:PHE:HB3	1.96	0.47
1:A:65:VAL:HG22	1:A:68:ARG:HH12	1.80	0.47
1:J:299:ARG:HB2	1:J:299:ARG:NH1	2.30	0.47
1:E:169:TYR:CD2	1:E:194:GLY:HA3	2.50	0.47
1:E:49:LEU:HD13	1:E:63:ARG:HG3	1.97	0.47
1:I:266:LEU:HB3	1:I:304:VAL:HG11	1.96	0.47
1:J:296:ILE:HG23	1:J:299:ARG:HH22	1.80	0.47
1:C:48:ILE:HG21	1:C:70:ILE:HG21	1.96	0.47
1:E:280:HIS:CG	1:E:281:PRO:HA	2.49	0.47
1:E:90:GLN:HE22	1:F:24:GLY:HA3	1.80	0.47
1:J:203:THR:CG2	1:K:256:ARG:HH21	2.28	0.47
1:H:10:ARG:HD3	1:H:233:ARG:NH2	2.30	0.47
1:L:85:SER:O	1:L:95:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HD13	1:A:63:ARG:HG3	1.97	0.46
1:F:54:GLU:OE2	1:F:264:LYS:NZ	2.46	0.46
1:B:280:HIS:CG	1:B:281:PRO:HA	2.49	0.46
1:K:184:LEU:CD1	1:K:192:ILE:HG21	2.45	0.46
1:E:256:ARG:NH1	1:H:199:GLU:OE2	2.49	0.46
1:K:223:ASP:OD1	1:K:223:ASP:N	2.48	0.46
1:F:126:PHE:HA	1:F:160:MET:CE	2.46	0.46
1:G:49:LEU:HD13	1:G:63:ARG:HG3	1.98	0.46
1:H:183:GLU:OE1	1:H:186:ARG:NH2	2.49	0.46
1:K:155:PRO:HA	1:K:187:LEU:HD23	1.97	0.46
1:K:48:ILE:HA	2:K:411:HOH:O	2.14	0.46
1:L:44:ASP:OD1	1:L:226:ARG:NH2	2.43	0.46
1:I:268:ARG:NH1	1:I:274:ALA:O	2.49	0.46
1:J:209:HIS:CE1	1:J:232:TRP:HH2	2.34	0.46
1:A:169:TYR:CD2	1:A:194:GLY:HA3	2.51	0.46
1:B:48:ILE:HG21	1:B:70:ILE:HG21	1.98	0.46
1:C:6:THR:N	1:C:7:PRO:HD2	2.31	0.46
1:J:296:ILE:HG12	1:J:299:ARG:HH21	1.80	0.46
1:L:152:LEU:HB3	1:L:157:LEU:HD21	1.98	0.46
1:K:51:ASN:HA	2:K:402:HOH:O	2.15	0.46
1:L:50:ALA:HA	1:L:83:THR:HG21	1.98	0.46
1:D:297:ALA:O	1:D:302:PRO:HD3	2.15	0.46
1:F:183:GLU:OE1	1:F:186:ARG:NH2	2.48	0.45
1:G:45:GLY:HA2	1:G:78:VAL:HB	1.98	0.45
1:J:302:PRO:HG2	1:J:305:LEU:CD2	2.46	0.45
1:I:48:ILE:N	2:I:410:HOH:O	2.49	0.45
1:J:36:ASP:CG	1:J:73:HIS:HE2	2.19	0.45
1:K:39:ILE:HG21	1:K:77:ARG:HD2	1.98	0.45
1:A:22:ASP:CB	1:A:277:ARG:HH11	2.27	0.45
1:F:32:LYS:HG2	1:F:73:HIS:CG	2.52	0.45
1:D:153:SER:HB2	1:D:155:PRO:HD2	1.99	0.45
1:G:200:GLU:HG2	1:G:254:GLU:HG2	1.98	0.45
1:C:186:ARG:O	1:J:186:ARG:HG3	2.17	0.45
1:D:36:ASP:OD2	2:D:401:HOH:O	2.21	0.45
1:J:101:GLN:OE1	1:J:101:GLN:HA	2.17	0.45
1:K:126:PHE:CD2	1:K:160:MET:HG2	2.52	0.45
1:L:177:ALA:O	1:L:181:LEU:HD23	2.16	0.45
1:G:280:HIS:CG	1:G:281:PRO:HA	2.50	0.45
1:B:223:ASP:N	1:B:223:ASP:OD1	2.49	0.45
1:H:261:LEU:HD21	1:H:278:PRO:HB3	1.97	0.45
1:B:200:GLU:HG2	1:B:254:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:233:ARG:HE	1:K:234:GLU:HG3	1.82	0.45
1:E:136:ILE:HD11	1:E:166:GLN:HG3	1.99	0.45
1:H:141:MET:HE3	1:H:141:MET:HB2	1.79	0.45
1:I:122:GLU:OE1	2:I:403:HOH:O	2.21	0.45
1:I:144:ASP:OD2	1:I:180:LYS:NZ	2.45	0.45
1:K:245:GLN:OE1	2:K:417:HOH:O	2.21	0.45
1:L:89:THR:HG21	1:L:131:ARG:HD2	1.99	0.45
1:L:141:MET:HE3	1:L:169:TYR:HB3	1.99	0.45
1:L:243:ARG:HD2	1:L:247:TRP:CD1	2.51	0.45
1:B:161:ALA:HB2	1:B:170:PHE:HZ	1.82	0.44
1:E:199:GLU:HG3	1:E:255:ASN:ND2	2.31	0.44
1:I:16:VAL:HG13	1:I:38:MET:HE1	1.99	0.44
1:J:60:ASP:OD1	1:J:95:ARG:NH1	2.50	0.44
1:G:48:ILE:HG21	1:G:70:ILE:HG21	1.99	0.44
1:H:118:PHE:O	1:H:119:ARG:NH1	2.46	0.44
1:A:163:GLU:HB3	1:J:126:PHE:CE1	2.52	0.44
1:C:254:GLU:HB2	1:C:262:THR:HG21	1.98	0.44
1:L:263:ALA:O	1:L:267:MET:HG3	2.17	0.44
1:B:227:PRO:HB2	1:B:243:ARG:CD	2.47	0.44
1:C:276:GLU:OE2	1:C:290:ARG:NH2	2.43	0.44
1:B:119:ARG:HH21	1:B:149:GLY:HA3	1.83	0.44
1:I:233:ARG:HH21	1:I:233:ARG:HB3	1.83	0.44
1:J:176:GLY:N	2:J:422:HOH:O	2.51	0.44
1:I:247:TRP:CD2	1:I:300:LEU:HD22	2.53	0.44
1:J:141:MET:HE1	1:J:196:TRP:CZ3	2.52	0.44
1:C:81:ILE:HG12	1:C:106:MET:HB3	2.00	0.44
1:I:201:ALA:HB1	1:I:204:LEU:HB2	1.99	0.44
1:I:223:ASP:N	1:I:223:ASP:OD1	2.49	0.44
1:I:24:GLY:HA3	1:J:90:GLN:OE1	2.17	0.44
1:J:280:HIS:CG	1:J:281:PRO:HA	2.53	0.44
1:J:209:HIS:NE2	1:J:232:TRP:HH2	2.16	0.44
1:I:231:ALA:HB1	1:I:239:ASP:HB2	1.98	0.43
1:C:202:ILE:HG23	1:C:203:THR:HG23	1.99	0.43
1:E:13:PHE:O	1:E:216:MET:HG3	2.18	0.43
1:I:181:LEU:HD23	1:I:181:LEU:HA	1.80	0.43
1:J:74:VAL:HA	1:J:77:ARG:HH21	1.83	0.43
1:E:227:PRO:HB2	1:E:243:ARG:HD3	2.00	0.43
1:I:60:ASP:OD1	1:I:95:ARG:NH1	2.51	0.43
1:B:141:MET:HE3	1:B:141:MET:HB2	1.91	0.43
1:B:119:ARG:NH2	1:B:149:GLY:HA3	2.32	0.43
1:D:40:ASP:OD1	2:D:402:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:THR:HG23	1:G:7:PRO:HD3	2.01	0.43
1:J:296:ILE:HG23	1:J:299:ARG:NH2	2.33	0.43
1:K:6:THR:N	1:K:7:PRO:HD2	2.34	0.43
1:F:280:HIS:CG	1:F:281:PRO:HA	2.53	0.43
1:I:13:PHE:CD2	1:I:45:GLY:HA3	2.54	0.43
1:G:12:ILE:HG12	1:G:14:PRO:HD3	2.00	0.43
1:I:280:HIS:CG	1:I:281:PRO:HA	2.54	0.43
1:J:13:PHE:O	1:J:216:MET:HG3	2.18	0.43
1:J:303:LEU:HD23	1:J:303:LEU:O	2.18	0.43
1:K:32:LYS:CE	1:K:70:ILE:HD13	2.48	0.43
1:C:280:HIS:CG	1:C:281:PRO:HA	2.54	0.43
1:G:13:PHE:CE2	1:G:45:GLY:HA3	2.53	0.43
1:J:203:THR:CG2	1:K:256:ARG:NH2	2.82	0.43
1:L:290:ARG:N	2:L:403:HOH:O	2.52	0.43
1:J:37:PHE:CE1	1:J:303:LEU:HD22	2.54	0.43
1:J:303:LEU:CD2	1:J:307:TRP:CD1	3.01	0.43
1:E:227:PRO:HB2	1:E:243:ARG:CD	2.49	0.42
1:C:200:GLU:HG2	1:C:254:GLU:HG2	2.00	0.42
1:H:6:THR:N	1:H:7:PRO:CD	2.82	0.42
1:L:267:MET:HB3	1:L:272:VAL:HB	2.01	0.42
1:H:71:LEU:HA	1:H:71:LEU:HD13	1.93	0.42
1:K:32:LYS:HZ3	1:K:73:HIS:HB2	1.83	0.42
1:J:262:THR:HG23	1:J:293:LEU:CD1	2.48	0.42
1:J:37:PHE:CZ	1:J:304:VAL:HB	2.54	0.42
1:K:302:PRO:HB2	2:K:450:HOH:O	2.19	0.42
1:L:67:THR:O	1:L:71:LEU:HB2	2.19	0.42
1:D:52:PHE:HA	1:D:260:ILE:HG12	2.01	0.42
1:E:153:SER:HB2	1:E:155:PRO:HD2	2.01	0.42
1:G:54:GLU:OE2	1:G:264:LYS:NZ	2.34	0.42
1:J:71:LEU:HD21	1:J:80:VAL:HB	2.02	0.42
1:L:196:TRP:CD2	1:L:214:GLY:HA3	2.54	0.42
1:F:13:PHE:O	1:F:216:MET:HG3	2.20	0.42
1:J:241:TYR:CE2	1:K:296:ILE:HD12	2.55	0.42
1:I:286:HIS:HB3	1:I:289:THR:CG2	2.50	0.42
1:L:226:ARG:HA	1:L:229:LEU:HD12	2.02	0.42
1:B:192:ILE:HG22	1:B:195:PRO:HD3	2.01	0.42
1:B:276:GLU:OE2	1:B:290:ARG:NH1	2.47	0.42
1:E:224:GLY:HA2	1:E:243:ARG:HH12	1.85	0.42
1:F:9:HIS:O	2:F:401:HOH:O	2.21	0.42
1:K:107:VAL:HG13	1:K:138:ILE:HD11	2.02	0.42
1:K:49:LEU:CD1	1:K:67:THR:HG22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:207:ASP:O	1:L:210:ALA:HB3	2.20	0.42
1:I:208:LEU:HD11	1:I:229:LEU:HD13	2.02	0.42
1:K:168:ALA:HB1	1:K:193:GLU:HB2	2.01	0.42
1:J:203:THR:HG23	2:K:409:HOH:O	2.19	0.42
1:L:280:HIS:CG	1:L:281:PRO:HA	2.54	0.42
1:D:68:ARG:HD3	1:D:98:ARG:NH2	2.35	0.41
1:L:108:MET:HG3	1:L:141:MET:HB3	2.01	0.41
1:I:247:TRP:CE2	1:I:300:LEU:HD22	2.55	0.41
1:K:107:VAL:HA	2:K:418:HOH:O	2.19	0.41
1:K:81:ILE:HG22	2:K:418:HOH:O	2.20	0.41
1:L:108:MET:HA	1:L:141:MET:O	2.20	0.41
1:A:26:LEU:HD11	1:A:62:GLU:HB3	2.01	0.41
1:H:48:ILE:HD11	1:H:82:VAL:HG22	2.03	0.41
1:J:228:ILE:HG13	1:J:243:ARG:HG2	2.03	0.41
1:E:48:ILE:HG21	1:E:70:ILE:HG21	2.02	0.41
1:J:247:TRP:HH2	1:J:302:PRO:HB3	1.85	0.41
1:B:161:ALA:HB2	1:B:170:PHE:CZ	2.55	0.41
1:K:256:ARG:CZ	2:K:404:HOH:O	2.57	0.41
1:I:261:LEU:HD21	1:I:278:PRO:HB3	2.03	0.41
1:B:228:ILE:HG13	1:B:243:ARG:HG2	2.02	0.41
1:E:136:ILE:HD12	1:E:136:ILE:C	2.41	0.41
1:I:82:VAL:O	1:I:107:VAL:HA	2.20	0.41
1:J:247:TRP:CH2	1:J:302:PRO:HB3	2.56	0.41
1:K:35:VAL:HG21	1:K:70:ILE:HG23	2.02	0.41
1:J:203:THR:OG1	1:K:256:ARG:NH2	2.54	0.41
1:K:254:GLU:HG3	1:K:262:THR:OG1	2.21	0.41
1:K:252:ASN:ND2	2:K:409:HOH:O	2.13	0.41
1:K:296:ILE:O	1:K:299:ARG:HB3	2.20	0.41
1:L:277:ARG:HG2	1:L:284:GLU:OE2	2.21	0.41
1:B:169:TYR:CD2	1:B:194:GLY:HA3	2.56	0.41
1:B:74:VAL:HA	1:B:77:ARG:HH21	1.86	0.41
1:I:303:LEU:HD21	1:I:307:TRP:HD1	1.85	0.41
1:L:118:PHE:O	1:L:119:ARG:HD3	2.21	0.41
1:L:14:PRO:HB3	1:L:218:GLY:O	2.21	0.41
1:D:276:GLU:OE2	1:D:290:ARG:NH1	2.54	0.40
1:B:13:PHE:CE2	1:B:45:GLY:HA3	2.55	0.40
1:B:246:ALA:O	1:B:300:LEU:HD21	2.21	0.40
1:C:12:ILE:HG12	1:C:14:PRO:HD3	2.04	0.40
1:F:278:PRO:HB2	1:F:282:MET:HB3	2.03	0.40
1:I:37:PHE:CZ	1:I:304:VAL:HB	2.57	0.40
1:J:114:HIS:O	1:J:118:PHE:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:224:GLY:CA	1:L:243:ARG:HH21	2.27	0.40
1:D:72:GLU:OE1	2:D:403:HOH:O	2.21	0.40
1:L:38:MET:HE2	1:L:46:LEU:HD22	2.02	0.40
1:A:186:ARG:HG3	1:L:186:ARG:O	2.21	0.40
1:C:168:ALA:HB1	1:C:193:GLU:HB2	2.04	0.40
1:J:48:ILE:HD11	1:J:82:VAL:HG13	2.04	0.40
1:L:244:TYR:O	1:L:248:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	301/320 (94%)	291 (97%)	10 (3%)	0	100	100
1	B	299/320 (93%)	292 (98%)	7 (2%)	0	100	100
1	C	301/320 (94%)	293 (97%)	8 (3%)	0	100	100
1	D	300/320 (94%)	295 (98%)	5 (2%)	0	100	100
1	E	301/320 (94%)	292 (97%)	9 (3%)	0	100	100
1	F	299/320 (93%)	292 (98%)	7 (2%)	0	100	100
1	G	300/320 (94%)	294 (98%)	6 (2%)	0	100	100
1	H	300/320 (94%)	292 (97%)	8 (3%)	0	100	100
1	I	301/320 (94%)	293 (97%)	8 (3%)	0	100	100
1	J	301/320 (94%)	294 (98%)	7 (2%)	0	100	100
1	K	300/320 (94%)	293 (98%)	7 (2%)	0	100	100
1	L	298/320 (93%)	291 (98%)	7 (2%)	0	100	100
All	All	3601/3840 (94%)	3512 (98%)	89 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	236/250 (94%)	234 (99%)	2 (1%)	81 90
1	B	235/250 (94%)	233 (99%)	2 (1%)	78 88
1	C	236/250 (94%)	232 (98%)	4 (2%)	60 74
1	D	234/250 (94%)	229 (98%)	5 (2%)	53 67
1	E	236/250 (94%)	235 (100%)	1 (0%)	91 96
1	F	235/250 (94%)	231 (98%)	4 (2%)	60 74
1	G	234/250 (94%)	232 (99%)	2 (1%)	78 88
1	H	234/250 (94%)	233 (100%)	1 (0%)	91 96
1	I	235/250 (94%)	230 (98%)	5 (2%)	53 67
1	J	235/250 (94%)	232 (99%)	3 (1%)	69 81
1	K	235/250 (94%)	231 (98%)	4 (2%)	60 74
1	L	233/250 (93%)	231 (99%)	2 (1%)	78 88
All	All	2818/3000 (94%)	2783 (99%)	35 (1%)	71 83

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	52	PHE
1	B	52	PHE
1	B	268	ARG
1	C	10	ARG
1	C	52	PHE
1	C	63	ARG
1	C	98	ARG
1	D	22	ASP
1	D	52	PHE
1	D	238	ASP
1	D	268	ARG
1	D	277	ARG
1	E	52	PHE

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Mol	Chain	Res	Type
1	F	52	PHE
1	F	63	ARG
1	F	233	ARG
1	F	268	ARG
1	G	37	PHE
1	G	52	PHE
1	H	277	ARG
1	I	10	ARG
1	I	52	PHE
1	I	190	ASP
1	I	226	ARG
1	I	277	ARG
1	J	52	PHE
1	J	268	ARG
1	J	277	ARG
1	K	52	PHE
1	K	90	GLN
1	K	256	ARG
1	K	298	ARG
1	L	52	PHE
1	L	238	ASP

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

Mol	Chain	Res	Type
1	I	286	HIS
1	J	100	GLN
1	J	253	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FF9	J	171	1	7,8,15	0.49	0	3,8,18	0.38	0
1	FF9	C	171	1	7,8,15	0.52	0	3,8,18	0.62	0
1	FF9	F	171	1	7,8,15	0.49	0	3,8,18	0.26	0
1	FF9	A	171	1	10,14,15	1.13	1 (10%)	6,16,18	1.73	1 (16%)
1	FF9	D	171	1	7,8,15	0.46	0	3,8,18	0.50	0
1	FF9	G	171	1	7,8,15	0.50	0	3,8,18	0.27	0
1	FF9	E	171	1	7,8,15	0.52	0	3,8,18	0.43	0
1	FF9	H	171	1	7,8,15	0.52	0	3,8,18	0.71	0
1	FF9	K	171	1	7,8,15	0.53	0	3,8,18	0.45	0
1	FF9	I	171	1	7,8,15	0.51	0	3,8,18	0.57	0
1	FF9	L	171	1	7,8,15	0.53	0	3,8,18	0.52	0
1	FF9	B	171	1	7,8,15	0.51	0	3,8,18	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FF9	J	171	1	-	3/6/7/18	-
1	FF9	C	171	1	-	0/6/7/18	-
1	FF9	F	171	1	-	2/6/7/18	-
1	FF9	A	171	1	-	1/10/16/18	-
1	FF9	D	171	1	-	1/6/7/18	-
1	FF9	G	171	1	-	0/6/7/18	-
1	FF9	E	171	1	-	0/6/7/18	-
1	FF9	H	171	1	-	1/6/7/18	-
1	FF9	K	171	1	-	1/6/7/18	-
1	FF9	I	171	1	-	1/6/7/18	-
1	FF9	L	171	1	-	1/6/7/18	-
1	FF9	B	171	1	-	2/6/7/18	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	FF9	CX2-CX1	-3.22	1.47	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	FF9	CD-CE-NZ	-3.06	105.09	110.66

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	J	171	FF9	O-C-CA-CB
1	F	171	FF9	O-C-CA-CB
1	A	171	FF9	O-C-CA-CB
1	D	171	FF9	O-C-CA-CB
1	H	171	FF9	O-C-CA-CB
1	I	171	FF9	O-C-CA-CB
1	L	171	FF9	O-C-CA-CB
1	B	171	FF9	O-C-CA-CB
1	B	171	FF9	CE-CD-CG-CB
1	K	171	FF9	CA-CB-CG-CD
1	J	171	FF9	CE-CD-CG-CB
1	J	171	FF9	CA-CB-CG-CD
1	F	171	FF9	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	171	FF9	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	303/320 (94%)	-0.24	4 (1%) 77 75	19, 28, 42, 65	0
1	B	301/320 (94%)	-0.07	4 (1%) 77 75	23, 32, 45, 67	0
1	C	303/320 (94%)	-0.24	3 (0%) 82 81	21, 27, 38, 62	0
1	D	302/320 (94%)	-0.21	2 (0%) 87 86	22, 30, 43, 77	0
1	E	303/320 (94%)	-0.27	3 (0%) 82 81	21, 30, 42, 82	0
1	F	301/320 (94%)	-0.22	0 100 100	20, 30, 40, 57	0
1	G	302/320 (94%)	-0.29	1 (0%) 94 93	23, 28, 40, 71	0
1	H	302/320 (94%)	-0.23	2 (0%) 87 86	22, 30, 42, 57	0
1	I	303/320 (94%)	0.89	54 (17%) 1 1	23, 47, 59, 74	0
1	J	303/320 (94%)	0.72	31 (10%) 6 6	20, 44, 58, 73	0
1	K	302/320 (94%)	1.17	53 (17%) 1 1	35, 43, 53, 75	0
1	L	300/320 (93%)	1.14	55 (18%) 1 1	34, 46, 55, 70	0
All	All	3625/3840 (94%)	0.18	212 (5%) 23 22	19, 32, 52, 82	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	6	THR	6.7
1	I	240	ALA	6.3
1	E	6	THR	6.2
1	J	71	LEU	6.1
1	A	308	ALA	5.8
1	I	228	ILE	5.5
1	A	309	HIS	5.3
1	G	6	THR	5.3
1	L	130	ALA	5.3
1	J	304	VAL	5.2
1	C	6	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	6	THR	5.1
1	K	7	PRO	4.9
1	I	309	HIS	4.9
1	K	41	ALA	4.6
1	J	35	VAL	4.6
1	K	185	ILE	4.6
1	L	118	PHE	4.6
1	I	24	GLY	4.5
1	D	7	PRO	4.5
1	L	208	LEU	4.4
1	L	229	LEU	4.4
1	L	244	TYR	4.4
1	E	7	PRO	4.1
1	J	229	LEU	4.1
1	I	293	LEU	4.0
1	I	74	VAL	4.0
1	J	222	PRO	4.0
1	A	6	THR	4.0
1	I	43	SER	3.9
1	B	7	PRO	3.9
1	J	287	PRO	3.9
1	K	265	ALA	3.8
1	I	203	THR	3.8
1	J	240	ALA	3.8
1	K	57	ALA	3.8
1	I	6	THR	3.8
1	K	79	PRO	3.8
1	L	297	ALA	3.7
1	J	272	VAL	3.7
1	I	305	LEU	3.7
1	K	261	LEU	3.5
1	L	210	ALA	3.5
1	K	256	ARG	3.5
1	J	297	ALA	3.5
1	L	102	LEU	3.5
1	A	22	ASP	3.5
1	K	140	ILE	3.4
1	K	215	ALA	3.3
1	K	308	ALA	3.3
1	L	237	HIS	3.3
1	J	305	LEU	3.3
1	K	172	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	232	TRP	3.2
1	K	16	VAL	3.2
1	K	65	VAL	3.2
1	L	46	LEU	3.2
1	I	190	ASP	3.2
1	I	12	ILE	3.1
1	L	293	LEU	3.1
1	I	269	GLU	3.1
1	J	308	ALA	3.1
1	K	190	ASP	3.1
1	I	236	ARG	3.0
1	I	277	ARG	3.0
1	I	187	LEU	3.0
1	L	225	ILE	3.0
1	I	80	VAL	3.0
1	K	189	GLY	3.0
1	I	225	ILE	3.0
1	I	21	ALA	2.9
1	C	7	PRO	2.9
1	J	309	HIS	2.9
1	B	6	THR	2.9
1	L	177	ALA	2.9
1	L	80	VAL	2.8
1	L	42	GLY	2.8
1	J	102	LEU	2.8
1	L	43	SER	2.8
1	L	39	ILE	2.8
1	I	221	PHE	2.8
1	K	34	ALA	2.8
1	I	7	PRO	2.8
1	K	132	VAL	2.8
1	J	205	LEU	2.7
1	K	227	PRO	2.7
1	L	220	GLY	2.7
1	K	17	PRO	2.7
1	K	232	TRP	2.7
1	L	19	THR	2.7
1	K	196	TRP	2.6
1	K	296	ILE	2.6
1	I	205	LEU	2.6
1	L	196	TRP	2.6
1	L	35	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	138	ILE	2.6
1	L	307	TRP	2.6
1	H	6	THR	2.6
1	L	250	LEU	2.6
1	K	277	ARG	2.6
1	J	291	ALA	2.6
1	K	99	ALA	2.6
1	L	25	GLU	2.6
1	K	225	ILE	2.6
1	K	18	THR	2.5
1	J	307	TRP	2.5
1	I	42	GLY	2.5
1	K	281	PRO	2.5
1	I	8	ARG	2.5
1	K	74	VAL	2.5
1	K	120	VAL	2.5
1	L	308	ALA	2.5
1	I	30	SER	2.5
1	I	265	ALA	2.5
1	L	23	THR	2.5
1	I	79	PRO	2.5
1	I	268	ARG	2.4
1	E	309	HIS	2.4
1	I	238	ASP	2.4
1	L	190	ASP	2.4
1	J	294	LEU	2.4
1	H	52	PHE	2.4
1	L	13	PHE	2.4
1	K	214	GLY	2.4
1	K	69	THR	2.4
1	B	211	GLY	2.4
1	I	11	GLY	2.4
1	K	11	GLY	2.4
1	L	230	GLU	2.4
1	L	232	TRP	2.4
1	I	211	GLY	2.4
1	L	151	ALA	2.4
1	J	46	LEU	2.3
1	I	186	ARG	2.3
1	J	237	HIS	2.3
1	J	29	ALA	2.3
1	K	71	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	71	LEU	2.3
1	L	10	ARG	2.3
1	B	190	ASP	2.3
1	K	126	PHE	2.3
1	I	198	GLY	2.3
1	I	246	ALA	2.3
1	L	289	THR	2.3
1	J	300	LEU	2.3
1	I	52	PHE	2.3
1	L	268	ARG	2.3
1	J	75	ALA	2.3
1	J	274	ALA	2.3
1	L	305	LEU	2.3
1	J	211	GLY	2.3
1	I	272	VAL	2.3
1	I	215	ALA	2.3
1	K	97	LEU	2.2
1	L	97	LEU	2.2
1	K	8	ARG	2.2
1	L	304	VAL	2.2
1	K	129	TYR	2.2
1	I	39	ILE	2.2
1	J	303	LEU	2.2
1	I	229	LEU	2.2
1	I	233	ARG	2.2
1	L	87	TYR	2.2
1	L	169	TYR	2.2
1	I	266	LEU	2.2
1	L	233	ARG	2.2
1	L	181	LEU	2.2
1	L	222	PRO	2.2
1	L	226	ARG	2.1
1	K	221	PHE	2.1
1	I	25	GLU	2.1
1	K	12	ILE	2.1
1	L	261	LEU	2.1
1	I	38	MET	2.1
1	L	182	ARG	2.1
1	I	237	HIS	2.1
1	K	113	TYR	2.1
1	I	105	ALA	2.1
1	J	81	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	232	TRP	2.1
1	I	23	THR	2.1
1	C	8	ARG	2.1
1	I	300	LEU	2.1
1	K	14	PRO	2.1
1	K	228	ILE	2.1
1	K	287	PRO	2.1
1	L	228	ILE	2.1
1	K	286	HIS	2.1
1	L	212	ALA	2.1
1	L	73	HIS	2.1
1	K	50	ALA	2.1
1	I	304	VAL	2.1
1	K	96	SER	2.1
1	K	166	GLN	2.0
1	I	46	LEU	2.0
1	I	250	LEU	2.0
1	L	251	ILE	2.0
1	I	179	ASN	2.0
1	I	214	GLY	2.0
1	L	116	ALA	2.0
1	J	74	VAL	2.0
1	I	244	TYR	2.0
1	K	10	ARG	2.0
1	L	52	PHE	2.0
1	K	106	MET	2.0
1	L	271	GLY	2.0
1	J	227	PRO	2.0
1	L	120	VAL	2.0
1	K	157	LEU	2.0
1	L	72	GLU	2.0
1	J	6	THR	2.0
1	K	67	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	FF9	K	171	9/16	0.80	0.24	36,46,49,51	0
1	FF9	L	171	9/16	0.82	0.25	36,48,50,50	0
1	FF9	A	171	15/16	0.85	0.20	21,26,33,34	6
1	FF9	I	171	9/16	0.87	0.19	38,42,49,52	0
1	FF9	D	171	9/16	0.93	0.13	24,30,33,36	0
1	FF9	J	171	9/16	0.93	0.16	31,37,43,44	0
1	FF9	E	171	9/16	0.94	0.17	23,26,39,40	0
1	FF9	F	171	9/16	0.94	0.13	24,26,31,32	0
1	FF9	C	171	9/16	0.95	0.14	21,23,31,36	0
1	FF9	G	171	9/16	0.95	0.14	24,25,28,35	0
1	FF9	H	171	9/16	0.96	0.11	24,28,35,37	0
1	FF9	B	171	9/16	0.98	0.13	27,28,34,36	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.