



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:56 PM UTC

PDB ID : 7C0E / pdb_00007c0e
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 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
Mogul : 2022.3.0, CSD as543be (2022)
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

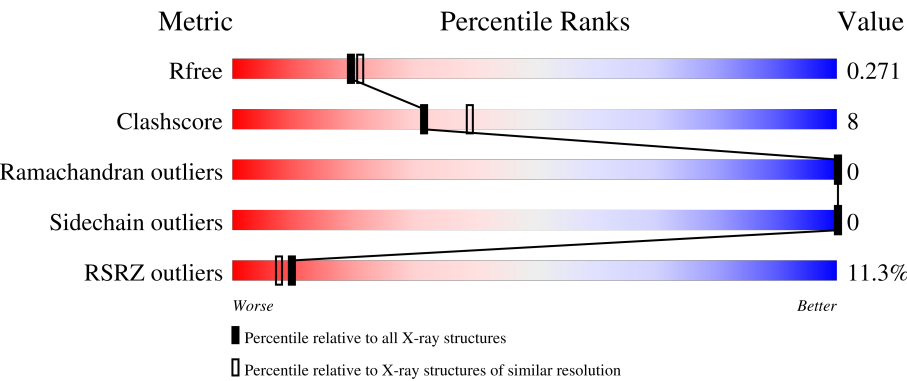
1 Overall quality at a glance i

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	86%9%5%
1	B	320	83%11%6%
1	C	320	85%10%5%
1	D	320	86%8%5%
1	E	320	83%12%5%

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Mol	Chain	Length	Quality of chain
1	F	320	82%12%6%
1	G	320	87%8%5%
1	H	320	%83%12%5%
1	I	320	31%74%21%5%
1	J	320	27%69%26%5%
1	K	320	30%67%28%5%
1	L	320	32%68%26%6%

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.

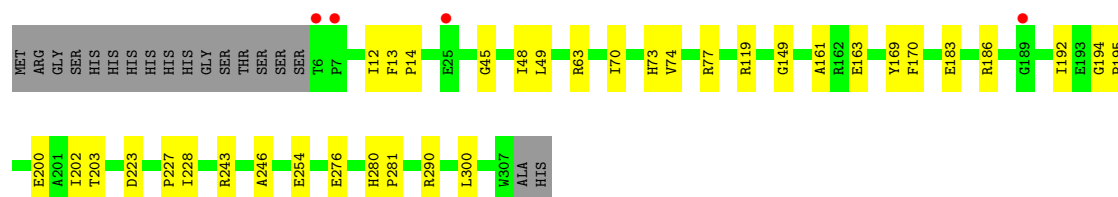
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain A: 



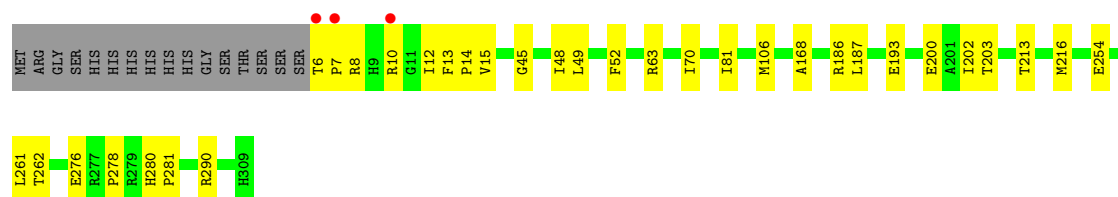
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain B: 



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

Chain C: 



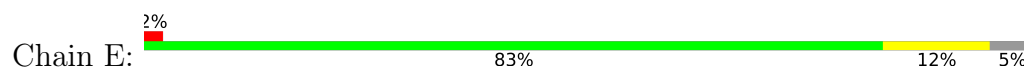
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

Chain D: 

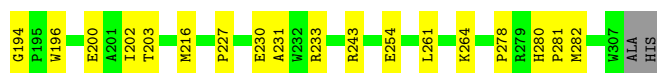
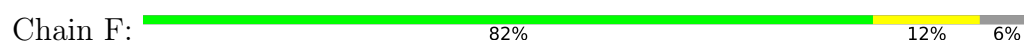




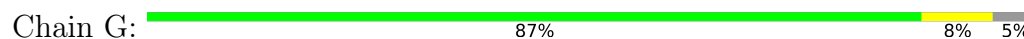
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



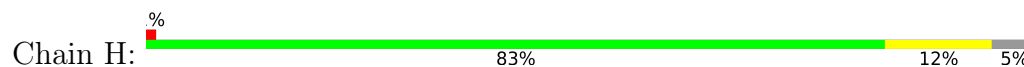
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



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

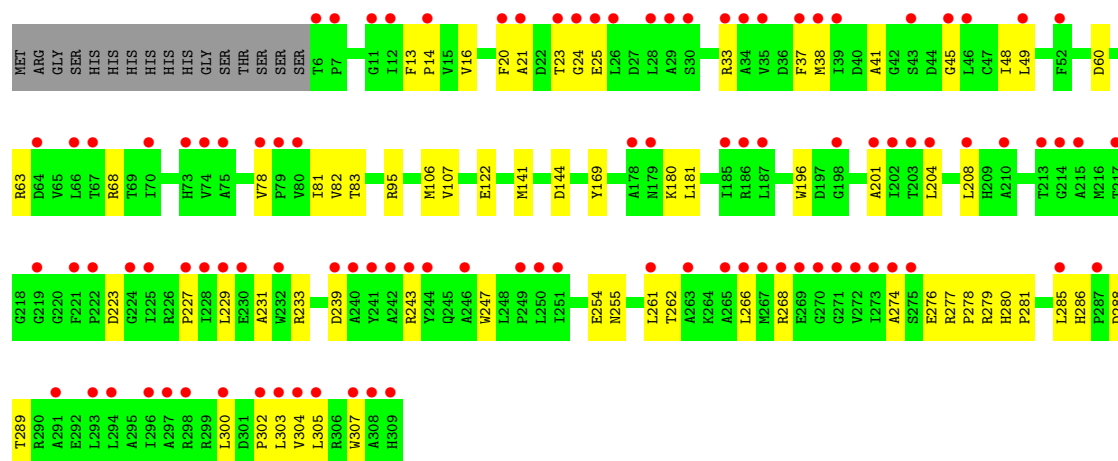


- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

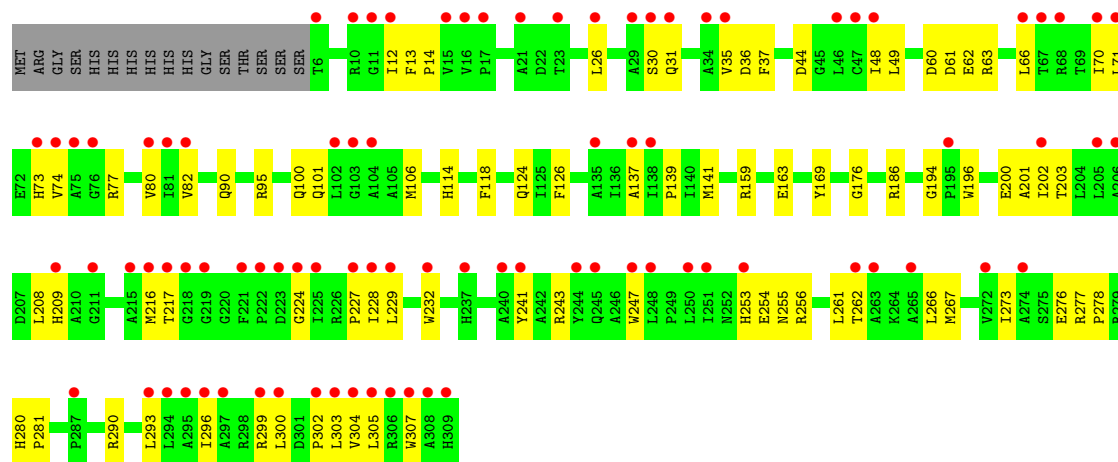


- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase

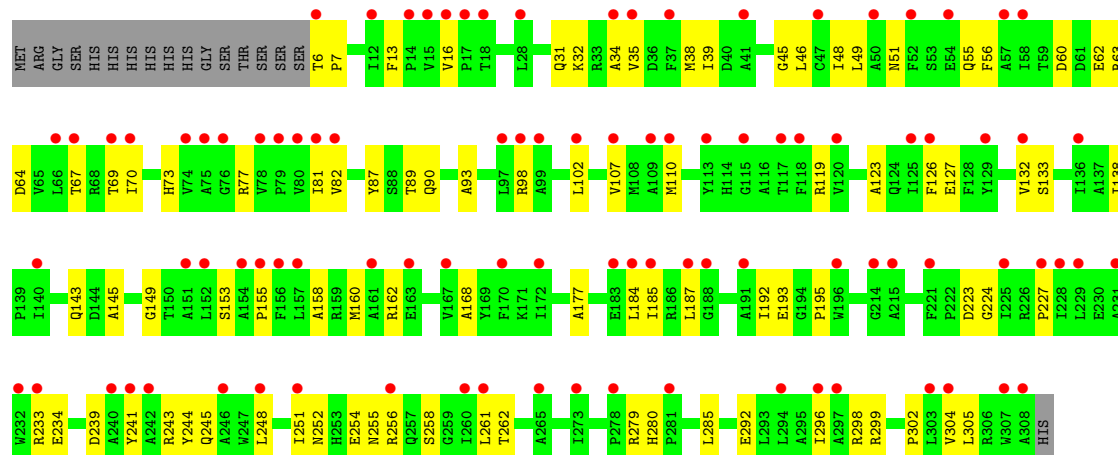




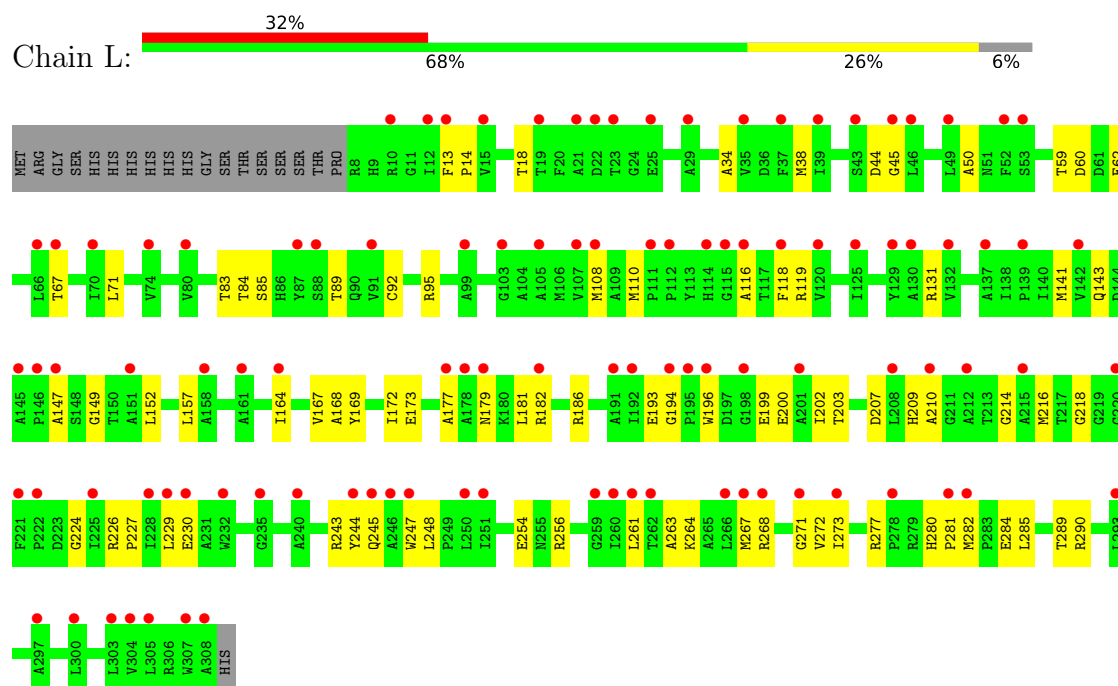
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, 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
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.221 , 0.269 0.227 , 0.271	Depositor DCC
R_{free} test set	8087 reflections (4.96%)	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)	0.36 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.15	0/2386	0.36	0/3244
1	B	0.14	0/2369	0.35	0/3222
1	C	0.14	0/2386	0.34	0/3244
1	D	0.14	0/2368	0.35	0/3222
1	E	0.14	0/2386	0.36	0/3244
1	F	0.14	0/2369	0.36	0/3222
1	G	0.14	0/2368	0.35	0/3222
1	H	0.14	0/2368	0.35	0/3222
1	I	0.17	0/2380	0.39	0/3237
1	J	0.18	0/2380	0.39	0/3237
1	K	0.17	0/2374	0.44	0/3229
1	L	0.18	0/2359	0.38	0/3207
All	All	0.15	0/28493	0.37	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2348	0	2308	21	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	19	0
1	D	2325	0	2290	16	0
1	E	2342	0	2308	27	0
1	F	2326	0	2296	32	0
1	G	2325	0	2290	15	0
1	H	2325	0	2290	25	0
1	I	2336	0	2297	56	0
1	J	2336	0	2297	82	0
1	K	2331	0	2301	96	0
1	L	2317	0	2287	64	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	448	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 (448) 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: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:K:32:LYS:HZ2	1:K:69:THR:HG22	1.46	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: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:L:84:THR:OG1	2:L:401:HOH:O	1.95	0.74
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:F:126:PHE:HA	1:F:160:MET:HE3	1.71	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:I:141:MET:HE3	1:I:169:TYR:HB3	1.75	0.67
1:K:299:ARG:NH2	2:K:423:HOH:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:55:GLN:NE2	2:K:402:HOH:O	2.32	0.62
1:K:162:ARG:NH1	2:K:414:HOH:O	2.18	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:O	1:L:268:ARG:NE	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:F:129:TYR:CD2	1:F:160:MET:HE1	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:49:LEU:HD11	1:K:67:THR:HG22	1.84	0.59
1:K:254:GLU:HB2	1:K:262:THR:HG21	1.83	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:I:16:VAL:HG13	1:I:38:MET:HE1	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD2	1:K:32:LYS:N	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:184:LEU:C	1:K:184:LEU:HD13	2.32	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:L:108:MET:HE3	1:L:143:GLN:HB2	1.91	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:K:32:LYS:HZ1	1:K:73:HIS:HB2	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:141:MET:HE1	1:I:196:TRP:CE3	2.45	0.52
1:J:61:ASP:OD1	2:J:403:HOH:O	2.18	0.52
1:J:100:GLN:HE22	1:J:137:ALA:N	1.94	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: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:L:141:MET:HE2	1:L:169:TYR:HB3	1.93	0.51
1:J:66:LEU:O	1:J:70:ILE:HG22	2.10	0.51
1:K:110:MET:HE1	1:K:145:ALA:HB3	1.93	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: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:J:36:ASP:CG	1:J:73:HIS:HE2	2.19	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:F:129:TYR:HD2	1:F:160:MET:HE1	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:VAL:HG11	1:D:52:PHE:HB3	1.95	0.48
1:G:54:GLU:OE2	1:G:264:LYS:NZ	2.34	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:8:ARG:HG3	1:E:8:ARG:HH11	1.79	0.48
1:E:294:LEU:O	1:E:298:ARG:HG3	2.13	0.48
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:38:MET:HE2	1:K:46:LEU:HD22	1.95	0.47
1:K:261:LEU:HB2	1:K:285:LEU:HD11	1.94	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:HE1	1:D:196:TRP:CE3	2.49	0.47
1:K:304:VAL:HG13	1:K:305:LEU:HG	1.96	0.47
1:I:41:ALA:HA	1:I:303:LEU:HD13	1.94	0.47
1:I:286:HIS:HB3	1:I:289:THR:HG23	1.95	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:A:65:VAL:HG22	1:A:68:ARG:HH12	1.80	0.47
1:C:15:VAL:HG11	1:C:52:PHE:HB3	1.96	0.47
1:J:299:ARG:HB2	1:J:299:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:LEU:HD13	1:E:63:ARG:HG3	1.97	0.47
1:E:169:TYR:CD2	1:E:194:GLY:HA3	2.50	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:90:GLN:HE22	1:F:24:GLY:HA3	1.80	0.47
1:E:280:HIS:CG	1:E:281:PRO:HA	2.49	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
1:A:49:LEU:HD13	1:A:63:ARG:HG3	1.97	0.46
1:K:62:GLU:CD	1:K:279:ARG:HH22	2.23	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:G:49:LEU:HD13	1:G:63:ARG:HG3	1.98	0.46
1:G:141:MET:HE1	1:G:196:TRP:CE3	2.50	0.46
1:H:183:GLU:OE1	1:H:186:ARG:NH2	2.49	0.46
1:K:48:ILE:HA	2:K:411:HOH:O	2.14	0.46
1:K:155:PRO:HA	1:K:187:LEU:HD23	1.97	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:E:136:ILE:HD12	1:E:136:ILE:C	2.41	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: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:C:186:ARG:O	1:J:186:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:36:ASP:OD2	2:D:401:HOH:O	2.21	0.45
1:J:101:GLN:HA	1:J:101:GLN:OE1	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:OD1	1:B:223:ASP:N	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
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: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: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: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:18:THR:O	1:L:264:LYS:NZ	2.44	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:L:141:MET:HE1	1:L:196:TRP:CE3	2.52	0.44
1:C:276:GLU:OE2	1:C:290:ARG:NH2	2.43	0.44
1:F:141:MET:HE2	1:F:169:TYR:HB3	2.00	0.44
1:B:119:ARG:HH21	1:B:149:GLY:HA3	1.83	0.44
1:I:233:ARG:HB3	1:I:233:ARG:HH21	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:C:81:ILE:HG12	1:C:106:MET:HB3	2.00	0.44
1:I:24:GLY:HA3	1:J:90:GLN:OE1	2.17	0.44
1:I:201:ALA:HB1	1:I:204:LEU:HB2	1.99	0.44
1:I:223:ASP:OD1	1:I:223:ASP:N	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ILE:HG23	1:C:203:THR:HG23	1.99	0.43
1:D:110:MET:HE1	1:D:145:ALA:HB3	2.00	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:H:141:MET:HE2	1:H:169:TYR:HB3	2.00	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: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
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:K:119:ARG:HE	1:K:149:GLY:C	2.26	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:O	1:J:303:LEU:HD23	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:F:141:MET:HE1	1:F:196:TRP:CE3	2.54	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:F:54:GLU:OE2	1:F:264:LYS:NZ	2.46	0.42
1:H:6:THR:N	1:H:7:PRO:CD	2.82	0.42
1:L:110:MET:HE1	1:L:147:ALA:HB3	2.00	0.42
1:L:267:MET:HB3	1:L:272:VAL:HB	2.01	0.42
1:H:71:LEU:HD13	1:H:71:LEU:HA	1.93	0.42
1:F:126:PHE:HA	1:F:160:MET:CE	2.46	0.42
1:J:37:PHE:CZ	1:J:304:VAL:HB	2.54	0.42
1:J:262:THR:HG23	1:J:293:LEU:CD1	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:SER:HB2	1:E:155:PRO:HD2	2.01	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:49:LEU:CD1	1:K:67:THR:HG22	2.50	0.42
1:K:107:VAL:HG13	1:K:138:ILE:HD11	2.02	0.42
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:L:216:MET:HE3	1:L:216:MET:HB2	1.85	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:B:183:GLU:CD	1:B:186:ARG:HH21	2.27	0.41
1:I:247:TRP:CE2	1:I:300:LEU:HD22	2.55	0.41
1:K:81:ILE:HG22	2:K:418:HOH:O	2.20	0.41
1:K:107:VAL:HA	2:K:418:HOH:O	2.19	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:C:216:MET:HE3	1:C:216:MET:HB2	1.84	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:A:141:MET:HE1	1:A:196:TRP:CE3	2.56	0.41
1:B:228:ILE:HG13	1:B:243:ARG:HG2	2.02	0.41
1:H:106:MET:SD	1:H:141:MET:HE3	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:74:VAL:HA	1:B:77:ARG:HH21	1.86	0.41
1:B:169:TYR:CD2	1:B:194:GLY:HA3	2.56	0.41
1:J:141:MET:HE1	1:J:196:TRP:CZ3	2.56	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:I:303:LEU:HD21	1:I:307:TRP:HD1	1.85	0.41
1:L:14:PRO:HB3	1:L:218:GLY:O	2.21	0.41
1:L:118:PHE:O	1:L:119:ARG:HD3	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
1:K:32:LYS:HZ3	1:K:73:HIS:HB2	1.85	0.40
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:F:14:PRO:HB2	1:F:38:MET:HE3	2.03	0.40
1:J:37:PHE:CD2	1:J:267:MET:HE2	2.56	0.40
1:H:36:ASP:CG	1:H:73:HIS:HE2	2.30	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 ⓘ

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	192/250 (77%)	192 (100%)	0	100	100
1	B	235/250 (94%)	235 (100%)	0	100	100
1	C	236/250 (94%)	236 (100%)	0	100	100
1	D	234/250 (94%)	234 (100%)	0	100	100
1	E	236/250 (94%)	236 (100%)	0	100	100
1	F	235/250 (94%)	235 (100%)	0	100	100
1	G	234/250 (94%)	234 (100%)	0	100	100
1	H	234/250 (94%)	234 (100%)	0	100	100
1	I	235/250 (94%)	235 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	235/250 (94%)	235 (100%)	0	100	100
1	K	235/250 (94%)	235 (100%)	0	100	100
1	L	233/250 (93%)	233 (100%)	0	100	100
All	All	2774/3000 (92%)	2774 (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 (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	252	ASN
1	B	124	GLN
1	B	245	GLN
1	C	143	GLN
1	D	143	GLN
1	D	252	ASN
1	E	124	GLN
1	E	252	ASN
1	E	309	HIS
1	F	124	GLN
1	F	166	GLN
1	F	252	ASN
1	G	55	GLN
1	G	124	GLN
1	G	209	HIS
1	G	252	ASN
1	H	124	GLN
1	H	252	ASN
1	I	286	HIS
1	J	100	GLN
1	J	252	ASN
1	J	253	HIS
1	L	166	GLN

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	E	171	1	7,8,15	0.53	0	3,8,18	0.40	0
1	FF9	D	171	1	7,8,15	0.47	0	3,8,18	0.47	0
1	FF9	F	171	1	7,8,15	0.50	0	3,8,18	0.23	0
1	FF9	G	171	1	7,8,15	0.51	0	3,8,18	0.24	0
1	FF9	H	171	1	7,8,15	0.52	0	3,8,18	0.66	0
1	FF9	C	171	1	7,8,15	0.52	0	3,8,18	0.58	0
1	FF9	K	171	1	7,8,15	0.54	0	3,8,18	0.42	0
1	FF9	J	171	1	7,8,15	0.50	0	3,8,18	0.36	0
1	FF9	I	171	1	7,8,15	0.51	0	3,8,18	0.53	0
1	FF9	A	171	1	12,14,15	0.84	1 (8%)	6,16,18	1.59	1 (16%)
1	FF9	B	171	1	7,8,15	0.51	0	3,8,18	0.37	0
1	FF9	L	171	1	7,8,15	0.53	0	3,8,18	0.48	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	E	171	1	-	0/6/7/18	-
1	FF9	D	171	1	-	1/6/7/18	-
1	FF9	F	171	1	-	2/6/7/18	-
1	FF9	G	171	1	-	0/6/7/18	-
1	FF9	H	171	1	-	1/6/7/18	-
1	FF9	C	171	1	-	0/6/7/18	-
1	FF9	K	171	1	-	2/6/7/18	-
1	FF9	J	171	1	-	3/6/7/18	-
1	FF9	I	171	1	-	1/6/7/18	-
1	FF9	A	171	1	-	5/14/16/18	-
1	FF9	B	171	1	-	2/6/7/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FF9	L	171	1	-	1/6/7/18	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	FF9	O1-CX2	-2.05	1.25	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	FF9	CD-CE-NZ	-3.15	105.09	110.67

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	171	FF9	O-C-CA-CB
1	A	171	FF9	C1-CX1-CX2-O1
1	A	171	FF9	C1-CX1-CX2-O2
1	A	171	FF9	NZ-CX1-CX2-O1
1	A	171	FF9	NZ-CX1-CX2-O2
1	B	171	FF9	O-C-CA-CB
1	D	171	FF9	O-C-CA-CB
1	F	171	FF9	O-C-CA-CB
1	H	171	FF9	O-C-CA-CB
1	I	171	FF9	O-C-CA-CB
1	J	171	FF9	O-C-CA-CB
1	L	171	FF9	O-C-CA-CB
1	B	171	FF9	CE-CD-CG-CB
1	J	171	FF9	CE-CD-CG-CB
1	K	171	FF9	CA-CB-CG-CD
1	K	171	FF9	C-CA-CB-CG
1	F	171	FF9	CE-CD-CG-CB
1	J	171	FF9	CA-CB-CG-CD

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 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	303/320 (94%)	0.04	4 (1%) 75 73	19, 28, 42, 65	0
1	B	301/320 (94%)	0.27	4 (1%) 75 73	23, 32, 45, 67	0
1	C	303/320 (94%)	-0.04	3 (0%) 79 77	21, 27, 38, 62	0
1	D	302/320 (94%)	0.12	4 (1%) 75 73	22, 30, 43, 77	0
1	E	303/320 (94%)	0.06	5 (1%) 69 66	21, 30, 42, 82	0
1	F	301/320 (94%)	0.08	1 (0%) 90 88	20, 30, 40, 57	0
1	G	302/320 (94%)	-0.00	1 (0%) 90 88	23, 28, 40, 71	0
1	H	302/320 (94%)	0.11	2 (0%) 84 82	22, 30, 42, 57	0
1	I	303/320 (94%)	1.47	100 (33%) 1 0	23, 47, 59, 74	0
1	J	303/320 (94%)	1.35	87 (28%) 1 1	20, 44, 58, 73	0
1	K	302/320 (94%)	1.75	96 (31%) 1 1	35, 43, 53, 75	0
1	L	300/320 (93%)	1.73	104 (34%) 1 0	34, 46, 55, 70	0
All	All	3625/3840 (94%)	0.58	411 (11%) 10 8	19, 32, 52, 82	0

All (411) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	240	ALA	6.1
1	A	308	ALA	5.5
1	E	6	THR	5.2
1	I	21	ALA	4.8
1	I	228	ILE	4.6
1	K	140	ILE	4.5
1	L	118	PHE	4.3
1	J	35	VAL	4.2
1	J	308	ALA	4.2
1	I	78	VAL	4.2
1	L	297	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	J	304	VAL	4.1
1	J	305	LEU	4.1
1	L	210	ALA	4.0
1	I	221	PHE	4.0
1	I	74	VAL	4.0
1	I	203	THR	4.0
1	I	24	GLY	4.0
1	I	43	SER	4.0
1	J	222	PRO	3.9
1	D	6	THR	3.9
1	I	80	VAL	3.9
1	J	102	LEU	3.9
1	J	297	ALA	3.9
1	K	18	THR	3.8
1	J	71	LEU	3.8
1	I	23	THR	3.8
1	I	270	GLY	3.7
1	J	272	VAL	3.7
1	J	75	ALA	3.7
1	I	305	LEU	3.7
1	J	229	LEU	3.7
1	K	261	LEU	3.7
1	J	241	TYR	3.7
1	K	256	ARG	3.7
1	A	309	HIS	3.7
1	I	250	LEU	3.6
1	K	57	ALA	3.6
1	L	244	TYR	3.6
1	I	274	ALA	3.6
1	K	41	ALA	3.6
1	J	294	LEU	3.5
1	K	191	ALA	3.5
1	L	130	ALA	3.5
1	J	300	LEU	3.5
1	B	7	PRO	3.5
1	K	132	VAL	3.5
1	J	303	LEU	3.4
1	K	167	VAL	3.4
1	L	229	LEU	3.4
1	K	16	VAL	3.4
1	K	172	ILE	3.3
1	K	229	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	L	177	ALA	3.3
1	J	81	ILE	3.3
1	K	281	PRO	3.3
1	B	6	THR	3.3
1	C	6	THR	3.3
1	L	52	PHE	3.3
1	J	206	ALA	3.3
1	L	303	LEU	3.3
1	J	307	TRP	3.3
1	I	225	ILE	3.3
1	J	70	ILE	3.3
1	J	232	TRP	3.3
1	L	266	LEU	3.2
1	K	126	PHE	3.2
1	L	208	LEU	3.2
1	L	251	ILE	3.2
1	K	6	THR	3.2
1	K	12	ILE	3.2
1	K	265	ALA	3.2
1	A	22	ASP	3.2
1	I	213	THR	3.2
1	I	52	PHE	3.1
1	L	220	GLY	3.1
1	K	156	PHE	3.1
1	L	43	SER	3.1
1	J	274	ALA	3.1
1	I	46	LEU	3.1
1	I	208	LEU	3.1
1	K	294	LEU	3.1
1	L	305	LEU	3.1
1	K	228	ILE	3.1
1	H	52	PHE	3.1
1	L	80	VAL	3.1
1	L	304	VAL	3.1
1	E	7	PRO	3.0
1	I	14	PRO	3.0
1	I	294	LEU	3.0
1	L	192	ILE	3.0
1	J	218	GLY	3.0
1	I	242	ALA	3.0
1	I	246	ALA	3.0
1	J	74	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	138	ILE	3.0
1	I	186	ARG	3.0
1	K	76	GLY	3.0
1	I	308	ALA	3.0
1	I	293	LEU	3.0
1	H	6	THR	3.0
1	I	20	PHE	2.9
1	L	293	LEU	2.9
1	K	120	VAL	2.9
1	K	113	TYR	2.9
1	L	87	TYR	2.9
1	I	38	MET	2.9
1	K	99	ALA	2.9
1	I	39	ILE	2.9
1	G	6	THR	2.9
1	I	30	SER	2.9
1	L	115	GLY	2.9
1	I	7	PRO	2.9
1	K	97	LEU	2.9
1	I	304	VAL	2.9
1	K	78	VAL	2.9
1	K	109	ALA	2.9
1	K	184	LEU	2.9
1	I	25	GLU	2.9
1	I	12	ILE	2.9
1	I	271	GLY	2.8
1	J	211	GLY	2.8
1	J	263	ALA	2.8
1	I	45	GLY	2.8
1	I	198	GLY	2.8
1	J	17	PRO	2.8
1	K	241	TYR	2.8
1	K	152	LEU	2.8
1	J	295	ALA	2.8
1	K	52	PHE	2.8
1	K	215	ALA	2.8
1	L	116	ALA	2.8
1	L	142	VAL	2.8
1	I	307	TRP	2.8
1	L	182	ARG	2.8
1	E	309	HIS	2.8
1	J	244	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	28	LEU	2.8
1	J	46	LEU	2.8
1	J	265	ALA	2.8
1	L	158	ALA	2.8
1	K	118	PHE	2.8
1	L	35	VAL	2.8
1	K	117	THR	2.8
1	L	23	THR	2.8
1	K	196	TRP	2.8
1	I	214	GLY	2.8
1	J	11	GLY	2.8
1	K	115	GLY	2.8
1	D	7	PRO	2.8
1	K	157	LEU	2.8
1	K	187	LEU	2.8
1	I	34	ALA	2.8
1	L	246	ALA	2.8
1	L	308	ALA	2.8
1	J	221	PHE	2.8
1	J	67	THR	2.7
1	J	31	GLN	2.7
1	B	189	GLY	2.7
1	K	14	PRO	2.7
1	I	37	PHE	2.7
1	I	11	GLY	2.7
1	I	219	GLY	2.7
1	K	54	GLU	2.7
1	I	261	LEU	2.7
1	J	26	LEU	2.7
1	J	215	ALA	2.7
1	J	80	VAL	2.7
1	I	6	THR	2.7
1	L	19	THR	2.7
1	J	302	PRO	2.7
1	K	79	PRO	2.7
1	K	35	VAL	2.7
1	K	304	VAL	2.7
1	I	273	ILE	2.7
1	I	187	LEU	2.7
1	J	104	ALA	2.6
1	J	135	ALA	2.6
1	L	99	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	35	VAL	2.6
1	L	262	THR	2.6
1	L	45	GLY	2.6
1	L	228	ILE	2.6
1	K	248	LEU	2.6
1	K	50	ALA	2.6
1	J	6	THR	2.6
1	L	194	GLY	2.6
1	K	185	ILE	2.6
1	J	309	HIS	2.6
1	L	25	GLU	2.6
1	L	151	ALA	2.6
1	L	307	TRP	2.6
1	L	107	VAL	2.6
1	L	282	MET	2.6
1	J	228	ILE	2.6
1	L	70	ILE	2.6
1	L	164	ILE	2.6
1	J	237	HIS	2.6
1	J	205	LEU	2.6
1	E	8	ARG	2.6
1	L	212	ALA	2.6
1	K	232	TRP	2.6
1	K	307	TRP	2.6
1	F	6	THR	2.6
1	I	249	PRO	2.6
1	J	287	PRO	2.6
1	K	17	PRO	2.6
1	L	15	VAL	2.6
1	J	251	ILE	2.6
1	J	253	HIS	2.6
1	K	303	LEU	2.5
1	L	261	LEU	2.5
1	I	215	ALA	2.5
1	K	308	ALA	2.5
1	L	247	TRP	2.5
1	I	227	PRO	2.5
1	L	67	THR	2.5
1	I	272	VAL	2.5
1	K	74	VAL	2.5
1	K	225	ILE	2.5
1	J	223	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	154	ALA	2.5
1	K	240	ALA	2.5
1	L	22	ASP	2.5
1	L	137	ALA	2.5
1	L	198	GLY	2.5
1	J	16	VAL	2.5
1	J	30	SER	2.5
1	I	202	ILE	2.5
1	I	75	ALA	2.5
1	K	75	ALA	2.5
1	K	161	ALA	2.5
1	I	287	PRO	2.5
1	I	302	PRO	2.5
1	K	47	CYS	2.5
1	I	269	GLU	2.5
1	K	183	GLU	2.5
1	K	221	PHE	2.5
1	L	53	SER	2.5
1	I	251	ILE	2.5
1	I	79	PRO	2.5
1	L	103	GLY	2.5
1	A	6	THR	2.4
1	I	185	ILE	2.4
1	K	70	ILE	2.4
1	K	80	VAL	2.4
1	L	125	ILE	2.4
1	I	232	TRP	2.4
1	I	300	LEU	2.4
1	C	7	PRO	2.4
1	D	308	ALA	2.4
1	J	21	ALA	2.4
1	K	34	ALA	2.4
1	L	215	ALA	2.4
1	I	224	GLY	2.4
1	I	296	ILE	2.4
1	J	296	ILE	2.4
1	L	13	PHE	2.4
1	L	74	VAL	2.4
1	L	91	VAL	2.4
1	I	297	ALA	2.4
1	L	139	PRO	2.4
1	J	76	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	161	ALA	2.4
1	K	15	VAL	2.4
1	K	296	ILE	2.4
1	L	132	VAL	2.4
1	I	204	LEU	2.4
1	J	248	LEU	2.4
1	L	250	LEU	2.4
1	L	300	LEU	2.4
1	L	196	TRP	2.4
1	I	243	ARG	2.4
1	I	222	PRO	2.4
1	J	240	ALA	2.4
1	K	188	GLY	2.4
1	L	29	ALA	2.4
1	K	67	THR	2.4
1	K	69	THR	2.4
1	K	107	VAL	2.4
1	I	266	LEU	2.4
1	K	28	LEU	2.4
1	K	98	ARG	2.4
1	L	129	TYR	2.3
1	K	227	PRO	2.3
1	L	111	PRO	2.3
1	L	278	PRO	2.3
1	I	265	ALA	2.3
1	K	231	ALA	2.3
1	K	246	ALA	2.3
1	L	191	ALA	2.3
1	L	267	MET	2.3
1	I	70	ILE	2.3
1	K	82	VAL	2.3
1	L	120	VAL	2.3
1	I	26	LEU	2.3
1	I	303	LEU	2.3
1	J	293	LEU	2.3
1	I	239	ASP	2.3
1	I	244	TYR	2.3
1	J	247	TRP	2.3
1	L	195	PRO	2.3
1	J	219	GLY	2.3
1	L	259	GLY	2.3
1	J	225	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	81	ILE	2.3
1	L	114	HIS	2.3
1	J	47	CYS	2.3
1	L	66	LEU	2.3
1	J	227	PRO	2.3
1	L	232	TRP	2.3
1	I	263	ALA	2.3
1	L	10	ARG	2.3
1	I	309	HIS	2.3
1	J	209	HIS	2.3
1	K	125	ILE	2.3
1	K	251	ILE	2.3
1	K	66	LEU	2.3
1	L	222	PRO	2.3
1	J	224	GLY	2.3
1	L	145	ALA	2.3
1	L	201	ALA	2.3
1	I	67	THR	2.3
1	I	229	LEU	2.2
1	K	102	LEU	2.2
1	J	68	ARG	2.2
1	L	268	ARG	2.2
1	K	297	ALA	2.2
1	J	23	THR	2.2
1	L	88	SER	2.2
1	L	12	ILE	2.2
1	L	46	LEU	2.2
1	J	299	ARG	2.2
1	K	278	PRO	2.2
1	L	281	PRO	2.2
1	E	308	ALA	2.2
1	L	21	ALA	2.2
1	L	147	ALA	2.2
1	J	202	ILE	2.2
1	L	260	ILE	2.2
1	I	285	LEU	2.2
1	J	66	LEU	2.2
1	K	214	GLY	2.2
1	L	235	GLY	2.2
1	J	262	THR	2.2
1	K	242	ALA	2.2
1	L	39	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	179	ASN	2.2
1	J	216	MET	2.2
1	K	155	PRO	2.2
1	L	245	GLN	2.2
1	J	137	ALA	2.2
1	J	217	THR	2.2
1	K	151	ALA	2.2
1	J	250	LEU	2.1
1	K	136	ILE	2.1
1	K	260	ILE	2.1
1	L	225	ILE	2.1
1	I	267	MET	2.1
1	K	37	PHE	2.1
1	K	170	PHE	2.1
1	L	146	PRO	2.1
1	J	245	GLN	2.1
1	I	178	ALA	2.1
1	I	201	ALA	2.1
1	I	275	SER	2.1
1	I	33	ARG	2.1
1	I	268	ARG	2.1
1	L	49	LEU	2.1
1	L	179	ASN	2.1
1	J	73	HIS	2.1
1	L	221	PHE	2.1
1	J	103	GLY	2.1
1	K	233	ARG	2.1
1	J	29	ALA	2.1
1	B	25	GLU	2.1
1	D	22	ASP	2.1
1	K	129	TYR	2.1
1	L	112	PRO	2.1
1	I	291	ALA	2.1
1	K	163	GLU	2.1
1	I	49	LEU	2.1
1	I	64	ASP	2.1
1	J	12	ILE	2.1
1	L	273	ILE	2.1
1	J	15	VAL	2.1
1	L	271	GLY	2.1
1	J	10	ARG	2.1
1	I	29	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	230	GLU	2.0
1	J	34	ALA	2.0
1	K	110	MET	2.0
1	L	105	ALA	2.0
1	L	178	ALA	2.0
1	L	240	ALA	2.0
1	I	73	HIS	2.0
1	I	66	LEU	2.0
1	I	241	TYR	2.0
1	C	10	ARG	2.0
1	I	298	ARG	2.0
1	J	82	VAL	2.0
1	L	37	PHE	2.0
1	L	108	MET	2.0
1	I	217	THR	2.0
1	L	230	GLU	2.0
1	I	210	ALA	2.0
1	J	48	ILE	2.0
1	J	195	PRO	2.0
1	J	306	ARG	2.0
1	K	58	ILE	2.0
1	K	273	ILE	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, 95th 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	0.72	0.18	36,46,49,51	0
1	FF9	L	171	9/16	0.74	0.17	36,48,50,50	0
1	FF9	A	171	15/16	0.77	0.15	21,26,33,34	6
1	FF9	I	171	9/16	0.84	0.14	38,42,49,52	0
1	FF9	J	171	9/16	0.89	0.11	31,37,43,44	0
1	FF9	D	171	9/16	0.91	0.08	24,30,33,36	0
1	FF9	E	171	9/16	0.91	0.12	23,26,39,40	0
1	FF9	G	171	9/16	0.92	0.09	24,25,28,35	0
1	FF9	F	171	9/16	0.93	0.08	24,26,31,32	0
1	FF9	H	171	9/16	0.93	0.09	24,28,35,37	0
1	FF9	C	171	9/16	0.94	0.08	21,23,31,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	FF9	B	171	9/16	0.95	0.09	27,28,34,36	0

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.