



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:49 PM UTC

PDB ID : 7C0D / pdb_00007c0d
Title : Crystal structure of Azospirillum brasilense L-2-keto-3-deoxyarabonate dehydratase (Hydroxypyruvate-bound form)
Authors : Watanabe, Y.; Watanabe, S.
Deposited on : 2020-05-01
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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

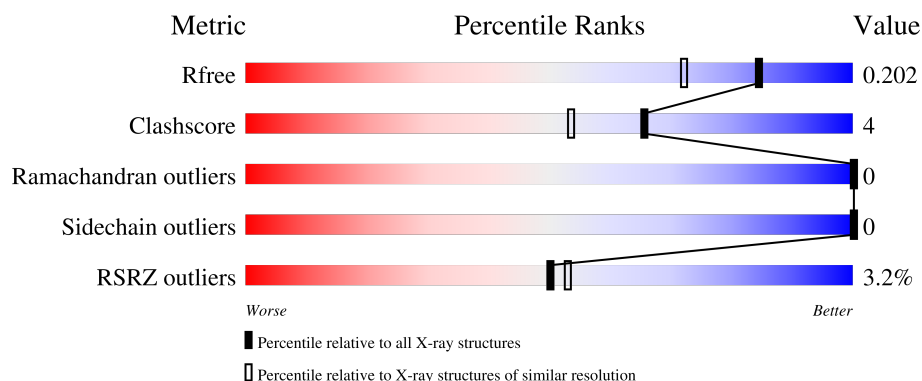
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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

Mol	Chain	Length	Quality of chain
1	A	320	 2% 88% 7% 5%
1	B	320	 2% 87% 8% 5%
1	C	320	 % 88% 7% 5%
1	D	320	 % 91% • 5%
1	E	320	 2% 88% 7% 5%

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Mol	Chain	Length	Quality of chain
1	F	320	2% 91% 5%
1	G	320	% 90% 5%
1	H	320	2% 88% 8% 5%
1	I	320	11% 85% 9% 6%
1	J	320	% 86% 9% 6%
1	K	320	% 87% 8% 6%
1	L	320	12% 83% 12% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 144 discrepancies between the modelled and reference sequences:

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

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

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

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

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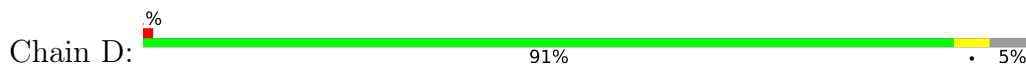
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Chain	Residue	Modelled	Actual	Comment	Reference
K	1	SER	-	expression tag	UNP Q1JUQ0
L	-10	MET	-	expression tag	UNP Q1JUQ0
L	-9	ARG	-	expression tag	UNP Q1JUQ0
L	-8	GLY	-	expression tag	UNP Q1JUQ0
L	-7	SER	-	expression tag	UNP Q1JUQ0
L	-6	HIS	-	expression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

- Molecule 2 is water.

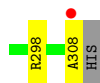
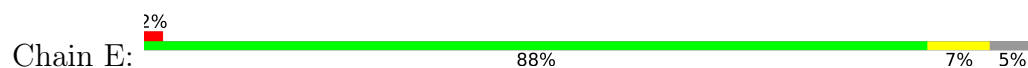
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	444	Total O 444 444	0	0
2	B	391	Total O 391 391	0	0
2	C	405	Total O 405 405	0	0
2	D	418	Total O 418 418	0	0
2	E	331	Total O 331 331	0	0
2	F	334	Total O 334 334	0	0
2	G	389	Total O 389 389	0	0
2	H	289	Total O 289 289	0	0
2	I	233	Total O 233 233	0	0
2	J	350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

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

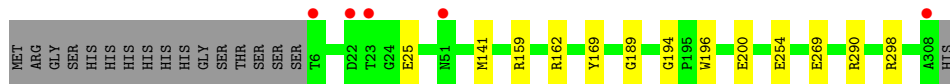
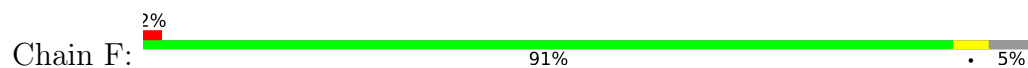




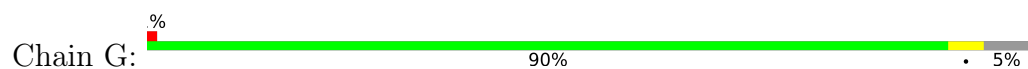
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



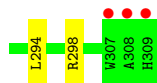
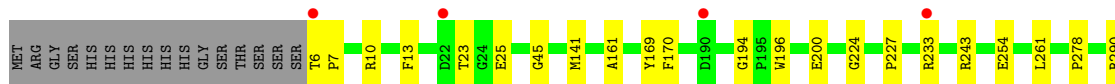
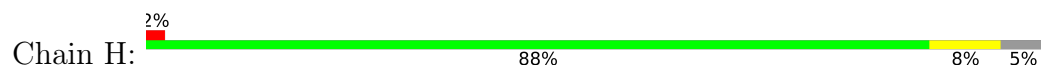
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



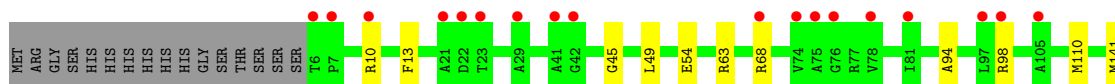
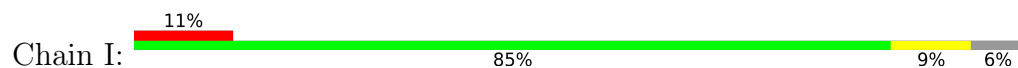
- Molecule 1: L-2-keto-3-deoxyarabonate dehydratase



- 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	76.38Å 88.47Å 143.70Å 84.83° 86.00° 73.21°	Depositor
Resolution (Å)	48.81 – 1.60 48.81 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.1 (48.81-1.60) 95.1 (48.81-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.170 , 0.199 0.176 , 0.202	Depositor DCC
R_{free} test set	23151 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32122	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	1/2386 (0.0%)	0.55	0/3244
1	B	0.32	0/2386	0.56	0/3244
1	C	0.29	0/2374	0.52	0/3229
1	D	0.30	0/2374	0.53	0/3229
1	E	0.26	0/2374	0.48	0/3229
1	F	0.26	0/2374	0.49	0/3229
1	G	0.27	0/2374	0.52	0/3229
1	H	0.25	0/2386	0.46	0/3244
1	I	0.24	0/2369	0.46	0/3222
1	J	0.30	0/2367	0.52	0/3218
1	K	0.23	0/2367	0.47	0/3218
1	L	0.24	0/2369	0.45	0/3222
All	All	0.28	1/28500 (0.0%)	0.50	0/38757

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	ARG	CD-NE	5.68	1.54	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2342	0	2317	30	0
1	B	2348	0	2320	19	0
1	C	2337	0	2313	14	0
1	D	2331	0	2310	8	0
1	E	2331	0	2310	18	0
1	F	2331	0	2310	9	0
1	G	2331	0	2310	9	0
1	H	2342	0	2317	19	0
1	I	2326	0	2305	25	0
1	J	2324	0	2304	20	0
1	K	2324	0	2304	17	0
1	L	2326	0	2305	28	0
2	A	444	0	0	11	0
2	B	391	0	0	6	2
2	C	405	0	0	5	0
2	D	418	0	0	2	1
2	E	331	0	0	8	0
2	F	334	0	0	5	0
2	G	389	0	0	3	0
2	H	289	0	0	2	0
2	I	233	0	0	8	0
2	J	350	0	0	6	1
2	K	310	0	0	4	0
2	L	235	0	0	6	0
All	All	32122	0	27725	213	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (213) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:10:ARG:HD3	1:I:233:ARG:HH11	1.42	0.82
1:E:277:ARG:NH2	2:E:402:HOH:O	2.12	0.81
1:B:173:GLU:OE2	1:B:199:GLU:N	2.13	0.81
1:L:230:GLU:OE2	1:L:233:ARG:NH1	2.15	0.79
1:B:290:ARG:NH2	2:B:403:HOH:O	2.17	0.77
1:A:268:ARG:NH2	1:A:276:GLU:H	1.83	0.76
1:B:10:ARG:NH1	2:B:401:HOH:O	2.02	0.75
1:B:230:GLU:OE2	1:B:233:ARG:NH1	2.19	0.74
1:A:268:ARG:HH21	1:A:276:GLU:N	1.85	0.74
1:H:10:ARG:CZ	1:H:233:ARG:NE	2.51	0.73
1:G:268:ARG:NH1	2:G:401:HOH:O	2.22	0.72
1:A:233:ARG:NH1	2:A:405:HOH:O	2.23	0.71
1:E:233:ARG:NH2	2:E:404:HOH:O	2.23	0.69
1:I:49:LEU:HD13	1:I:63:ARG:HG3	1.74	0.69
1:C:90:GLN:OE1	2:C:403:HOH:O	2.12	0.68
1:A:268:ARG:CZ	1:A:276:GLU:HG2	2.24	0.68
1:J:68:ARG:NH2	2:J:401:HOH:O	2.25	0.68
1:I:268:ARG:NH1	2:I:404:HOH:O	2.26	0.67
1:A:309:HIS:OXT	2:A:403:HOH:O	2.12	0.67
1:I:68:ARG:NH1	2:I:405:HOH:O	2.27	0.67
1:H:10:ARG:NH2	1:H:233:ARG:NE	2.44	0.66
1:K:10:ARG:NH2	2:K:401:HOH:O	2.08	0.66
1:A:122:GLU:OE2	2:A:404:HOH:O	2.13	0.66
1:E:261:LEU:HD21	1:E:278:PRO:HB3	1.77	0.65
1:A:268:ARG:NE	1:A:276:GLU:HG2	2.11	0.65
1:L:10:ARG:HE	1:L:233:ARG:HH22	1.45	0.64
1:D:56:PHE:HZ	1:D:282:MET:HE1	1.62	0.64
1:F:189:GLY:O	2:F:402:HOH:O	2.15	0.64
1:L:63:ARG:NH2	2:L:409:HOH:O	2.30	0.64
1:A:10:ARG:NH1	2:A:407:HOH:O	2.30	0.64
1:L:163:GLU:OE2	2:L:402:HOH:O	2.15	0.63
1:B:171:KYQ:HEA	1:B:173:GLU:CD	2.24	0.63
1:G:22:ASP:O	1:G:277:ARG:NH2	2.32	0.63
1:K:23:THR:OG1	1:K:25:GLU:HG2	1.98	0.62
1:K:227:PRO:HB2	1:K:243:ARG:HD3	1.81	0.62
1:I:277:ARG:NH2	2:I:408:HOH:O	2.32	0.62
1:I:54:GLU:HG2	1:I:282:MET:HE1	1.83	0.60
1:E:49:LEU:HD13	1:E:63:ARG:HG3	1.83	0.60
1:L:77:ARG:NH1	2:L:408:HOH:O	2.29	0.60
1:D:230:GLU:OE2	1:D:233:ARG:NH1	2.32	0.59
1:J:290:ARG:NH2	2:J:405:HOH:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HD3	2:A:474:HOH:O	2.02	0.59
1:E:308:ALA:O	2:E:403:HOH:O	2.16	0.59
1:H:10:ARG:NH2	1:H:233:ARG:HE	2.00	0.59
1:C:261:LEU:HD21	1:C:278:PRO:HB3	1.85	0.58
1:I:94:ALA:O	2:I:402:HOH:O	2.17	0.58
1:H:10:ARG:CZ	1:H:233:ARG:CD	2.81	0.58
1:B:10:ARG:NH2	2:B:404:HOH:O	2.31	0.58
1:H:298:ARG:NH1	2:H:403:HOH:O	2.24	0.57
1:A:49:LEU:HD13	1:A:63:ARG:HG3	1.86	0.57
1:A:22:ASP:CG	2:A:402:HOH:O	2.46	0.57
1:A:268:ARG:HE	1:A:276:GLU:H	1.52	0.57
1:I:224:GLY:HA2	1:I:243:ARG:HH11	1.70	0.57
1:J:63:ARG:HD2	2:J:411:HOH:O	2.05	0.57
1:L:10:ARG:NE	1:L:233:ARG:NH2	2.50	0.57
1:A:290:ARG:HD3	2:A:681:HOH:O	2.05	0.56
1:F:162:ARG:NH2	2:F:403:HOH:O	2.33	0.56
1:A:268:ARG:NE	1:A:276:GLU:H	2.05	0.55
1:D:56:PHE:CZ	1:D:282:MET:HE1	2.41	0.55
1:F:290:ARG:HD3	2:F:640:HOH:O	2.06	0.55
1:H:6:THR:HG23	1:H:7:PRO:HD3	1.89	0.55
1:B:277:ARG:HD3	1:B:284:GLU:OE2	2.07	0.54
1:L:40:ASP:OD1	2:L:403:HOH:O	2.18	0.54
1:A:268:ARG:HE	1:A:276:GLU:N	2.06	0.54
1:B:49:LEU:HD13	1:B:63:ARG:HG3	1.89	0.54
1:D:189:GLY:O	2:D:401:HOH:O	2.19	0.54
1:H:290:ARG:NH1	1:H:294:LEU:HD11	2.22	0.54
1:E:10:ARG:HE	1:E:233:ARG:NE	2.06	0.53
1:G:261:LEU:HD21	1:G:278:PRO:HB3	1.91	0.53
1:B:63:ARG:HD3	2:B:432:HOH:O	2.08	0.53
1:I:261:LEU:HD21	1:I:278:PRO:HB3	1.91	0.53
1:C:298:ARG:NH2	2:C:410:HOH:O	2.38	0.52
1:E:290:ARG:HD3	2:E:633:HOH:O	2.09	0.52
1:K:63:ARG:NH2	2:K:405:HOH:O	2.40	0.52
1:H:141:MET:HE1	1:H:196:TRP:CE3	2.45	0.52
1:K:13:PHE:CE2	1:K:45:GLY:HA3	2.45	0.51
1:A:268:ARG:CZ	1:A:276:GLU:H	2.23	0.51
1:B:10:ARG:HE	1:B:233:ARG:HH21	1.58	0.51
1:K:224:GLY:HA2	1:K:243:ARG:HH21	1.75	0.51
1:F:169:TYR:CD2	1:F:194:GLY:HA3	2.46	0.51
1:K:268:ARG:NH1	2:K:406:HOH:O	2.43	0.51
1:L:169:TYR:CD2	1:L:194:GLY:HA3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:GLN:OE1	1:C:63:ARG:NH1	2.43	0.51
1:A:141:MET:HE1	1:A:196:TRP:CE3	2.46	0.51
1:L:202:ILE:HG23	1:L:203:THR:HG23	1.93	0.51
1:I:10:ARG:NH1	2:I:410:HOH:O	2.44	0.51
1:G:243:ARG:HD2	2:G:668:HOH:O	2.10	0.50
1:I:200:GLU:HG2	1:I:254:GLU:HG2	1.93	0.50
1:A:10:ARG:HD2	1:A:233:ARG:CZ	2.41	0.50
1:G:245:GLN:NE2	2:G:407:HOH:O	2.45	0.49
1:C:14:PRO:HG3	1:C:222:PRO:HB3	1.93	0.49
1:E:169:TYR:CD2	1:E:194:GLY:HA3	2.47	0.49
1:L:36:ASP:CG	1:L:73:HIS:HE2	2.20	0.49
1:F:269:GLU:OE1	1:F:298:ARG:NH2	2.40	0.49
1:H:10:ARG:NH1	1:H:233:ARG:CD	2.76	0.49
1:L:224:GLY:HA2	1:L:243:ARG:HH11	1.78	0.49
1:I:169:TYR:CD2	1:I:194:GLY:HA3	2.48	0.48
1:C:141:MET:HE1	1:C:196:TRP:CE3	2.48	0.48
1:D:200:GLU:HG2	1:D:254:GLU:HG2	1.95	0.48
1:L:110:MET:HE1	1:L:147:ALA:HB3	1.96	0.48
1:E:298:ARG:NH1	2:E:417:HOH:O	2.47	0.48
1:L:49:LEU:HD13	1:L:63:ARG:HG3	1.94	0.48
1:G:141:MET:HE1	1:G:196:TRP:CE3	2.48	0.48
1:K:49:LEU:HD13	1:K:63:ARG:HG3	1.96	0.48
1:J:200:GLU:HG2	1:J:254:GLU:HG2	1.96	0.48
1:A:268:ARG:NH2	1:A:276:GLU:HG2	2.29	0.48
1:L:10:ARG:NE	1:L:233:ARG:HH21	2.12	0.48
1:J:169:TYR:CD2	1:J:194:GLY:HA3	2.49	0.47
1:J:68:ARG:HG3	1:J:102:LEU:HD13	1.95	0.47
1:H:224:GLY:HA2	1:H:243:ARG:HH21	1.79	0.47
1:L:261:LEU:HD21	1:L:278:PRO:HB3	1.97	0.47
1:B:7:PRO:HG3	2:B:401:HOH:O	2.14	0.47
1:E:13:PHE:CE2	1:E:45:GLY:HA3	2.49	0.47
1:F:200:GLU:HG2	1:F:254:GLU:HG2	1.96	0.47
1:L:277:ARG:NH1	1:L:284:GLU:CD	2.72	0.47
1:D:169:TYR:CD2	1:D:194:GLY:HA3	2.50	0.47
1:J:277:ARG:NH1	2:J:404:HOH:O	2.31	0.47
1:F:141:MET:HE1	1:F:196:TRP:CE3	2.50	0.46
1:J:162:ARG:NH1	2:J:410:HOH:O	2.42	0.46
1:I:277:ARG:HD3	1:I:284:GLU:OE1	2.15	0.46
1:E:224:GLY:HA2	1:E:243:ARG:HH11	1.80	0.46
1:I:110:MET:HE1	1:I:147:ALA:HB3	1.98	0.46
1:L:90:GLN:NE2	2:L:417:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ASN:OD1	1:C:256:ARG:NH1	2.49	0.46
1:H:10:ARG:NH2	2:H:401:HOH:O	1.91	0.46
1:B:56:PHE:HZ	1:B:282:MET:CE	2.29	0.45
1:I:141:MET:HE1	1:I:196:TRP:CE3	2.51	0.45
1:B:169:TYR:CD2	1:B:194:GLY:HA3	2.52	0.45
1:D:141:MET:HE1	1:D:196:TRP:CE3	2.51	0.45
1:J:280:HIS:CG	1:J:281:PRO:HA	2.52	0.45
1:K:159:ARG:NE	2:K:404:HOH:O	2.40	0.45
1:C:271:GLY:HA2	2:C:401:HOH:O	2.16	0.45
1:H:227:PRO:HB2	1:H:243:ARG:HD3	1.97	0.45
1:B:13:PHE:CE2	1:B:45:GLY:HA3	2.51	0.45
1:H:13:PHE:CE2	1:H:45:GLY:HA3	2.52	0.45
1:I:141:MET:HE1	1:I:196:TRP:CZ3	2.52	0.45
1:G:55:GLN:OE1	1:G:63:ARG:NH2	2.50	0.45
1:B:141:MET:HE1	1:B:196:TRP:CE3	2.52	0.44
1:C:169:TYR:CD2	1:C:194:GLY:HA3	2.51	0.44
1:I:98:ARG:HG3	2:I:402:HOH:O	2.18	0.44
1:A:10:ARG:HD2	1:A:233:ARG:NH1	2.33	0.44
1:H:261:LEU:HD21	1:H:278:PRO:HB3	2.00	0.44
1:L:56:PHE:HZ	1:L:282:MET:HE1	1.83	0.44
1:K:141:MET:HE1	1:K:196:TRP:CE3	2.53	0.43
1:B:200:GLU:HG2	1:B:254:GLU:HG2	2.01	0.43
1:I:13:PHE:CE2	1:I:45:GLY:HA3	2.53	0.43
1:K:169:TYR:CD2	1:K:194:GLY:HA3	2.53	0.43
1:H:169:TYR:CD2	1:H:194:GLY:HA3	2.54	0.43
1:C:200:GLU:HG2	1:C:254:GLU:HG2	2.00	0.43
1:I:278:PRO:HG2	2:I:401:HOH:O	2.18	0.43
1:I:141:MET:HE2	1:I:169:TYR:HB3	1.99	0.43
1:I:216:MET:HE3	1:I:216:MET:HB2	1.89	0.43
1:K:200:GLU:HG2	1:K:254:GLU:HG2	1.99	0.43
1:L:269:GLU:OE1	1:L:298:ARG:NH2	2.50	0.43
1:A:169:TYR:CD2	1:A:194:GLY:HA3	2.52	0.43
1:J:110:MET:HE1	1:J:147:ALA:HB3	2.01	0.43
1:E:141:MET:HE1	1:E:196:TRP:CE3	2.53	0.43
1:K:56:PHE:HZ	1:K:282:MET:HE1	1.84	0.43
1:A:176:GLY:HA2	2:D:403:HOH:O	2.19	0.43
1:E:10:ARG:HG3	2:E:401:HOH:O	2.19	0.43
1:B:261:LEU:HD21	1:B:278:PRO:HB3	2.00	0.42
1:A:21:ALA:HB3	2:A:401:HOH:O	2.18	0.42
1:A:277:ARG:NH1	2:A:417:HOH:O	2.52	0.42
1:C:110:MET:HE1	1:C:147:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:GLY:N	2:E:401:HOH:O	2.51	0.42
1:L:13:PHE:O	1:L:216:MET:HG3	2.19	0.42
1:E:200:GLU:HG2	1:E:254:GLU:HG2	2.01	0.42
1:H:23:THR:OG1	1:H:25:GLU:CD	2.62	0.42
1:J:64:ASP:O	1:J:68:ARG:HD3	2.19	0.42
1:L:13:PHE:CE2	1:L:45:GLY:HA3	2.53	0.42
1:E:141:MET:HE1	1:E:196:TRP:CZ3	2.54	0.42
1:L:10:ARG:HE	1:L:233:ARG:HH21	1.56	0.42
1:E:10:ARG:HE	1:E:233:ARG:HE	1.66	0.42
1:H:200:GLU:HG2	1:H:254:GLU:HG2	2.01	0.42
1:L:297:ALA:O	1:L:302:PRO:HD3	2.20	0.42
1:G:13:PHE:CE2	1:G:45:GLY:HA3	2.54	0.42
1:A:13:PHE:CE2	1:A:45:GLY:HA3	2.55	0.41
1:A:261:LEU:HD21	1:A:278:PRO:HB3	2.01	0.41
1:G:277:ARG:HD2	1:G:284:GLU:OE1	2.20	0.41
1:I:10:ARG:HH11	1:I:233:ARG:HH11	1.68	0.41
1:I:230:GLU:HA	1:I:233:ARG:HH22	1.85	0.41
1:J:261:LEU:HD21	1:J:278:PRO:HB3	2.02	0.41
1:C:13:PHE:CE2	1:C:45:GLY:HA3	2.55	0.41
1:I:199:GLU:CD	1:L:256:ARG:HH22	2.27	0.41
1:J:171:KYQ:HE	1:J:216:MET:HB3	2.02	0.41
1:J:186:ARG:NH1	2:J:419:HOH:O	2.53	0.41
1:K:280:HIS:CG	1:K:281:PRO:HA	2.56	0.41
1:F:159:ARG:HD2	2:F:525:HOH:O	2.20	0.41
1:J:141:MET:HE1	1:J:196:TRP:CE3	2.55	0.41
1:J:141:MET:HE1	1:J:196:TRP:CZ3	2.56	0.41
1:K:141:MET:HE1	1:K:196:TRP:CZ3	2.56	0.41
1:K:261:LEU:HD21	1:K:278:PRO:HB3	2.02	0.41
1:A:277:ARG:NH1	1:A:284:GLU:CD	2.79	0.41
1:H:10:ARG:NH1	1:H:233:ARG:HD3	2.36	0.41
1:H:161:ALA:HB2	1:H:170:PHE:HZ	1.86	0.41
1:J:97:LEU:O	1:J:101:GLN:HG2	2.20	0.41
1:J:256:ARG:NH1	1:K:255:ASN:OD1	2.54	0.40
1:C:51:ASN:ND2	2:C:402:HOH:O	2.11	0.40
1:L:22:ASP:OD1	1:L:275:SER:HB2	2.21	0.40
1:L:200:GLU:HG2	1:L:254:GLU:HG2	2.04	0.40
1:J:233:ARG:HE	1:J:233:ARG:HB2	1.68	0.40
1:D:6:THR:N	1:D:7:PRO:CD	2.84	0.40
1:J:14:PRO:HD2	1:J:45:GLY:O	2.21	0.40

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

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	301/320 (94%)	294 (98%)	7 (2%)	0	100	100
1	B	301/320 (94%)	293 (97%)	8 (3%)	0	100	100
1	C	300/320 (94%)	293 (98%)	7 (2%)	0	100	100
1	D	300/320 (94%)	293 (98%)	7 (2%)	0	100	100
1	E	300/320 (94%)	295 (98%)	5 (2%)	0	100	100
1	F	300/320 (94%)	294 (98%)	6 (2%)	0	100	100
1	G	300/320 (94%)	293 (98%)	7 (2%)	0	100	100
1	H	301/320 (94%)	294 (98%)	7 (2%)	0	100	100
1	I	299/320 (93%)	293 (98%)	6 (2%)	0	100	100
1	J	299/320 (93%)	295 (99%)	4 (1%)	0	100	100
1	K	299/320 (93%)	292 (98%)	7 (2%)	0	100	100
1	L	299/320 (93%)	293 (98%)	6 (2%)	0	100	100
All	All	3599/3840 (94%)	3522 (98%)	77 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	236/250 (94%)	236 (100%)	0	100	100
1	B	236/250 (94%)	236 (100%)	0	100	100
1	C	235/250 (94%)	235 (100%)	0	100	100
1	D	235/250 (94%)	235 (100%)	0	100	100
1	E	235/250 (94%)	235 (100%)	0	100	100
1	F	235/250 (94%)	235 (100%)	0	100	100
1	G	235/250 (94%)	235 (100%)	0	100	100
1	H	236/250 (94%)	236 (100%)	0	100	100
1	I	235/250 (94%)	235 (100%)	0	100	100
1	J	234/250 (94%)	234 (100%)	0	100	100
1	K	234/250 (94%)	234 (100%)	0	100	100
1	L	235/250 (94%)	235 (100%)	0	100	100
All	All	2821/3000 (94%)	2821 (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 (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	252	ASN
1	A	257	GLN
1	A	309	HIS
1	B	124	GLN
1	B	252	ASN
1	B	257	GLN
1	C	166	GLN
1	C	252	ASN
1	D	124	GLN
1	D	179	ASN
1	D	252	ASN
1	E	124	GLN
1	F	124	GLN
1	F	252	ASN
1	G	124	GLN
1	G	252	ASN
1	G	257	GLN

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Mol	Chain	Res	Type
1	H	124	GLN
1	I	124	GLN
1	J	124	GLN
1	J	237	HIS
1	J	252	ASN
1	J	257	GLN
1	K	124	GLN
1	K	179	ASN
1	K	245	GLN
1	K	252	ASN
1	K	257	GLN
1	L	55	GLN
1	L	124	GLN
1	L	252	ASN

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	KYQ	G	171	1	7,8,15	0.55	0	3,8,18	0.60	0
1	KYQ	K	171	1	7,8,15	0.56	0	3,8,18	0.52	0
1	KYQ	J	171	1	7,8,15	0.54	0	3,8,18	0.77	0
1	KYQ	H	171	1	7,8,15	0.55	0	3,8,18	0.54	0
1	KYQ	B	171	1	12,14,15	0.90	0	6,16,18	1.31	1 (16%)
1	KYQ	L	171	1	7,8,15	0.58	0	3,8,18	0.68	0
1	KYQ	F	171	1	7,8,15	0.54	0	3,8,18	0.52	0
1	KYQ	C	171	1	12,14,15	1.04	0	6,16,18	1.06	0
1	KYQ	E	171	1	7,8,15	0.58	0	3,8,18	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KYQ	D	171	1	7,8,15	0.51	0	3,8,18	0.59	0
1	KYQ	I	171	1	7,8,15	0.57	0	3,8,18	0.59	0
1	KYQ	A	171	1	7,8,15	0.65	0	3,8,18	0.67	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	KYQ	G	171	1	-	1/6/7/18	-
1	KYQ	K	171	1	-	1/6/7/18	-
1	KYQ	J	171	1	-	1/6/7/18	-
1	KYQ	H	171	1	-	1/6/7/18	-
1	KYQ	B	171	1	-	6/12/16/18	-
1	KYQ	L	171	1	-	1/6/7/18	-
1	KYQ	F	171	1	-	1/6/7/18	-
1	KYQ	C	171	1	-	5/12/16/18	-
1	KYQ	E	171	1	-	1/6/7/18	-
1	KYQ	D	171	1	-	1/6/7/18	-
1	KYQ	I	171	1	-	1/6/7/18	-
1	KYQ	A	171	1	-	1/6/7/18	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	KYQ	O16-C12-O15	-2.08	118.94	123.90

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	171	KYQ	O-C-CA-CB
1	B	171	KYQ	O-C-CA-CB
1	B	171	KYQ	NZ-C11-C12-O16
1	B	171	KYQ	NZ-C11-C12-O15
1	B	171	KYQ	C13-C11-C12-O16
1	B	171	KYQ	C12-C11-C13-O14
1	C	171	KYQ	O-C-CA-CB
1	C	171	KYQ	NZ-C11-C12-O16

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	171	KYQ	1	0
1	B	171	KYQ	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%)	-0.27	6 (1%) 65 69	9, 14, 23, 43	0
1	B	303/320 (94%)	-0.33	5 (1%) 69 72	8, 12, 22, 42	0
1	C	302/320 (94%)	-0.31	3 (0%) 79 83	8, 14, 23, 46	0
1	D	302/320 (94%)	-0.33	3 (0%) 79 83	9, 13, 21, 38	0
1	E	302/320 (94%)	0.12	6 (1%) 65 69	12, 19, 29, 45	0
1	F	302/320 (94%)	0.04	5 (1%) 69 72	11, 18, 27, 46	0
1	G	302/320 (94%)	-0.28	2 (0%) 84 87	10, 15, 24, 46	0
1	H	303/320 (94%)	0.20	7 (2%) 61 64	12, 20, 31, 56	0
1	I	301/320 (94%)	1.05	35 (11%) 9 9	14, 24, 36, 49	0
1	J	301/320 (94%)	-0.10	2 (0%) 84 87	11, 15, 26, 38	0
1	K	301/320 (94%)	0.14	3 (0%) 79 83	11, 20, 31, 38	0
1	L	301/320 (94%)	1.20	39 (12%) 7 7	17, 26, 37, 52	0
All	All	3623/3840 (94%)	0.09	116 (3%) 50 53	8, 17, 31, 56	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	308	ALA	6.3
1	I	6	THR	4.3
1	A	6	THR	4.2
1	F	6	THR	4.0
1	G	308	ALA	3.9
1	L	22	ASP	3.8
1	C	6	THR	3.8
1	H	6	THR	3.8
1	L	23	THR	3.7
1	A	309	HIS	3.7
1	L	75	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	309	HIS	3.7
1	I	22	ASP	3.6
1	I	304	VAL	3.5
1	D	6	THR	3.4
1	I	42	GLY	3.4
1	H	22	ASP	3.4
1	L	6	THR	3.4
1	B	308	ALA	3.3
1	L	74	VAL	3.3
1	G	6	THR	3.2
1	L	244	TYR	3.2
1	I	75	ALA	3.2
1	B	309	HIS	3.2
1	E	6	THR	3.1
1	I	305	LEU	3.1
1	L	274	ALA	3.1
1	L	229	LEU	3.0
1	L	240	ALA	3.0
1	F	308	ALA	2.9
1	I	231	ALA	2.9
1	L	64	ASP	2.9
1	I	307	TRP	2.9
1	B	6	THR	2.8
1	D	47	CYS	2.8
1	I	68	ARG	2.8
1	L	307	TRP	2.8
1	I	229	LEU	2.8
1	L	76	GLY	2.8
1	A	268	ARG	2.8
1	A	22	ASP	2.8
1	L	137	ALA	2.7
1	E	308	ALA	2.7
1	L	232	TRP	2.7
1	L	21	ALA	2.7
1	E	22	ASP	2.7
1	I	277	ARG	2.7
1	A	233	ARG	2.6
1	I	295	ALA	2.6
1	F	23	THR	2.5
1	L	71	LEU	2.5
1	L	303	LEU	2.5
1	I	246	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	22	ASP	2.5
1	I	247	TRP	2.5
1	K	22	ASP	2.5
1	K	308	ALA	2.5
1	I	98	ARG	2.5
1	L	271	GLY	2.5
1	E	117	THR	2.5
1	I	10	ARG	2.4
1	L	42	GLY	2.4
1	I	240	ALA	2.4
1	L	90	GLN	2.4
1	J	277	ARG	2.4
1	I	97	LEU	2.4
1	L	46	LEU	2.4
1	B	23	THR	2.4
1	L	29	ALA	2.4
1	C	22	ASP	2.4
1	I	302	PRO	2.3
1	I	232	TRP	2.3
1	H	233	ARG	2.3
1	D	308	ALA	2.3
1	L	295	ALA	2.3
1	L	97	LEU	2.3
1	L	24	GLY	2.3
1	L	138	ILE	2.3
1	I	237	HIS	2.2
1	E	23	THR	2.2
1	I	23	THR	2.2
1	I	297	ALA	2.2
1	L	233	ARG	2.2
1	L	208	LEU	2.2
1	I	296	ILE	2.2
1	A	23	THR	2.2
1	I	233	ARG	2.2
1	I	41	ALA	2.2
1	L	39	ILE	2.2
1	F	51	ASN	2.2
1	I	7	PRO	2.2
1	I	78	VAL	2.2
1	L	35	VAL	2.1
1	I	76	GLY	2.1
1	L	103	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	21	ALA	2.1
1	I	29	ALA	2.1
1	I	74	VAL	2.1
1	I	105	ALA	2.1
1	L	210	ALA	2.1
1	L	294	LEU	2.1
1	H	190	ASP	2.1
1	L	7	PRO	2.1
1	L	273	ILE	2.1
1	L	235	GLY	2.1
1	L	297	ALA	2.1
1	I	272	VAL	2.1
1	L	102	LEU	2.1
1	K	23	THR	2.1
1	H	307	TRP	2.1
1	I	81	ILE	2.1
1	C	25	GLU	2.0
1	B	10	ARG	2.0
1	J	68	ARG	2.0
1	E	25	GLU	2.0
1	L	225	ILE	2.0

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

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	KYQ	L	171	9/16	0.89	0.11	20,22,28,29	0
1	KYQ	I	171	9/16	0.92	0.09	17,21,26,27	0
1	KYQ	H	171	9/16	0.94	0.08	15,16,22,23	0
1	KYQ	B	171	15/16	0.94	0.09	8,13,24,26	6
1	KYQ	C	171	15/16	0.94	0.09	8,14,25,25	6
1	KYQ	F	171	9/16	0.95	0.08	14,14,21,23	0
1	KYQ	G	171	9/16	0.96	0.07	14,14,18,23	0
1	KYQ	D	171	9/16	0.96	0.07	14,14,17,20	0
1	KYQ	E	171	9/16	0.96	0.07	14,14,21,22	0
1	KYQ	J	171	9/16	0.96	0.06	11,12,21,23	0
1	KYQ	A	171	9/16	0.96	0.08	14,14,17,22	0
1	KYQ	K	171	9/16	0.97	0.07	14,16,23,30	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.