



wwPDB EM Model Validation Summary Report ⓘ

Mar 18, 2020 – 09:46 AM EDT

PDB ID : 6KPE
EMDB ID : EMD-0743
Title : 343 K cryoEM structure of Sso-KARI in complex with Mg²⁺
Authors : Chen, C.Y.; Chang, Y.C.; Lin, B.L.; Huang, C.H.; Tsai, M.D.
Deposited on : 2019-08-15
Resolution : 2.83 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

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:

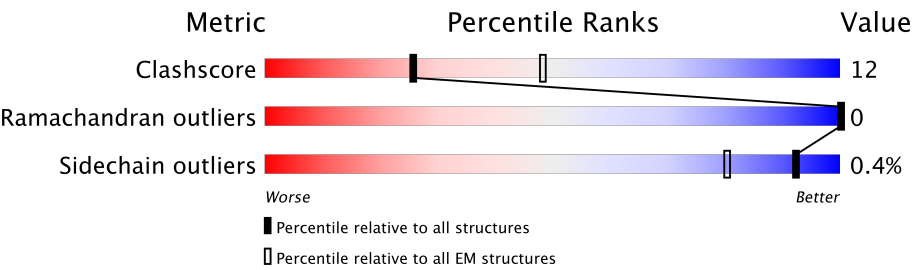
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	333	<div><div>70%28%..</div></div>
1	B	333	<div><div>70%28%..</div></div>
1	C	333	<div><div>70%28%..</div></div>
1	D	333	<div><div>70%28%..</div></div>
1	E	333	<div><div>71%27%..</div></div>
1	F	333	<div><div>71%27%..</div></div>
1	G	333	<div><div>69%29%..</div></div>
1	H	333	<div><div>69%29%..</div></div>
1	I	333	<div><div>69%29%..</div></div>

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Mol	Chain	Length	Quality of chain
1	J	333	 70% 28% ..
1	K	333	 70% 28% ..
1	L	333	 71% 27% ..

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 62184 atoms, of which 31212 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ketol-acid reductoisomerase.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	328	Total	C	H	N	O	S	0	0
			5181	1667	2601	423	480	10		
1	B	328	Total	C	H	N	O	S	0	0
			5181	1667	2601	423	480	10		
1	C	328	Total	C	H	N	O	S	0	0
			5181	1667	2601	423	480	10		
1	D	328	Total	C	H	N	O	S	0	0
			5181	1667	2601	423	480	10		
1	E	328	Total	C	H	N	O	S	0	0
			5181	1667	2601	423	480	10		
1	F	328	Total	C	H	N	O	S	0	0
			5181	1667	2601	423	480	10		
1	G	328	Total	C	H	N	O	S	0	0
			5181	1667	2601	423	480	10		
1	H	328	Total	C	H	N	O	S	0	0
			5181	1667	2601	423	480	10		
1	I	328	Total	C	H	N	O	S	0	0
			5181	1667	2601	423	480	10		
1	J	328	Total	C	H	N	O	S	0	0
			5181	1667	2601	423	480	10		
1	K	328	Total	C	H	N	O	S	0	0
			5181	1667	2601	423	480	10		
1	L	328	Total	C	H	N	O	S	0	0
			5181	1667	2601	423	480	10		

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		AltConf
2	G	1	Total	Mg	0
			1	1	
2	J	1	Total	Mg	0
			1	1	

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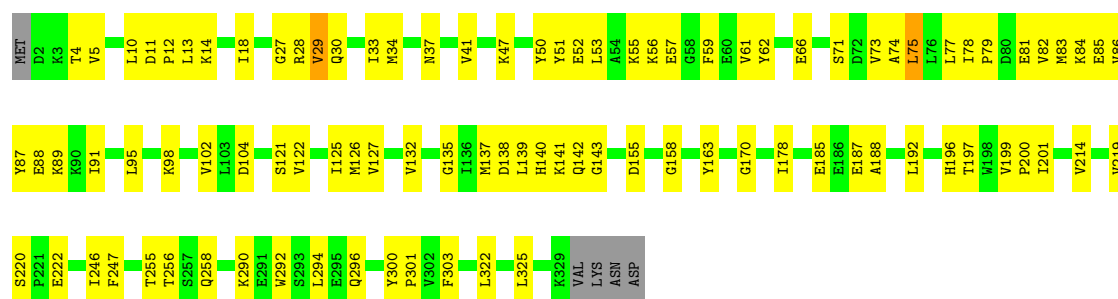
Mol	Chain	Residues	Atoms		AltConf
2	D	1	Total 1	Mg 1	0
2	K	1	Total 1	Mg 1	0
2	E	1	Total 1	Mg 1	0
2	H	1	Total 1	Mg 1	0
2	B	1	Total 1	Mg 1	0
2	I	1	Total 1	Mg 1	0
2	C	1	Total 1	Mg 1	0
2	A	1	Total 1	Mg 1	0
2	L	1	Total 1	Mg 1	0
2	F	1	Total 1	Mg 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

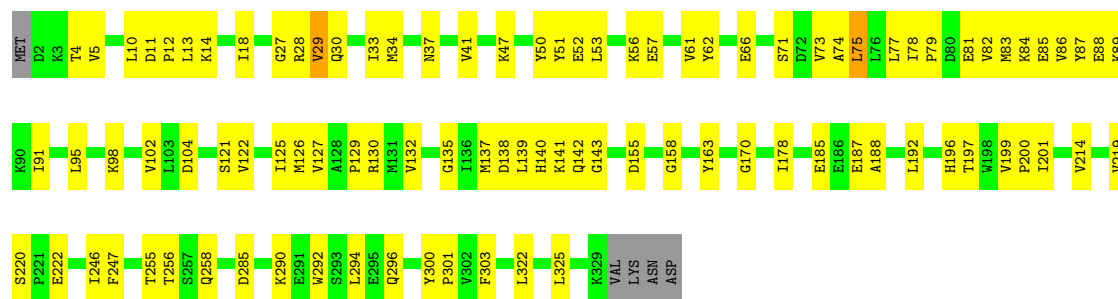
- Molecule 1: Ketol-acid reductoisomerase

Chain A: 



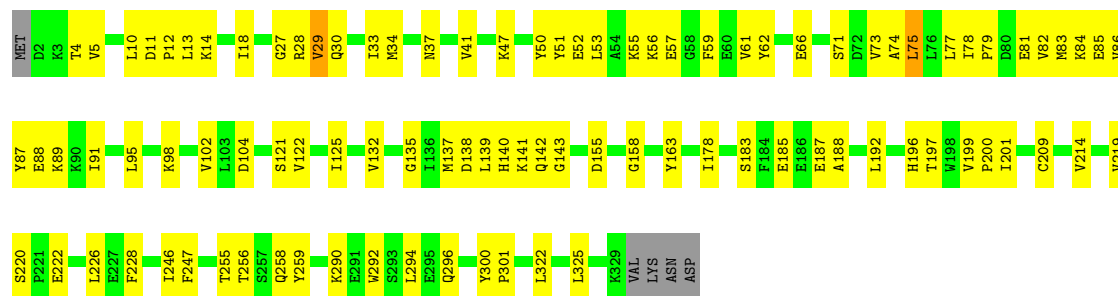
- Molecule 1: Ketol-acid reductoisomerase

Chain B: 



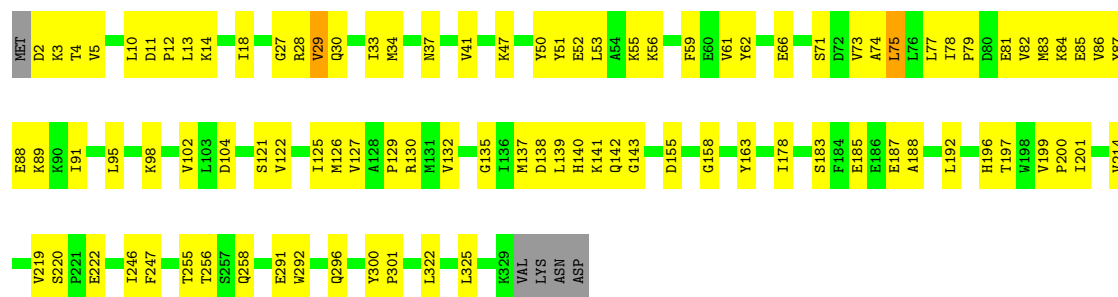
- Molecule 1: Ketol-acid reductoisomerase

Chain C: 



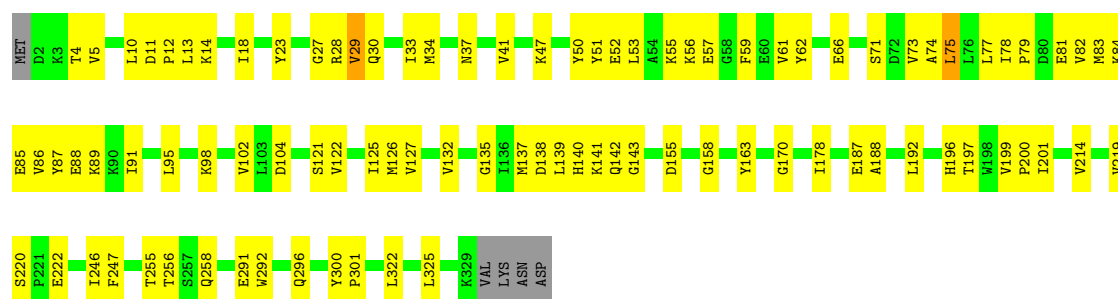
- Molecule 1: Ketol-acid reductoisomerase

Chain D:  70% 28% ..



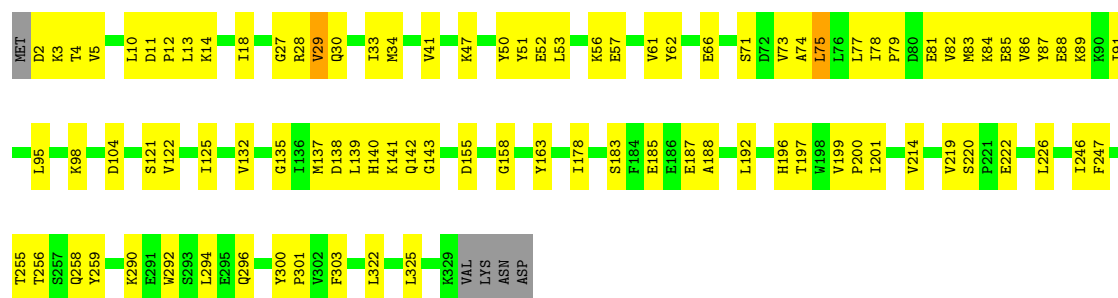
- Molecule 1: Ketol-acid reductoisomerase

Chain E:  71% 27% ..



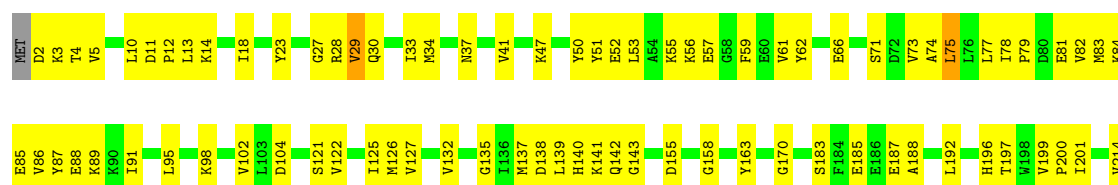
- Molecule 1: Ketol-acid reductoisomerase

Chain F:  71% 27% ..



- Molecule 1: Ketol-acid reductoisomerase

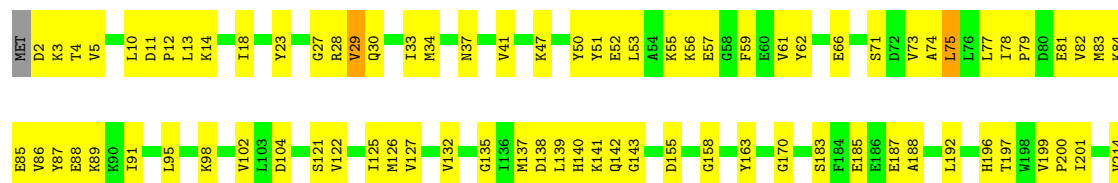
Chain G:  69% 29% ..





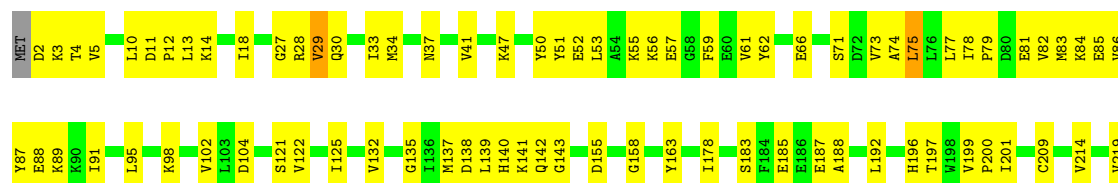
• Molecule 1: Ketol-acid reductoisomerase

Chain H: 69% 29% ..



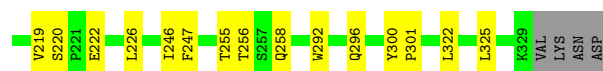
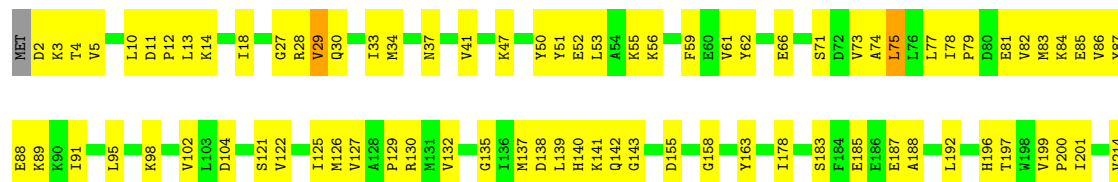
• Molecule 1: Ketol-acid reductoisomerase

Chain I: 69% 29% ..



• Molecule 1: Ketol-acid reductoisomerase

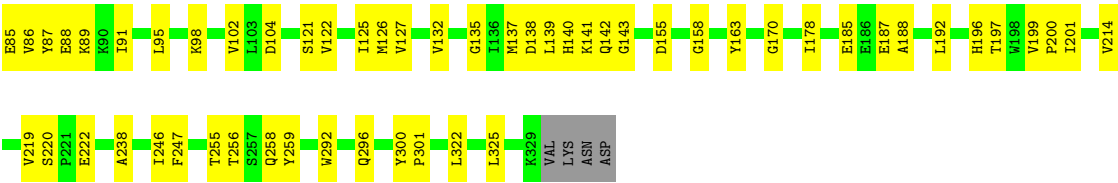
Chain J: 70% 28% ..



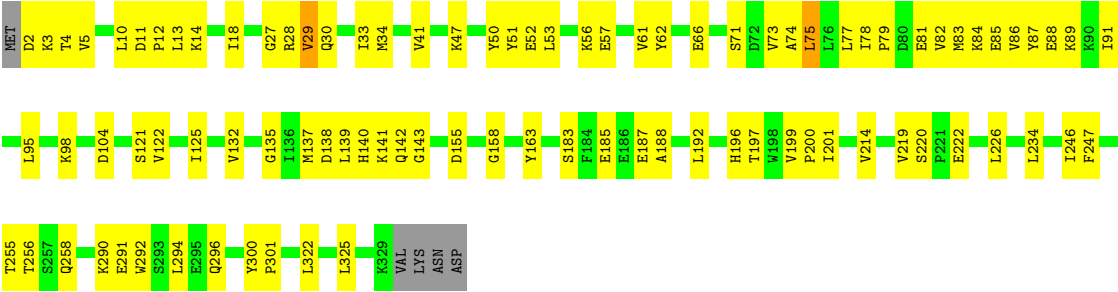
• Molecule 1: Ketol-acid reductoisomerase

Chain K: 70% 28% ..





• Molecule 1: Ketol-acid reductoisomerase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	58483	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.45	0/2633	0.53	4/3555 (0.1%)
1	B	0.45	0/2633	0.53	4/3555 (0.1%)
1	C	0.45	0/2633	0.53	4/3555 (0.1%)
1	D	0.45	0/2633	0.53	4/3555 (0.1%)
1	E	0.45	0/2633	0.53	4/3555 (0.1%)
1	F	0.45	0/2633	0.53	3/3555 (0.1%)
1	G	0.45	0/2633	0.53	4/3555 (0.1%)
1	H	0.45	0/2633	0.53	4/3555 (0.1%)
1	I	0.45	0/2633	0.53	4/3555 (0.1%)
1	J	0.45	0/2633	0.53	4/3555 (0.1%)
1	K	0.45	0/2633	0.53	4/3555 (0.1%)
1	L	0.45	0/2633	0.53	4/3555 (0.1%)
All	All	0.45	0/31596	0.53	47/42660 (0.1%)

There are no bond length outliers.

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	VAL	CG1-CB-CG2	7.03	122.15	110.90
1	A	82	VAL	CG1-CB-CG2	7.03	122.14	110.90
1	F	29	VAL	CG1-CB-CG2	7.03	122.14	110.90
1	K	82	VAL	CG1-CB-CG2	7.03	122.14	110.90
1	C	82	VAL	CG1-CB-CG2	7.03	122.14	110.90

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	2580	2601	2604	67	0
1	B	2580	2601	2604	68	0
1	C	2580	2601	2604	68	0
1	D	2580	2601	2604	67	0
1	E	2580	2601	2604	68	0
1	F	2580	2601	2604	68	0
1	G	2580	2601	2604	64	0
1	H	2580	2601	2604	64	0
1	I	2580	2601	2604	68	0
1	J	2580	2601	2604	65	0
1	K	2580	2601	2604	66	0
1	L	2580	2601	2604	65	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
All	All	30972	31212	31248	766	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 12.

The worst 5 of 766 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:G:222:GLU:OE1	1:G:222:GLU:N	2.21	0.74
1:H:222:GLU:OE1	1:H:222:GLU:N	2.21	0.74
1:G:81:GLU:OE2	1:H:256:THR:OG1	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:THR:OG1	1:H:81:GLU:OE2	2.05	0.73
1:A:222:GLU:OE1	1:A:222:GLU:N	2.20	0.73

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 PDB entries followed by that with respect to all EM entries.

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	326/333 (98%)	292 (90%)	34 (10%)	0	100	100
1	B	326/333 (98%)	292 (90%)	34 (10%)	0	100	100
1	C	326/333 (98%)	292 (90%)	34 (10%)	0	100	100
1	D	326/333 (98%)	292 (90%)	34 (10%)	0	100	100
1	E	326/333 (98%)	292 (90%)	34 (10%)	0	100	100
1	F	326/333 (98%)	292 (90%)	34 (10%)	0	100	100
1	G	326/333 (98%)	292 (90%)	34 (10%)	0	100	100
1	H	326/333 (98%)	292 (90%)	34 (10%)	0	100	100
1	I	326/333 (98%)	292 (90%)	34 (10%)	0	100	100
1	J	326/333 (98%)	292 (90%)	34 (10%)	0	100	100
1	K	326/333 (98%)	292 (90%)	34 (10%)	0	100	100
1	L	326/333 (98%)	292 (90%)	34 (10%)	0	100	100
All	All	3912/3996 (98%)	3504 (90%)	408 (10%)	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 PDB entries followed by that with respect to all EM entries.

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	267/272 (98%)	266 (100%)	1 (0%)	92	97
1	B	267/272 (98%)	266 (100%)	1 (0%)	92	97
1	C	267/272 (98%)	266 (100%)	1 (0%)	92	97
1	D	267/272 (98%)	266 (100%)	1 (0%)	92	97
1	E	267/272 (98%)	266 (100%)	1 (0%)	92	97
1	F	267/272 (98%)	266 (100%)	1 (0%)	92	97
1	G	267/272 (98%)	266 (100%)	1 (0%)	92	97
1	H	267/272 (98%)	266 (100%)	1 (0%)	92	97
1	I	267/272 (98%)	266 (100%)	1 (0%)	92	97
1	J	267/272 (98%)	266 (100%)	1 (0%)	92	97
1	K	267/272 (98%)	266 (100%)	1 (0%)	92	97
1	L	267/272 (98%)	266 (100%)	1 (0%)	92	97
All	All	3204/3264 (98%)	3192 (100%)	12 (0%)	92	97

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	28	ARG
1	G	28	ARG
1	J	28	ARG
1	E	28	ARG
1	I	28	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	154	GLN
1	G	296	GLN
1	L	96	GLN
1	F	278	ASN

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Mol	Chain	Res	Type
1	G	96	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.