



wwPDB EM Validation Summary Report ⓘ

Jul 16, 2025 – 01:05 AM JST

PDB ID : 8IVQ / pdb_00008ivq
EMDB ID : EMD-35759
Title : Cryo-EM structure of mouse BIRC6, Global map
Authors : Liu, S.; Jiang, T.; Bu, F.; Zhao, J.; Wang, G.; Li, N.; Gao, N.; Qiu, X.
Deposited on : 2023-03-28
Resolution : 3.60 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

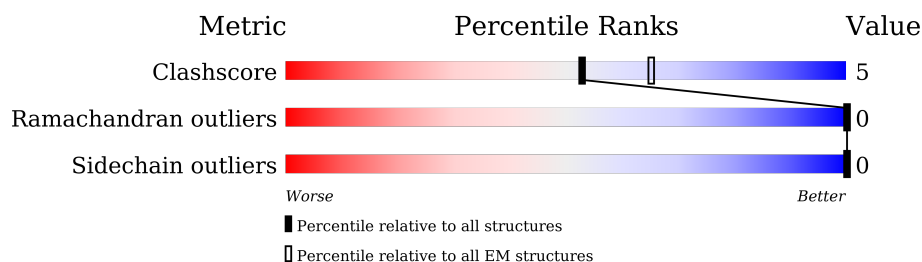
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 of 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	4896	
1	B	4896	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 41900 atoms, of which 0 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 Isoform 2 of Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2921	Total 20950	C 13236	N 3680	O 3904	S 130	0	0
1	B	2921	Total 20950	C 13236	N 3680	O 3904	S 130	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-50	MET	-	initiating methionine	UNP O88738
A	-49	ASP	-	expression tag	UNP O88738
A	-48	TYR	-	expression tag	UNP O88738
A	-47	LYS	-	expression tag	UNP O88738
A	-46	ASP	-	expression tag	UNP O88738
A	-45	HIS	-	expression tag	UNP O88738
A	-44	ASP	-	expression tag	UNP O88738
A	-43	GLY	-	expression tag	UNP O88738
A	-42	ASP	-	expression tag	UNP O88738
A	-41	TYR	-	expression tag	UNP O88738
A	-40	LYS	-	expression tag	UNP O88738
A	-39	ASP	-	expression tag	UNP O88738
A	-38	HIS	-	expression tag	UNP O88738
A	-37	ASP	-	expression tag	UNP O88738
A	-36	ILE	-	expression tag	UNP O88738
A	-35	ASP	-	expression tag	UNP O88738
A	-34	TYR	-	expression tag	UNP O88738
A	-33	LYS	-	expression tag	UNP O88738
A	-32	ASP	-	expression tag	UNP O88738
A	-31	ASP	-	expression tag	UNP O88738
A	-30	ASP	-	expression tag	UNP O88738
A	-29	ASP	-	expression tag	UNP O88738
A	-28	LYS	-	expression tag	UNP O88738
A	-27	ARG	-	expression tag	UNP O88738
A	-26	VAL	-	expression tag	UNP O88738
A	-25	VAL	-	expression tag	UNP O88738

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	PRO	-	expression tag	UNP O88738
A	-23	LEU	-	expression tag	UNP O88738
A	-22	GLU	-	expression tag	UNP O88738
A	-21	SER	-	expression tag	UNP O88738
A	-20	THR	-	expression tag	UNP O88738
A	-19	GLY	-	expression tag	UNP O88738
A	-18	LEU	-	expression tag	UNP O88738
A	-17	GLN	-	expression tag	UNP O88738
A	-16	GLU	-	expression tag	UNP O88738
A	-15	LEU	-	expression tag	UNP O88738
A	-14	ALA	-	expression tag	UNP O88738
A	-13	THR	-	expression tag	UNP O88738
A	-12	MET	-	expression tag	UNP O88738
A	-11	GLU	-	expression tag	UNP O88738
A	-10	GLN	-	expression tag	UNP O88738
A	-9	LYS	-	expression tag	UNP O88738
A	-8	LEU	-	expression tag	UNP O88738
A	-7	ILE	-	expression tag	UNP O88738
A	-6	SER	-	expression tag	UNP O88738
A	-5	GLU	-	expression tag	UNP O88738
A	-4	GLU	-	expression tag	UNP O88738
A	-3	ASP	-	expression tag	UNP O88738
A	-2	LEU	-	expression tag	UNP O88738
A	-1	GLU	-	expression tag	UNP O88738
A	0	PHE	-	expression tag	UNP O88738
A	178	ILE	THR	conflict	UNP O88738
A	690	THR	ALA	conflict	UNP O88738
A	2079	ARG	GLY	conflict	UNP O88738
A	2418	GLY	CYS	conflict	UNP O88738
A	2959	ILE	THR	conflict	UNP O88738
A	3226	THR	SER	conflict	UNP O88738
A	3914	VAL	MET	conflict	UNP O88738
A	3929	VAL	ILE	conflict	UNP O88738
A	4346	MET	VAL	conflict	UNP O88738
B	-50	MET	-	initiating methionine	UNP O88738
B	-49	ASP	-	expression tag	UNP O88738
B	-48	TYR	-	expression tag	UNP O88738
B	-47	LYS	-	expression tag	UNP O88738
B	-46	ASP	-	expression tag	UNP O88738
B	-45	HIS	-	expression tag	UNP O88738
B	-44	ASP	-	expression tag	UNP O88738
B	-43	GLY	-	expression tag	UNP O88738

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-42	ASP	-	expression tag	UNP O88738
B	-41	TYR	-	expression tag	UNP O88738
B	-40	LYS	-	expression tag	UNP O88738
B	-39	ASP	-	expression tag	UNP O88738
B	-38	HIS	-	expression tag	UNP O88738
B	-37	ASP	-	expression tag	UNP O88738
B	-36	ILE	-	expression tag	UNP O88738
B	-35	ASP	-	expression tag	UNP O88738
B	-34	TYR	-	expression tag	UNP O88738
B	-33	LYS	-	expression tag	UNP O88738
B	-32	ASP	-	expression tag	UNP O88738
B	-31	ASP	-	expression tag	UNP O88738
B	-30	ASP	-	expression tag	UNP O88738
B	-29	ASP	-	expression tag	UNP O88738
B	-28	LYS	-	expression tag	UNP O88738
B	-27	ARG	-	expression tag	UNP O88738
B	-26	VAL	-	expression tag	UNP O88738
B	-25	VAL	-	expression tag	UNP O88738
B	-24	PRO	-	expression tag	UNP O88738
B	-23	LEU	-	expression tag	UNP O88738
B	-22	GLU	-	expression tag	UNP O88738
B	-21	SER	-	expression tag	UNP O88738
B	-20	THR	-	expression tag	UNP O88738
B	-19	GLY	-	expression tag	UNP O88738
B	-18	LEU	-	expression tag	UNP O88738
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B	-8	LEU	-	expression tag	UNP O88738
B	-7	ILE	-	expression tag	UNP O88738
B	-6	SER	-	expression tag	UNP O88738
B	-5	GLU	-	expression tag	UNP O88738
B	-4	GLU	-	expression tag	UNP O88738
B	-3	ASP	-	expression tag	UNP O88738
B	-2	LEU	-	expression tag	UNP O88738
B	-1	GLU	-	expression tag	UNP O88738

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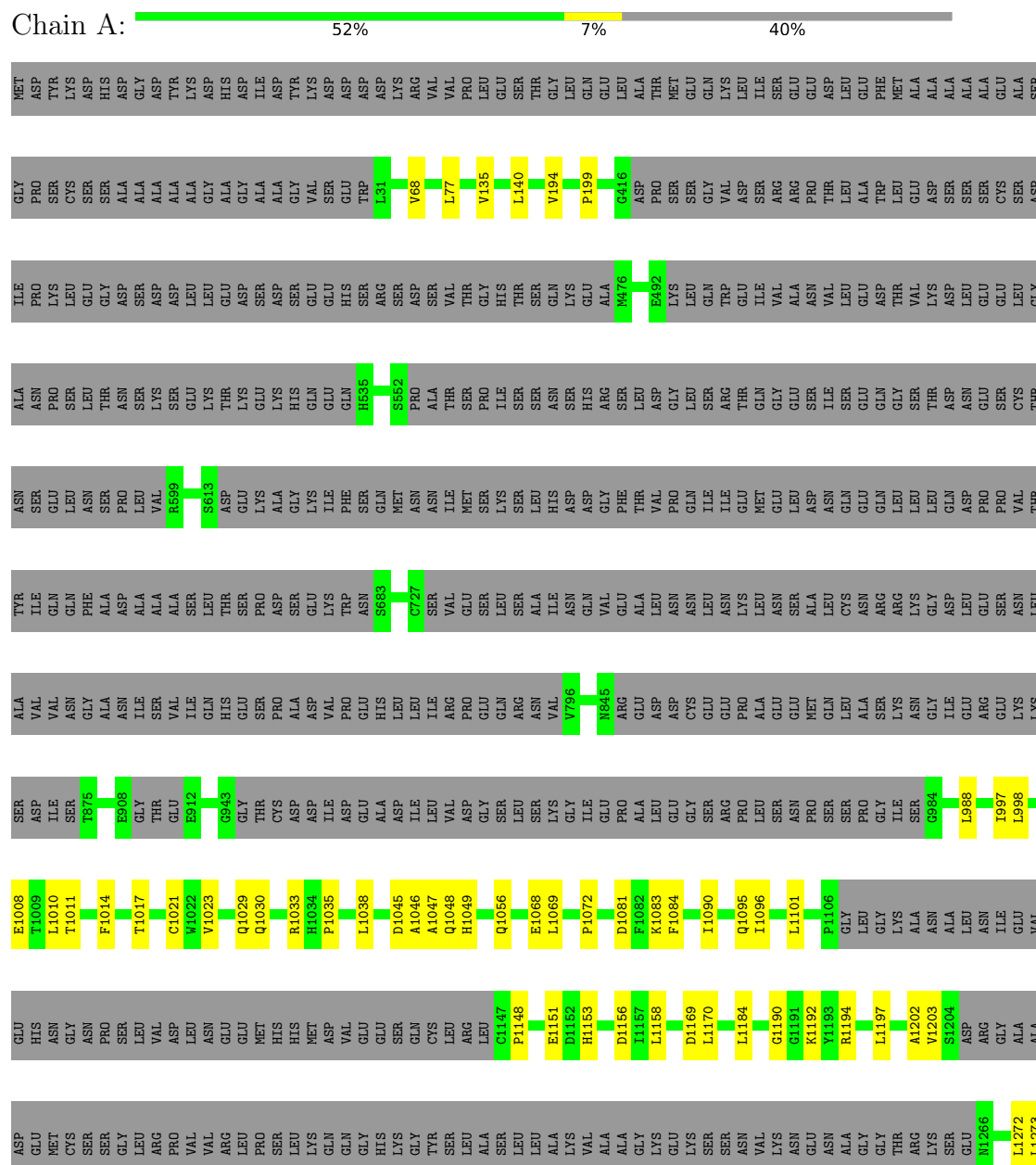
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	PHE	-	expression tag	UNP O88738
B	178	ILE	THR	conflict	UNP O88738
B	690	THR	ALA	conflict	UNP O88738
B	2079	ARG	GLY	conflict	UNP O88738
B	2418	GLY	CYS	conflict	UNP O88738
B	2959	ILE	THR	conflict	UNP O88738
B	3226	THR	SER	conflict	UNP O88738
B	3914	VAL	MET	conflict	UNP O88738
B	3929	VAL	ILE	conflict	UNP O88738
B	4346	MET	VAL	conflict	UNP O88738

3 Residue-property plots

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. 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: Isoform 2 of Baculoviral IAP repeat-containing protein 6

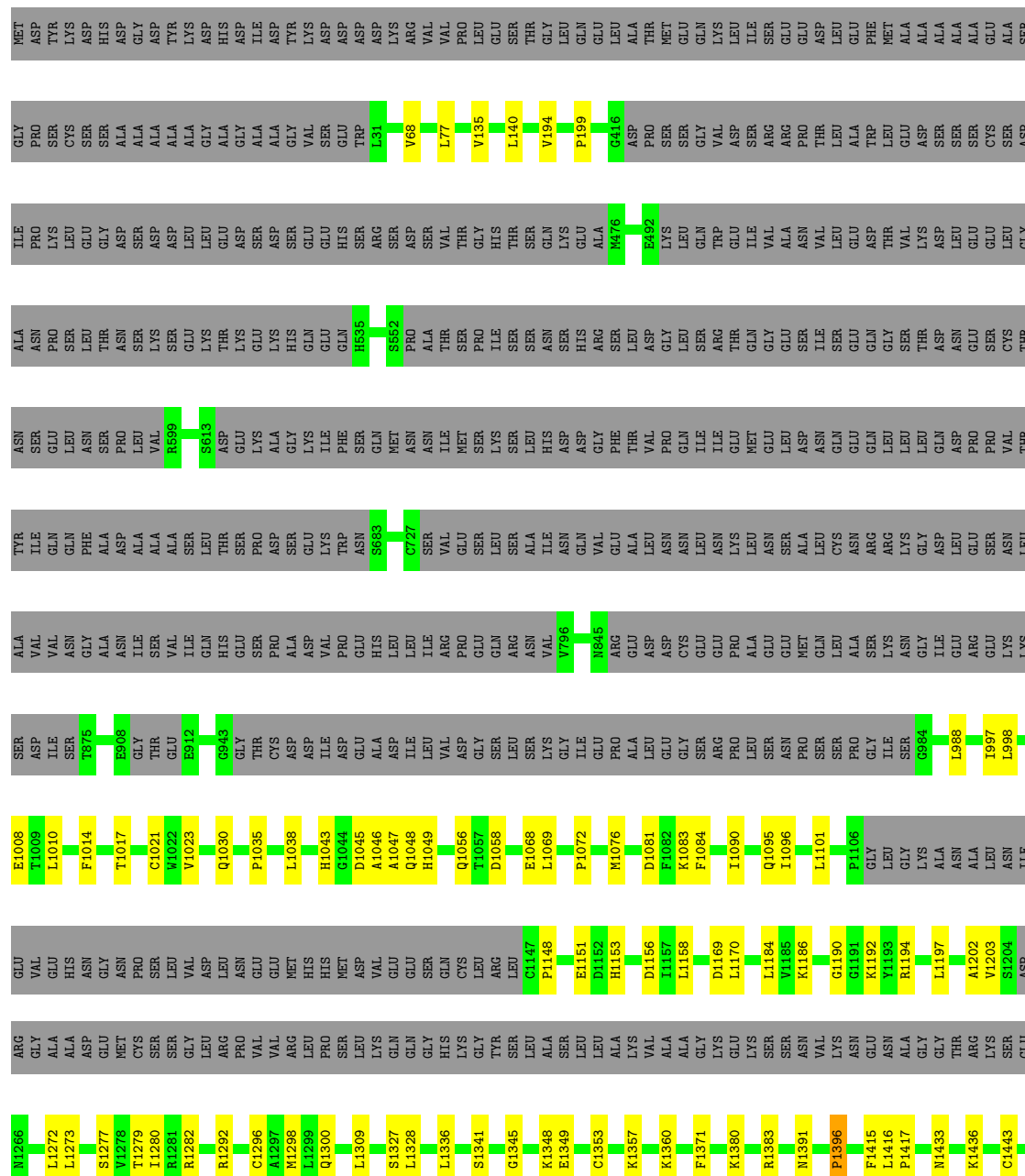






CYS	PRO	GLU	GLY	LEU	ASP	PRO	ASP	ILE	GLU	ASP	SER	ALA	SER	PRO	VAL	CYS	ARG	ALA	THR	THR	GLY	ALA	GLU	ASP	THR	LEU	THR	HIS	ASP	HIS	VAL	ASN	PRO	SER	SER	SER	LYS	ASP	LEU	PRO	SER	ASP	PHE	GLN	LEU
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- Molecule 1: Isoform 2 of Baculoviral IAP repeat-containing protein 6







ARG	HIS
GLN	HIS
ALA	ALA
THR	ALA
VAL	PHE
LYS	GLN
TRP	LEU
ALA	LYS
ALA	ARG
GLU	HIS
GLN	THR
ILE	LEU
ARG	ALA
ASN	GLU
PRO	GLU
SER	PRO
PRO	LEU
CYS	LYS
PHE	LEU
LYS	PRO
LYS	CYS
GLU	PRO
VAL	CYS
ILE	PRO
HIS	GLY
LYS	GLY
HIS	LEU
PHE	ASP
TYR	PRO
LEU	ASP
LYS	ILE
ARG	GLU
ILE	ASP
GLU	ALA
LEU	SER
MET	PRO
ALA	VAL
GLN	CYS
CYS	ARG
GLU	ALA
THR	ALA
GLU	ALA
TRP	GLY
ILE	ALA
ALA	GLU
ASP	ASP
ILE	THR
GLN	LEU
GLN	THR
TYR	HIS
SER	ASP
SER	HIS
ASP	VAL
LYS	ASN
ARG	PRO
VAL	SER
GLY	SER
ARG	SER
THR	LYS
MET	ASP
SER	LEU

PRO
SER
ASP
PHE
GLN
LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	68.4	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/21276	0.54	5/28980 (0.0%)
1	B	0.24	0/21276	0.54	4/28980 (0.0%)
All	All	0.24	0/42552	0.54	9/57960 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1396	PRO	CA-N-CD	-5.95	103.67	112.00
1	A	1396	PRO	CA-N-CD	-5.93	103.70	112.00
1	A	4321	MET	CA-CB-CG	5.34	124.79	114.10
1	B	4321	MET	CA-CB-CG	5.32	124.75	114.10
1	A	4305	GLU	CA-CB-CG	5.23	124.57	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1396	PRO	Peptide
1	A	1834	ILE	Peptide
1	B	1396	PRO	Peptide
1	B	1834	ILE	Peptide

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	20950	0	19684	215	0
1	B	20950	0	19684	224	0
All	All	41900	0	39368	413	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 5.

The worst 5 of 413 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:B:3798:PHE:O	1:B:3802:MET:HB3	1.81	0.81
1:A:3798:PHE:O	1:A:3802:MET:HB3	1.81	0.80
1:B:1383:ARG:HH21	1:B:2562:GLU:HB2	1.52	0.74
1:A:1383:ARG:HH21	1:A:2562:GLU:HB2	1.52	0.73
1:A:2375:GLY:HA2	1:A:2641:VAL:HA	1.76	0.68

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	2841/4896 (58%)	2786 (98%)	55 (2%)	0	100	100
1	B	2841/4896 (58%)	2787 (98%)	54 (2%)	0	100	100
All	All	5682/9792 (58%)	5573 (98%)	109 (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 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	2046/4236 (48%)	2046 (100%)	0	100	100
1	B	2046/4236 (48%)	2046 (100%)	0	100	100
All	All	4092/8472 (48%)	4092 (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. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3962	GLN
1	B	3513	ASN
1	B	1056	GLN
1	B	4169	GLN
1	B	3095	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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.