



Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 02:17 PM JST

PDB ID : 8IVQ
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 Full wwPDB EM 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/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 : 4.02b-467
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) : 2.39

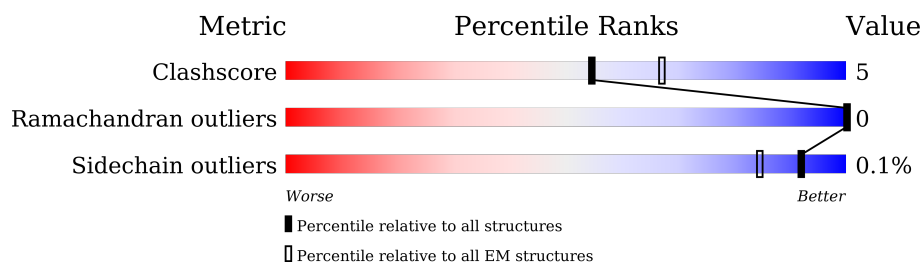
1 Overall quality at a glance

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	C	N	O	S	0	0
			20950	13236	3680	3904	130		
1	B	2921	Total	C	N	O	S	0	0
			20950	13236	3680	3904	130		

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
B	-17	GLN	-	expression tag	UNP O88738
B	-16	GLU	-	expression tag	UNP O88738
B	-15	LEU	-	expression tag	UNP O88738
B	-14	ALA	-	expression tag	UNP O88738
B	-13	THR	-	expression tag	UNP O88738
B	-12	MET	-	expression tag	UNP O88738
B	-11	GLU	-	expression tag	UNP O88738
B	-10	GLN	-	expression tag	UNP O88738
B	-9	LYS	-	expression tag	UNP O88738
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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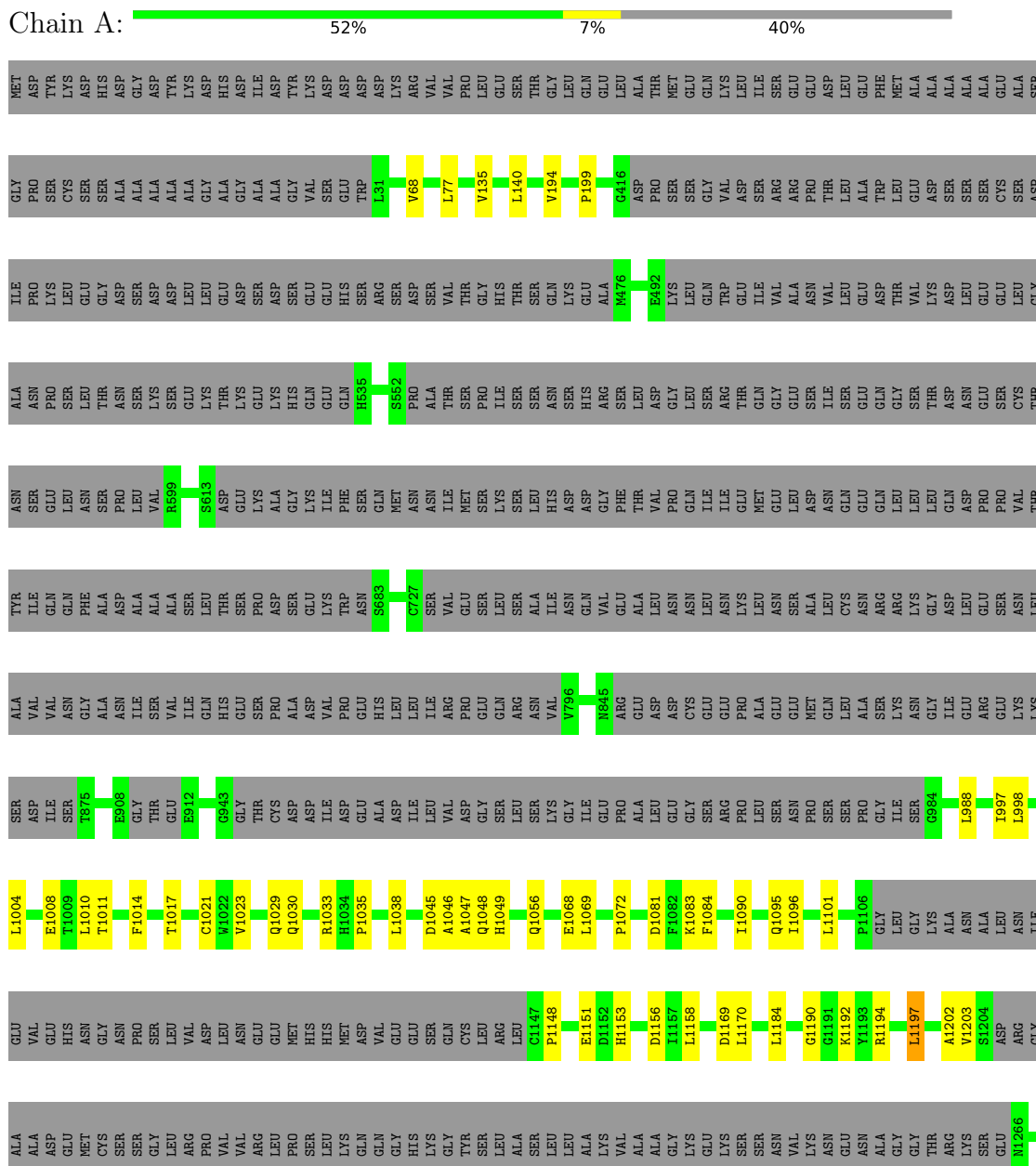
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	PHE	-	expression tag	UNP O88738
B	178	ILE	THR	conflict	UNP O88738
B	690	THR	ALA	conflict	UNP O88738
B	2079	ARG	GLY	conflict	UNP O88738
B	2418	GLY	CYS	conflict	UNP O88738
B	2959	ILE	THR	conflict	UNP 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



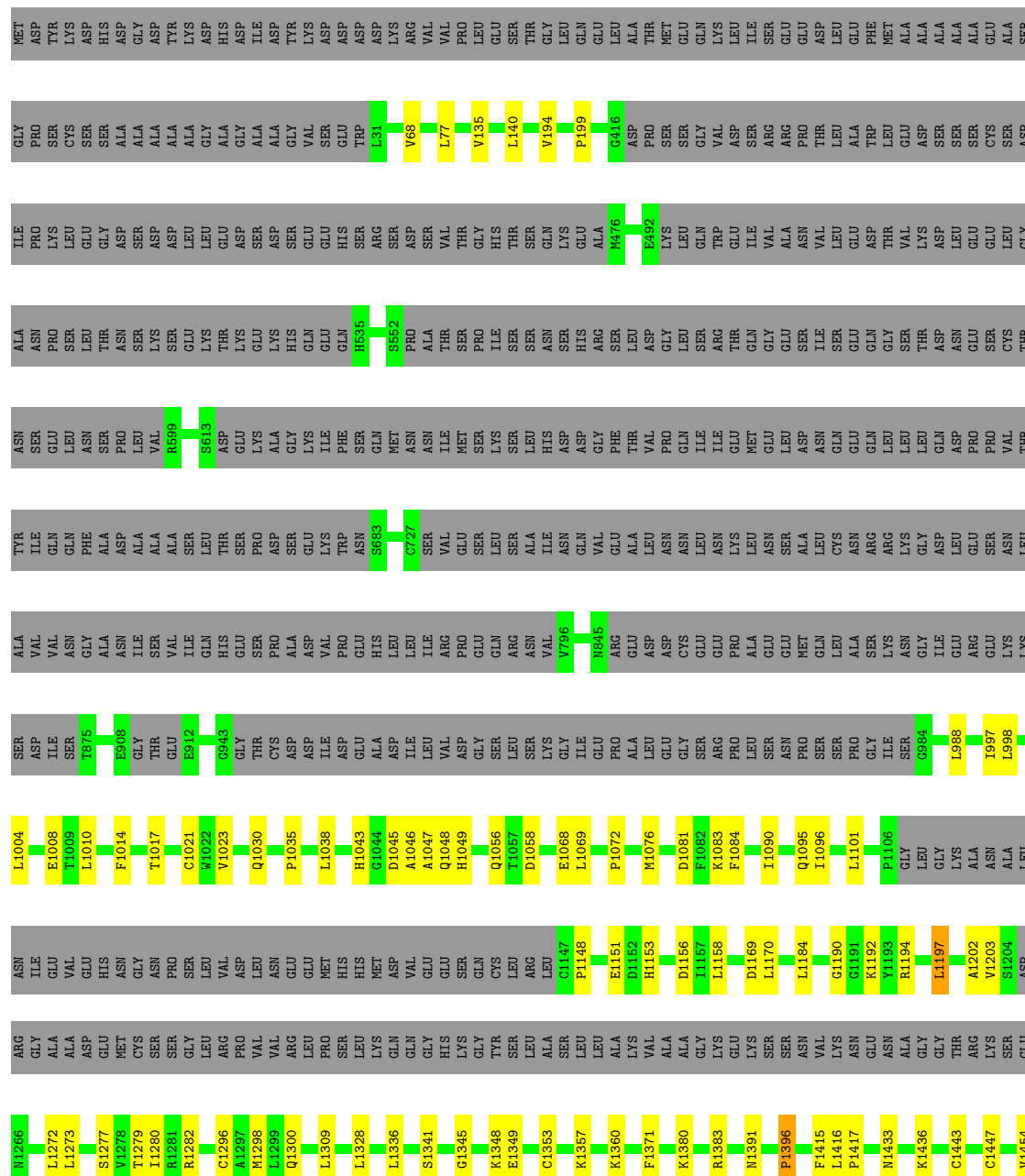


PRO	GLN	ARG	ALA	MET	LYS	THR	M4321	S4242	VAL	THR	SER	LYS	H3760	ASN	PRO	VAL	GLN	ILE	T2995
GLN	ARG	ALA	ARG	LYS	PRO	S4420	S4322	H4243	TYR	PRO	SER	GLU	L3774	SER	VAL	GLN	VAL	ILE	12995
TYR	ARG	ALA	ARG	PRO	ASP	V4421	G4323	H4243	GLU	SER	SER	LYS	F3775	GLN	GLN	VAL	GLN	ILE	12995
LEU	ARG	ALA	ARG	PRO	GLU	T4423	A4324	H4243	ALA	ASP	ALA	LYS	F3776	ASP	ASP	CYS	GLY	ILE	12995
LEU	ALA	ALA	ARG	VAL	THR	M4428	GLY	ARG	PRO	CYS	ALA	HIS	Q3776	LEU	ARG	ARG	GLY	ILE	12995
GLN	ALA	ALA	ALA	PRO	ILE	K4429	GLU	VAL	THR	MET	ALA	GLU	T3777	ARG	LEU	LEU	GLY	ILE	12995
LEU	ALA	ALA	ALA	PRO	ALA	V4432	GLN	SER	ALA	ASP	SER	LYS	Q3359	HIS	HIS	LEU	GLY	ILE	12995
LEU	ALA	ALA	ALA	PRO	ALA	Y4435	PRO	LEU	PRO	VAL	THR	VAL	L3382	THR	THR	THR	THR	THR	12995
LEU	ALA	ALA	ALA	PRO	ALA	T4436	GLU	SER	PRO	VAL	ASP	ASP	L3382	LYS	LYS	LYS	LYS	LYS	12995
GLU	ALA	ALA	ALA	GLU	GLU	M4437	GLU	GLN	PRO	GLU	SER	GLN	M3389	HIS	HIS	GLU	GLU	GLU	12995
THR	ALA	ALA	ALA	TYR	LYS	R4438	ARG	THR	VAL	PRO	THR	ASN	L3400	ASN	ASN	ASN	ASN	ASN	12995
THR	ALA	ALA	ALA	VAL	VAL	L4439	ALA	PRO	LYS	VAL	GLY	GLY	N3401	PHE	PHE	PHE	PHE	PHE	12995
GLY	ALA	ALA	ALA	ALA	ALA	K4442	GLN	GLN	SER	ALA	L3970	GLY	G3788	GLN	ASP	ASP	GLY	GLY	12995
HIS	ALA	ALA	ALA	ALA	ALA	ARG	V4339	VAL	VAL	ALA	G3985	PHE	L3797	LEU	LEU	LEU	GLY	GLY	12995
SER	ALA	ALA	ALA	ALA	ALA	GLU	R4339	SER	GLN	VAL	G3985	ASP	L3797	SER	SER	SER	GLY	GLY	12995
SER	ALA	ALA	ALA	ALA	ALA	ASN	L4347	ASN	ALA	ILE	V3993	ASP	F3798	SER	SER	SER	GLY	GLY	12995
ARG	ALA	ALA	ALA	ALA	ALA	LYS	L4350	SER	THR	ILE	G3996	TYR	Q3800	SER	SER	SER	GLY	GLY	12995
SER	ALA	ALA	ALA	ALA	ALA	GLN	L4356	ASN	SER	GLN	GLY	VAL	L3801	LEU	LEU	LEU	GLY	GLY	12995
ASN	ALA	ALA	ALA	ALA	ALA	VAL	L4357	THR	THR	VAL	SER	VAL	M3802	THR	ASP	ASP	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	14357	THR	THR	VAL	LYS	VAL	K3807	ASP	ASP	ASP	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	M4360	ALA	ILE	ILE	VAL	ALA	L3812	SER	SER	SER	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	L4364	ALA	GLN	GLN	THR	GLY	Q3813	ASN	ASN	ASN	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	ARG	GLU	VAL	VAL	SER	LYS	S3814	ALA	ALA	ALA	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	ASN	GLN	ALA	SER	LEU	LYS	Q3836	GLN	GLN	GLN	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	ASN	GLN	ALA	ALA	LEU	LYS	Q3836	ALA	ALA	ALA	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	P4367	GLN	PRO	PRO	SER	GLN	L3844	PRO	PRO	PRO	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	P4377	TYR	VAL	ILE	LYS	SER	H3845	GLY	GLY	GLY	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	P4377	TYR	VAL	ILE	LYS	SER	L3845	GLY	GLY	GLY	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	R4380	ALA	ALA	SER	ASP	ARG	L3846	HIS	ASN	ASN	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
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LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
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LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
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LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
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LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
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LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
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LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR	THR	SER	PHE	VAL	P3847	LEU	LEU	LEU	GLY	GLY	12995
LEU	ALA	ALA	ALA	ALA	ALA	VAL	V4396	THR											

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

Chain B:  52% 7% 40%







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

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	0.29	0/21276	0.60	14/28980 (0.0%)
1	B	0.29	0/21276	0.60	14/28980 (0.0%)
All	All	0.29	0/42552	0.60	28/57960 (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.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4162	LEU	CB-CG-CD2	-9.11	95.51	111.00
1	B	4162	LEU	CB-CG-CD2	-9.10	95.53	111.00
1	A	2337	LEU	CA-CB-CG	7.63	132.86	115.30
1	B	2337	LEU	CA-CB-CG	7.62	132.83	115.30
1	B	2129	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	2129	ASP	CB-CG-OD1	7.56	125.11	118.30
1	A	4241	LEU	CA-CB-CG	6.78	130.89	115.30
1	B	4241	LEU	CA-CB-CG	6.77	130.87	115.30
1	A	4321	MET	CA-CB-CG	6.76	124.79	113.30
1	B	4321	MET	CA-CB-CG	6.73	124.75	113.30
1	A	1004	LEU	CB-CG-CD1	5.62	120.55	111.00
1	B	1004	LEU	CB-CG-CD1	5.62	120.55	111.00
1	B	1396	PRO	CA-N-CD	-5.59	103.67	111.50
1	A	1396	PRO	CA-N-CD	-5.57	103.70	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4439	LEU	CA-CB-CG	5.23	127.32	115.30
1	A	4439	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	1004	LEU	CA-CB-CG	5.17	127.20	115.30
1	B	1004	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	1197	LEU	CA-CB-CG	5.15	127.15	115.30
1	B	1197	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	2372	LEU	CB-CG-CD1	5.12	119.70	111.00
1	B	2372	LEU	CB-CG-CD1	5.10	119.67	111.00
1	A	4305	GLU	CA-CB-CG	5.08	124.57	113.40
1	B	4428	MET	CG-SD-CE	-5.07	92.08	100.20
1	A	4428	MET	CG-SD-CE	-5.07	92.09	100.20
1	B	4305	GLU	CA-CB-CG	5.06	124.54	113.40
1	B	2344	LEU	CA-CB-CG	5.06	126.93	115.30
1	A	2344	LEU	CA-CB-CG	5.03	126.87	115.30

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

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	210	0
1	B	20950	0	19684	211	0
All	All	41900	0	39368	396	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.

All (396) 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
1:A:1349:GLU:O	1:A:1353:CYS:HB2	1.94	0.67
1:B:2375:GLY:HA2	1:B:2641:VAL:HA	1.76	0.67
1:B:1349:GLU:O	1:B:1353:CYS:HB2	1.94	0.66
1:A:1417:PRO:HG2	1:A:2001:ILE:HG12	1.78	0.65
1:B:1417:PRO:HG2	1:B:2001:ILE:HG12	1.78	0.65
1:A:2703:ARG:NH1	1:A:2706:CYS:SG	2.71	0.64
1:B:1298:MET:HG2	1:B:1336:LEU:HD21	1.80	0.64
1:B:2703:ARG:NH1	1:B:2706:CYS:SG	2.71	0.63
1:B:3353:MET:SD	1:B:3408:ARG:NH2	2.72	0.63
1:A:3353:MET:SD	1:A:3408:ARG:NH2	2.72	0.63
1:A:1298:MET:HG2	1:A:1336:LEU:HD21	1.80	0.62
1:B:1169:ASP:HA	1:B:2567:LEU:HD21	1.83	0.61
1:B:1789:ASP:HB2	1:B:1865:TYR:HB2	1.82	0.60
1:A:1169:ASP:HA	1:A:2567:LEU:HD21	1.83	0.60
1:B:3807:LYS:HE2	1:B:3847:PRO:HG3	1.83	0.60
1:A:4432:VAL:HG11	1:A:4470:GLN:HB2	1.84	0.60
1:A:3702:LEU:HD13	1:A:3774:LEU:HD22	1.83	0.60
1:A:3807:LYS:HE2	1:A:3847:PRO:HG3	1.83	0.60
1:A:4420:SER:N	1:A:4423:THR:HG1	2.00	0.60
1:A:1789:ASP:HB2	1:A:1865:TYR:HB2	1.82	0.60
1:A:1792:ILE:HB	1:A:1828:LEU:HB3	1.84	0.60
1:A:4198:THR:OG1	1:A:4309:CYS:SG	2.60	0.60
1:A:1443:CYS:O	1:A:1447:CYS:HB2	2.02	0.59
1:B:1341:SER:HB2	1:B:1391:ASN:HD22	1.67	0.59
1:B:4432:VAL:HG11	1:B:4470:GLN:HB2	1.84	0.59
1:B:3228:GLU:HB2	1:B:3265:CYS:HB3	1.84	0.59
1:B:4420:SER:N	1:B:4423:THR:HG1	2.00	0.59
1:B:2310:ALA:HB3	1:B:2313:ARG:HE	1.68	0.59
1:B:4198:THR:OG1	1:B:4309:CYS:SG	2.60	0.59
1:B:3702:LEU:HD13	1:B:3774:LEU:HD22	1.83	0.59
1:B:3206:LEU:HD21	1:B:3209:ILE:HD11	1.85	0.59
1:A:3228:GLU:HB2	1:A:3265:CYS:HB3	1.84	0.59
1:A:1341:SER:HB2	1:A:1391:ASN:HD22	1.67	0.58
1:A:2310:ALA:HB3	1:A:2313:ARG:HE	1.68	0.58
1:A:4234:ILE:HG23	1:A:4310:LEU:HD23	1.86	0.58
1:A:3206:LEU:HD21	1:A:3209:ILE:HD11	1.85	0.58
1:B:1443:CYS:O	1:B:1447:CYS:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4234:ILE:HG23	1:B:4310:LEU:HD23	1.86	0.58
1:B:4307:VAL:O	1:B:4311:LEU:HB3	2.04	0.58
1:B:1170:LEU:HD11	1:B:2551:GLN:HG2	1.86	0.58
1:B:1967:GLN:O	1:B:1971:ASN:ND2	2.37	0.58
1:A:1035:PRO:HD2	1:A:1038:LEU:HD12	1.86	0.58
1:A:1170:LEU:HD11	1:A:2551:GLN:HG2	1.86	0.58
1:B:1792:ILE:HB	1:B:1828:LEU:HB3	1.84	0.58
1:A:1967:GLN:O	1:A:1971:ASN:ND2	2.37	0.58
1:A:2308:THR:HG21	1:A:2352:ARG:HH21	1.69	0.57
1:B:4396:VAL:HG13	1:B:4483:LEU:HD13	1.87	0.57
1:A:2703:ARG:HE	1:B:3238:PRO:HB2	1.70	0.56
1:B:1035:PRO:HD2	1:B:1038:LEU:HD12	1.86	0.56
1:A:1534:LEU:HB3	1:A:1537:LEU:HD21	1.87	0.56
1:A:4307:VAL:O	1:A:4311:LEU:HB3	2.04	0.56
1:B:1345:GLY:H	1:B:1348:LYS:HD3	1.70	0.56
1:A:1017:THR:OG1	1:A:1068:GLU:OE2	2.23	0.56
1:A:1014:PHE:HA	1:A:1072:PRO:HD3	1.88	0.56
1:A:1190:GLY:HA3	1:A:1192:LYS:HE3	1.88	0.56
1:A:2809:ARG:O	1:B:2809:ARG:NH2	2.39	0.56
1:B:2370:LEU:HD22	1:B:2649:LEU:HD21	1.87	0.56
1:A:2809:ARG:NH2	1:B:2809:ARG:O	2.39	0.56
1:A:4396:VAL:HG13	1:A:4483:LEU:HD13	1.87	0.56
1:B:1014:PHE:HA	1:B:1072:PRO:HD3	1.88	0.56
1:B:1190:GLY:HA3	1:B:1192:LYS:HE3	1.88	0.55
1:A:2370:LEU:HD22	1:A:2649:LEU:HD21	1.87	0.55
1:B:2308:THR:HG21	1:B:2352:ARG:HH21	1.70	0.55
1:A:2185:ASN:HB2	1:A:2188:SER:HB3	1.88	0.55
1:A:4321:MET:SD	1:A:4322:SER:N	2.76	0.55
1:B:1017:THR:OG1	1:B:1068:GLU:OE2	2.23	0.55
1:B:3239:LEU:HD13	1:B:3255:LEU:HD21	1.89	0.55
1:B:4321:MET:SD	1:B:4322:SER:N	2.76	0.55
1:A:1008:GLU:OE2	1:A:1282:ARG:NH1	2.40	0.55
1:A:2101:ASP:OD1	1:A:2101:ASP:N	2.37	0.55
1:A:3238:PRO:HB2	1:B:2703:ARG:HE	1.70	0.55
1:A:1345:GLY:H	1:A:1348:LYS:HD3	1.70	0.55
1:B:1021:CYS:O	1:B:1056:GLN:NE2	2.40	0.55
1:B:1534:LEU:HB3	1:B:1537:LEU:HD21	1.87	0.55
1:B:2675:ASN:OD1	1:B:2781:ARG:NH1	2.40	0.55
1:B:1558:ARG:HA	1:B:1762:GLN:HA	1.89	0.55
1:A:1461:ARG:NH2	1:A:2002:GLN:O	2.39	0.55
1:A:2675:ASN:OD1	1:A:2781:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:GLU:OE2	1:B:1282:ARG:NH1	2.40	0.55
1:B:1461:ARG:NH2	1:B:2002:GLN:O	2.39	0.55
1:A:1461:ARG:NH2	1:A:2004:SER:O	2.40	0.54
1:A:1558:ARG:HA	1:A:1762:GLN:HA	1.89	0.54
1:A:1021:CYS:O	1:A:1056:GLN:NE2	2.40	0.54
1:A:2761:ASN:ND2	1:B:2865:SER:O	2.41	0.54
1:A:3239:LEU:HD13	1:A:3255:LEU:HD21	1.89	0.54
1:A:3412:LEU:HD21	1:B:1935:SER:HB2	1.90	0.54
1:A:4154:LEU:HD12	1:A:4155:PRO:HD2	1.90	0.54
1:B:1461:ARG:NH2	1:B:2004:SER:O	2.40	0.54
1:B:1084:PHE:HB2	1:B:1273:LEU:HD22	1.90	0.54
1:B:2185:ASN:HB2	1:B:2188:SER:HB3	1.88	0.54
1:B:3853:SER:HB2	1:B:3966:ALA:HB1	1.90	0.54
1:A:2755:THR:HB	1:A:2817:GLY:H	1.73	0.53
1:B:3345:LEU:HD12	1:B:3382:LEU:HD13	1.91	0.53
1:A:3621:LEU:HD23	1:A:3672:ILE:HG23	1.91	0.53
1:A:1935:SER:HB2	1:B:3412:LEU:HD21	1.91	0.53
1:A:1799:ALA:HB2	1:A:1849:ARG:HA	1.91	0.53
1:A:2865:SER:O	1:B:2761:ASN:ND2	2.41	0.53
1:A:3345:LEU:HD12	1:A:3382:LEU:HD13	1.91	0.53
1:A:4186:HIS:HB2	1:A:4189:GLN:HG2	1.90	0.53
1:B:1799:ALA:HB2	1:B:1849:ARG:HA	1.91	0.53
1:B:3621:LEU:HD23	1:B:3672:ILE:HG23	1.91	0.53
1:B:4186:HIS:HB2	1:B:4189:GLN:HG2	1.90	0.53
1:A:3797:LEU:O	1:A:3801:LEU:HB3	2.09	0.52
1:B:4154:LEU:HD12	1:B:4155:PRO:HD2	1.90	0.52
1:B:2755:THR:HB	1:B:2817:GLY:H	1.73	0.52
1:B:3797:LEU:O	1:B:3801:LEU:HB3	2.09	0.52
1:A:1084:PHE:HB2	1:A:1273:LEU:HD22	1.90	0.52
1:A:3400:LEU:HD13	1:B:2368:ARG:HG2	1.92	0.52
1:A:4435:TYR:HA	1:A:4438:ARG:HD2	1.92	0.52
1:A:2368:ARG:HG2	1:B:3400:LEU:HD13	1.92	0.52
1:A:3241:THR:OG1	1:B:2763:HIS:ND1	2.43	0.52
1:A:3853:SER:HB2	1:A:3966:ALA:HB1	1.90	0.52
1:B:3433:LYS:HG3	1:B:3502:LEU:HD21	1.92	0.52
1:A:2763:HIS:ND1	1:B:3241:THR:OG1	2.43	0.52
1:B:4435:TYR:HA	1:B:4438:ARG:HD2	1.92	0.52
1:A:3235:ASN:ND2	1:B:2670:PHE:O	2.39	0.52
1:B:3798:PHE:O	1:B:3802:MET:CB	2.57	0.52
1:A:2767:VAL:HG13	1:A:2818:PRO:HB3	1.92	0.51
1:B:1510:ASP:OD1	1:B:1510:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3622:VAL:HG23	1:B:3697:LEU:HD22	1.92	0.51
1:A:1030:GLN:HE22	1:A:1047:ALA:HB3	1.76	0.51
1:B:2703:ARG:HH12	1:B:2771:ALA:HB2	1.75	0.51
1:A:1510:ASP:N	1:A:1510:ASP:OD1	2.43	0.51
1:B:3322:HIS:O	1:B:3326:HIS:HB2	2.11	0.51
1:B:2767:VAL:HG13	1:B:2818:PRO:HB3	1.92	0.51
1:A:2049:PHE:HE1	1:A:2085:VAL:HG11	1.76	0.51
1:A:2674:ALA:O	1:A:2717:ASN:ND2	2.41	0.51
1:A:2703:ARG:HH12	1:A:2771:ALA:HB2	1.75	0.51
1:A:3622:VAL:HG23	1:A:3697:LEU:HD22	1.92	0.51
1:A:3415:ASP:HA	1:A:3418:ILE:HD12	1.93	0.51
1:A:3433:LYS:HG3	1:A:3502:LEU:HD21	1.92	0.51
1:B:1030:GLN:HE22	1:B:1047:ALA:HB3	1.75	0.51
1:A:3322:HIS:O	1:A:3326:HIS:HB2	2.11	0.50
1:B:3415:ASP:HA	1:B:3418:ILE:HD12	1.93	0.50
1:A:3401:ASN:OD1	1:B:2368:ARG:NH2	2.45	0.50
1:B:2101:ASP:OD1	1:B:2101:ASP:N	2.37	0.50
1:A:1309:LEU:HD21	1:A:1357:LYS:HB3	1.94	0.50
1:B:2125:LEU:HB3	1:B:2317:VAL:HG21	1.93	0.50
1:B:3389:ASN:HA	1:B:3410:ASN:HD21	1.76	0.50
1:A:1454:VAL:HG13	1:A:2009:LEU:HD22	1.94	0.50
1:B:4062:ALA:HB1	1:B:4158:ALA:HB1	1.94	0.50
1:A:3604:GLN:NE2	1:A:3678:GLU:O	2.45	0.50
1:A:4226:LEU:HD11	1:A:4347:LEU:HD23	1.94	0.50
1:B:1296:CYS:O	1:B:1300:GLN:HB2	2.12	0.50
1:A:3389:ASN:HA	1:A:3410:ASN:HD21	1.76	0.50
1:B:2049:PHE:HE1	1:B:2085:VAL:HG11	1.76	0.50
1:B:1790:VAL:HB	1:B:1830:LEU:HB2	1.93	0.49
1:A:1296:CYS:O	1:A:1300:GLN:HB2	2.12	0.49
1:B:4226:LEU:HD11	1:B:4347:LEU:HD23	1.94	0.49
1:A:2701:LEU:HD12	1:B:2862:LYS:HE2	1.95	0.49
1:A:4231:LEU:HA	1:A:4234:ILE:HD12	1.95	0.49
1:A:1010:LEU:HD13	1:A:1280:ILE:HG22	1.94	0.49
1:B:3210:HIS:HB2	1:B:3283:LYS:HB2	1.95	0.49
1:A:2125:LEU:HB3	1:A:2317:VAL:HG21	1.93	0.49
1:A:2368:ARG:NH2	1:B:3401:ASN:OD1	2.45	0.49
1:A:2861:ASP:OD1	1:A:2861:ASP:N	2.45	0.49
1:B:1309:LEU:HD21	1:B:1357:LYS:HB3	1.94	0.49
1:B:1466:GLU:HA	1:B:1469:LEU:HD12	1.94	0.49
1:B:2051:HIS:O	1:B:2055:SER:OG	2.31	0.49
1:B:2107:LEU:HA	1:B:2110:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3210:HIS:HB2	1:A:3283:LYS:HB2	1.95	0.49
1:B:1010:LEU:HD13	1:B:1280:ILE:HG22	1.94	0.49
1:A:2862:LYS:HE2	1:B:2701:LEU:HD12	1.95	0.49
1:A:3848:VAL:HA	1:A:3970:LEU:HB2	1.95	0.49
1:A:2563:GLN:OE1	1:A:2564:GLN:NE2	2.46	0.49
1:A:4062:ALA:HB1	1:A:4158:ALA:HB1	1.94	0.49
1:A:2739:VAL:HG13	1:A:2797:LEU:HD22	1.94	0.49
1:B:2861:ASP:OD1	1:B:2861:ASP:N	2.45	0.49
1:B:4231:LEU:HA	1:B:4234:ILE:HD12	1.94	0.49
1:A:3346:GLN:HB3	1:A:3405:LEU:HG	1.95	0.48
1:B:2129:ASP:O	1:B:2320:LYS:NZ	2.42	0.48
1:B:3515:SER:O	1:B:3525:LYS:NZ	2.44	0.48
1:A:1790:VAL:HB	1:A:1830:LEU:HB2	1.93	0.48
1:B:4347:LEU:HA	1:B:4350:LEU:HG	1.96	0.48
1:A:1466:GLU:HA	1:A:1469:LEU:HD12	1.94	0.48
1:A:1471:THR:HG21	1:A:2097:ILE:HG22	1.95	0.48
1:A:2051:HIS:O	1:A:2055:SER:OG	2.31	0.48
1:B:2563:GLN:OE1	1:B:2564:GLN:NE2	2.46	0.48
1:A:1909:ASP:OD2	1:A:1913:ARG:NH1	2.47	0.48
1:B:1454:VAL:HG13	1:B:2009:LEU:HD22	1.94	0.48
1:B:1471:THR:HG21	1:B:2097:ILE:HG22	1.95	0.48
1:B:1909:ASP:OD2	1:B:1913:ARG:NH1	2.47	0.48
1:B:2739:VAL:HG13	1:B:2797:LEU:HD22	1.94	0.48
1:B:3814:SER:HB2	1:B:3993:VAL:HB	1.95	0.48
1:A:3798:PHE:O	1:A:3802:MET:CB	2.57	0.48
1:A:1383:ARG:NH1	1:A:2566:GLU:OE1	2.47	0.48
1:A:3060:THR:O	1:B:2380:ARG:NH1	2.46	0.48
1:B:1383:ARG:NH1	1:B:2566:GLU:OE1	2.47	0.47
1:B:3346:GLN:HB3	1:B:3405:LEU:HG	1.95	0.47
1:B:1551:SER:O	1:B:1555:ARG:NH1	2.48	0.47
1:B:3604:GLN:NE2	1:B:3678:GLU:O	2.45	0.47
1:A:2380:ARG:NH1	1:B:3060:THR:O	2.47	0.47
1:B:2129:ASP:HB3	1:B:2317:VAL:HG22	1.97	0.47
1:A:3174:PRO:HG2	1:A:3280:SER:HB3	1.95	0.47
1:B:1786:LEU:HD21	1:B:1874:GLU:HB3	1.97	0.47
1:A:3218:LEU:HB2	1:B:3218:LEU:HB2	1.95	0.47
1:B:1058:ASP:OD2	1:B:1058:ASP:N	2.48	0.47
1:A:1551:SER:O	1:A:1555:ARG:NH1	2.47	0.47
1:A:1786:LEU:HD21	1:A:1874:GLU:HB3	1.97	0.47
1:A:2107:LEU:HA	1:A:2110:ILE:HG22	1.94	0.47
1:B:3812:LEU:HD22	1:B:3859:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3812:LEU:HD22	1:A:3859:VAL:HG11	1.96	0.47
1:A:4347:LEU:HA	1:A:4350:LEU:HG	1.96	0.47
1:B:3110:SER:OG	1:B:3111:MET:N	2.46	0.47
1:B:3848:VAL:HA	1:B:3970:LEU:HB2	1.95	0.47
1:A:3760:HIS:HD2	1:A:3985:GLY:HA3	1.79	0.47
1:B:3174:PRO:HG2	1:B:3280:SER:HB3	1.95	0.47
1:A:2670:PHE:O	1:B:3235:ASN:ND2	2.39	0.47
1:A:3520:CYS:HA	1:A:3525:LYS:HD3	1.96	0.47
1:B:3520:CYS:HA	1:B:3525:LYS:HD3	1.96	0.47
1:B:3775:PHE:O	1:B:4073:ARG:NH1	2.47	0.47
1:A:2842:ILE:HG23	1:A:2915:LEU:HD13	1.97	0.46
1:A:3775:PHE:O	1:A:4073:ARG:NH1	2.47	0.46
1:A:3814:SER:HB2	1:A:3993:VAL:HB	1.96	0.46
1:A:1911:GLN:HG3	1:A:1970:LEU:HD11	1.98	0.46
1:B:1096:ILE:HA	1:B:1202:ALA:HA	1.98	0.46
1:B:3760:HIS:HD2	1:B:3985:GLY:HA3	1.79	0.46
1:A:2129:ASP:HB3	1:A:2317:VAL:HG22	1.97	0.46
1:A:2553:LEU:HD23	1:A:2567:LEU:HD13	1.97	0.46
1:B:3629:CYS:HA	1:B:3704:LEU:HD13	1.98	0.46
1:B:2837:VAL:HG13	1:B:2842:ILE:HD11	1.97	0.46
1:B:1081:ASP:HB2	1:B:1279:THR:HB	1.98	0.46
1:A:2837:VAL:HG13	1:A:2842:ILE:HD11	1.97	0.46
1:B:1911:GLN:HG3	1:B:1970:LEU:HD11	1.98	0.46
1:B:2842:ILE:HG23	1:B:2915:LEU:HD13	1.97	0.46
1:B:4172:LEU:HA	1:B:4175:VAL:HG12	1.98	0.46
1:B:1045:ASP:HA	1:B:1048:GLN:HG3	1.98	0.46
1:A:1045:ASP:HA	1:A:1048:GLN:HG3	1.98	0.45
1:A:1046:ALA:HA	1:A:1049:HIS:CD2	2.51	0.45
1:A:4172:LEU:HA	1:A:4175:VAL:HG12	1.98	0.45
1:B:1076:MET:SD	1:B:1076:MET:N	2.87	0.45
1:A:2129:ASP:O	1:A:2320:LYS:NZ	2.42	0.45
1:A:3802:MET:HG3	1:A:4058:LEU:HD13	1.98	0.45
1:A:1096:ILE:HA	1:A:1202:ALA:HA	1.98	0.45
1:B:1153:HIS:HB3	1:B:1156:ASP:HB2	1.98	0.45
1:B:4428:MET:HB2	1:B:4428:MET:HE2	1.83	0.45
1:A:1081:ASP:HB2	1:A:1279:THR:HB	1.98	0.45
1:A:1014:PHE:HE1	1:A:1069:LEU:HD22	1.81	0.45
1:B:1046:ALA:HA	1:B:1049:HIS:CD2	2.51	0.45
1:A:3110:SER:OG	1:A:3111:MET:N	2.46	0.45
1:A:3222:PRO:HG3	1:A:3268:LEU:HD23	1.99	0.45
1:B:1534:LEU:HD23	1:B:1791:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3515:SER:O	1:A:3525:LYS:NZ	2.44	0.45
1:B:68:VAL:O	1:B:77:LEU:N	2.45	0.45
1:B:1095:GLN:O	1:B:1203:VAL:N	2.50	0.45
1:A:1153:HIS:HB3	1:A:1156:ASP:HB2	1.98	0.45
1:A:1534:LEU:HD23	1:A:1791:LEU:HD13	1.98	0.45
1:B:2553:LEU:HD23	1:B:2567:LEU:HD13	1.97	0.45
1:A:1095:GLN:O	1:A:1203:VAL:N	2.49	0.45
1:A:3629:CYS:HA	1:A:3704:LEU:HD13	1.98	0.45
1:B:2674:ALA:O	1:B:2717:ASN:ND2	2.41	0.45
1:B:3802:MET:HG3	1:B:4058:LEU:HD13	1.98	0.45
1:A:3187:PHE:HE2	1:A:3277:LEU:HB2	1.83	0.44
1:A:3485:ALA:HB1	1:A:3836:GLY:HA2	2.00	0.44
1:B:2557:LEU:HD21	1:B:2566:GLU:HB3	1.99	0.44
1:B:4307:VAL:O	1:B:4311:LEU:CB	2.65	0.44
1:B:4399:LEU:HB2	1:B:4421:VAL:HB	1.99	0.44
1:A:1779:LEU:HD21	1:A:1861:LEU:HD11	2.00	0.44
1:A:4307:VAL:O	1:A:4311:LEU:CB	2.65	0.44
1:B:3485:ALA:HB1	1:B:3836:GLY:HA2	1.99	0.44
1:B:3844:LEU:HD13	1:B:3858:ARG:HD2	2.00	0.44
1:A:2322:VAL:HG21	1:A:2360:ILE:HG12	2.00	0.44
1:B:3222:PRO:HG3	1:B:3268:LEU:HD23	1.99	0.44
1:A:1023:VAL:HG13	1:A:1056:GLN:HE22	1.82	0.44
1:A:3844:LEU:HD13	1:A:3858:ARG:HD2	1.99	0.44
1:B:1014:PHE:HE1	1:B:1069:LEU:HD22	1.81	0.44
1:B:1101:LEU:HB2	1:B:1197:LEU:HB2	1.99	0.44
1:A:3147:HIS:HE1	1:A:3293:THR:O	2.01	0.44
1:B:1779:LEU:HD21	1:B:1861:LEU:HD11	2.00	0.44
1:B:4059:GLN:HA	1:B:4162:LEU:HD21	1.99	0.44
1:A:4059:GLN:HA	1:A:4162:LEU:HD21	1.99	0.44
1:A:4399:LEU:HB2	1:A:4421:VAL:HB	1.99	0.44
1:B:1023:VAL:HG13	1:B:1056:GLN:HE22	1.82	0.44
1:B:3187:PHE:HE2	1:B:3277:LEU:HB2	1.83	0.44
1:B:4205:ARG:HG3	1:B:4312:GLN:HB3	1.99	0.44
1:A:2318:VAL:HG13	1:A:2344:LEU:HG	2.00	0.44
1:A:2557:LEU:HD21	1:A:2566:GLU:HB3	1.99	0.43
1:A:2632:LEU:HD22	1:A:2641:VAL:HG11	2.00	0.43
1:B:2082:LEU:HD12	1:B:2082:LEU:HA	1.84	0.43
1:A:1101:LEU:HB2	1:A:1197:LEU:HB2	1.99	0.43
1:A:1472:ARG:HD2	1:A:1930:LEU:HD13	2.01	0.43
1:A:4205:ARG:HG3	1:A:4312:GLN:HB3	1.99	0.43
1:B:988:LEU:HD12	1:B:997:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:ILE:HD13	1:A:1272:LEU:HD21	2.00	0.43
1:B:2322:VAL:HG21	1:B:2360:ILE:HG12	2.00	0.43
1:A:2783:GLN:HG3	1:A:2832:GLN:HE22	1.84	0.43
1:A:2798:LEU:HD13	1:A:2829:THR:HG22	2.00	0.43
1:B:2798:LEU:HD13	1:B:2829:THR:HG22	2.01	0.43
1:B:3352:LEU:HD11	1:B:3416:SER:HB3	2.00	0.43
1:A:2853:VAL:HG11	1:A:2909:LEU:HD21	2.01	0.43
1:B:1515:LEU:HD11	1:B:2062:LEU:HD21	2.00	0.43
1:B:1090:ILE:HD13	1:B:1272:LEU:HD21	2.00	0.43
1:B:1472:ARG:HD2	1:B:1930:LEU:HD13	2.01	0.43
1:B:2713:THR:O	1:B:2716:THR:OG1	2.31	0.43
1:B:2783:GLN:HG3	1:B:2832:GLN:HE22	1.84	0.43
1:A:68:VAL:O	1:A:77:LEU:N	2.45	0.43
1:A:3846:LEU:HD13	1:A:3850:THR:HG21	2.01	0.43
1:A:3051:TYR:CD1	1:A:3052:MET:HG2	2.54	0.42
1:B:2632:LEU:HD22	1:B:2641:VAL:HG11	2.00	0.42
1:A:1803:ILE:HG22	1:A:1818:VAL:HG12	2.01	0.42
1:B:1298:MET:HE3	1:B:1298:MET:HB2	1.96	0.42
1:B:3147:HIS:HE1	1:B:3293:THR:O	2.01	0.42
1:B:3552:ILE:HG21	1:B:3617:LEU:HD12	2.01	0.42
1:A:1194:ARG:HA	1:A:1194:ARG:HD3	1.88	0.42
1:A:3352:LEU:HD11	1:A:3416:SER:HB3	2.00	0.42
1:B:140:LEU:O	1:B:194:VAL:N	2.44	0.42
1:B:2318:VAL:HG13	1:B:2344:LEU:HG	2.00	0.42
1:B:3051:TYR:CD1	1:B:3052:MET:HG2	2.54	0.42
1:B:2021:LEU:HD13	1:B:2584:LEU:HD21	2.01	0.42
1:B:2311:HIS:HE1	1:B:2355:ILE:HG23	1.84	0.42
1:A:1487:LEU:HD22	1:A:1968:LEU:HD11	2.02	0.42
1:A:2135:LEU:HD12	1:A:2135:LEU:HA	1.91	0.42
1:A:1515:LEU:HD11	1:A:2062:LEU:HD21	2.00	0.42
1:B:3146:ILE:HG13	1:B:3285:LEU:HD23	2.02	0.42
1:A:140:LEU:O	1:A:194:VAL:N	2.43	0.42
1:A:3146:ILE:HG13	1:A:3285:LEU:HD23	2.02	0.42
1:A:3552:ILE:HG21	1:A:3617:LEU:HD12	2.01	0.42
1:A:1083:LYS:HB2	1:A:1277:SER:HB2	2.02	0.42
1:A:1158:LEU:HD12	1:A:1184:LEU:HA	2.02	0.42
1:A:2034:ALA:O	1:A:2038:SER:OG	2.32	0.42
1:B:1487:LEU:HD22	1:B:1968:LEU:HD11	2.02	0.42
1:B:1803:ILE:HG22	1:B:1818:VAL:HG12	2.01	0.42
1:B:3701:LEU:HD13	1:B:3749:THR:HG23	2.01	0.42
1:A:988:LEU:HD12	1:A:997:ILE:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:PHE:HE2	1:A:1416:LEU:HA	1.85	0.42
1:B:1542:PRO:HB2	1:B:1759:PRO:HD3	2.02	0.42
1:B:3846:LEU:HD13	1:B:3850:THR:HG21	2.01	0.42
1:A:2311:HIS:HE1	1:A:2355:ILE:HG23	1.84	0.41
1:A:1415:PHE:HB3	1:A:1991:LEU:HD23	2.02	0.41
1:A:2021:LEU:HD13	1:A:2584:LEU:HD21	2.02	0.41
1:A:4211:THR:HG21	1:A:4221:LEU:HD23	2.02	0.41
1:A:4428:MET:HE2	1:A:4428:MET:HB2	1.84	0.41
1:B:135:VAL:HA	1:B:199:PRO:HA	2.02	0.41
1:B:1371:PHE:HE2	1:B:1416:LEU:HA	1.85	0.41
1:B:1433:ASN:HA	1:B:1436:LYS:HZ3	1.84	0.41
1:B:2795:SER:HB3	1:B:2834:PHE:HD1	1.85	0.41
1:B:4211:THR:HG21	1:B:4221:LEU:HD23	2.02	0.41
1:A:1542:PRO:HB2	1:A:1759:PRO:HD3	2.02	0.41
1:A:2082:LEU:HD12	1:A:2082:LEU:HA	1.84	0.41
1:A:2795:SER:HB3	1:A:2834:PHE:HD1	1.84	0.41
1:B:2853:VAL:HG11	1:B:2909:LEU:HD21	2.01	0.41
1:A:135:VAL:HA	1:A:199:PRO:HA	2.02	0.41
1:A:1943:LEU:HG	1:B:3114:THR:HG22	2.03	0.41
1:A:2166:ASP:OD2	1:A:2342:LYS:NZ	2.44	0.41
1:A:3318:ARG:HG2	1:A:3359:MET:SD	2.61	0.41
1:B:1083:LYS:HB2	1:B:1277:SER:HB2	2.02	0.41
1:B:2554:ASP:N	1:B:2554:ASP:OD1	2.53	0.41
1:A:2151:ILE:HD13	1:A:2151:ILE:HA	1.91	0.41
1:A:4167:HIS:HB3	1:A:4199:LEU:HD21	2.02	0.41
1:A:4377:PRO:HA	1:A:4380:ARG:HE	1.86	0.41
1:B:1443:CYS:O	1:B:1447:CYS:CB	2.69	0.41
1:B:3797:LEU:O	1:B:3801:LEU:CB	2.68	0.41
1:B:1148:PRO:HA	1:B:1151:GLU:HB3	2.02	0.41
1:B:4432:VAL:HG13	1:B:4466:VAL:HG12	2.03	0.41
1:B:4436:THR:HA	1:B:4439:LEU:HG	2.03	0.41
1:A:998:LEU:HB3	1:A:1328:LEU:HB3	2.02	0.41
1:A:1029:GLN:HG3	1:A:1033:ARG:HE	1.86	0.41
1:A:1916:LEU:HD23	1:B:3800:GLN:HE21	1.85	0.41
1:A:4238:LEU:HD13	1:A:4356:LEU:HD13	2.03	0.41
1:B:2655:LEU:HD23	1:B:2655:LEU:HA	1.93	0.41
1:B:2826:LEU:HD23	1:B:2826:LEU:HA	1.91	0.41
1:B:3445:ASP:HB3	1:B:3472:LEU:HD13	2.03	0.41
1:A:1011:THR:O	1:A:1049:HIS:ND1	2.54	0.41
1:A:2036:LEU:HD23	1:A:2071:LEU:HD13	2.03	0.41
1:A:3330:LEU:O	1:A:3334:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3701:LEU:HD13	1:A:3749:THR:HG23	2.01	0.41
1:B:998:LEU:HB3	1:B:1328:LEU:HB3	2.02	0.41
1:A:4357:ILE:HA	1:A:4360:MET:HG3	2.03	0.41
1:A:1148:PRO:HA	1:A:1151:GLU:HB3	2.02	0.40
1:A:3800:GLN:HE21	1:B:1916:LEU:HD23	1.85	0.40
1:A:1511:LEU:HD12	1:A:2105:MET:HB3	2.04	0.40
1:A:2554:ASP:OD1	1:A:2554:ASP:N	2.53	0.40
1:A:2702:LEU:HG	1:A:2703:ARG:NH1	2.37	0.40
1:A:3797:LEU:O	1:A:3801:LEU:CB	2.68	0.40
1:B:1014:PHE:CE1	1:B:1069:LEU:HD22	2.56	0.40
1:B:1415:PHE:HB3	1:B:1991:LEU:HD23	2.02	0.40
1:B:2702:LEU:HG	1:B:2703:ARG:NH1	2.37	0.40
1:A:1380:LYS:HE2	1:A:1834:ILE:HG23	2.03	0.40
1:A:3114:THR:HG22	1:B:1943:LEU:HG	2.03	0.40
1:A:3599:LEU:HD23	1:A:3599:LEU:HA	1.98	0.40
1:A:3807:LYS:HA	1:A:3847:PRO:HA	2.03	0.40
1:B:1194:ARG:HA	1:B:1194:ARG:HD3	1.88	0.40
1:B:1380:LYS:HE2	1:B:1834:ILE:HG23	2.03	0.40
1:B:3613:LEU:HD23	1:B:3613:LEU:HA	1.95	0.40
1:A:4436:THR:HA	1:A:4439:LEU:HG	2.03	0.40
1:B:1158:LEU:HD12	1:B:1184:LEU:HA	2.02	0.40
1:B:1357:LYS:HA	1:B:1360:LYS:HD2	2.03	0.40
1:B:2651:LEU:HD21	1:B:2711:SER:HA	2.04	0.40
1:B:3318:ARG:HG2	1:B:3359:MET:SD	2.60	0.40
1:B:1043:HIS:CE1	1:B:1815:ARG:HA	2.57	0.40
1:B:2373:LEU:HD23	1:B:2373:LEU:HA	1.96	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 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%)	2043 (100%)	3 (0%)	92	97
1	B	2046/4236 (48%)	2043 (100%)	3 (0%)	92	97
All	All	4092/8472 (48%)	4086 (100%)	6 (0%)	92	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1775	ARG
1	A	2313	ARG
1	A	4429	LYS
1	B	1775	ARG
1	B	2313	ARG
1	B	4429	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1056	GLN
1	A	2311	HIS
1	A	2656	ASN
1	A	3147	HIS
1	B	1056	GLN
1	B	2311	HIS
1	B	2656	ASN

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Mol	Chain	Res	Type
1	B	3147	HIS

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.