



Full wwPDB EM Validation 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 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 : 4-5-2 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

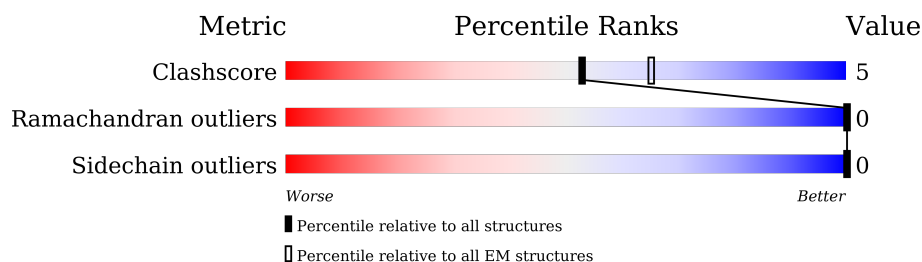
1 Overall quality at a glance

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	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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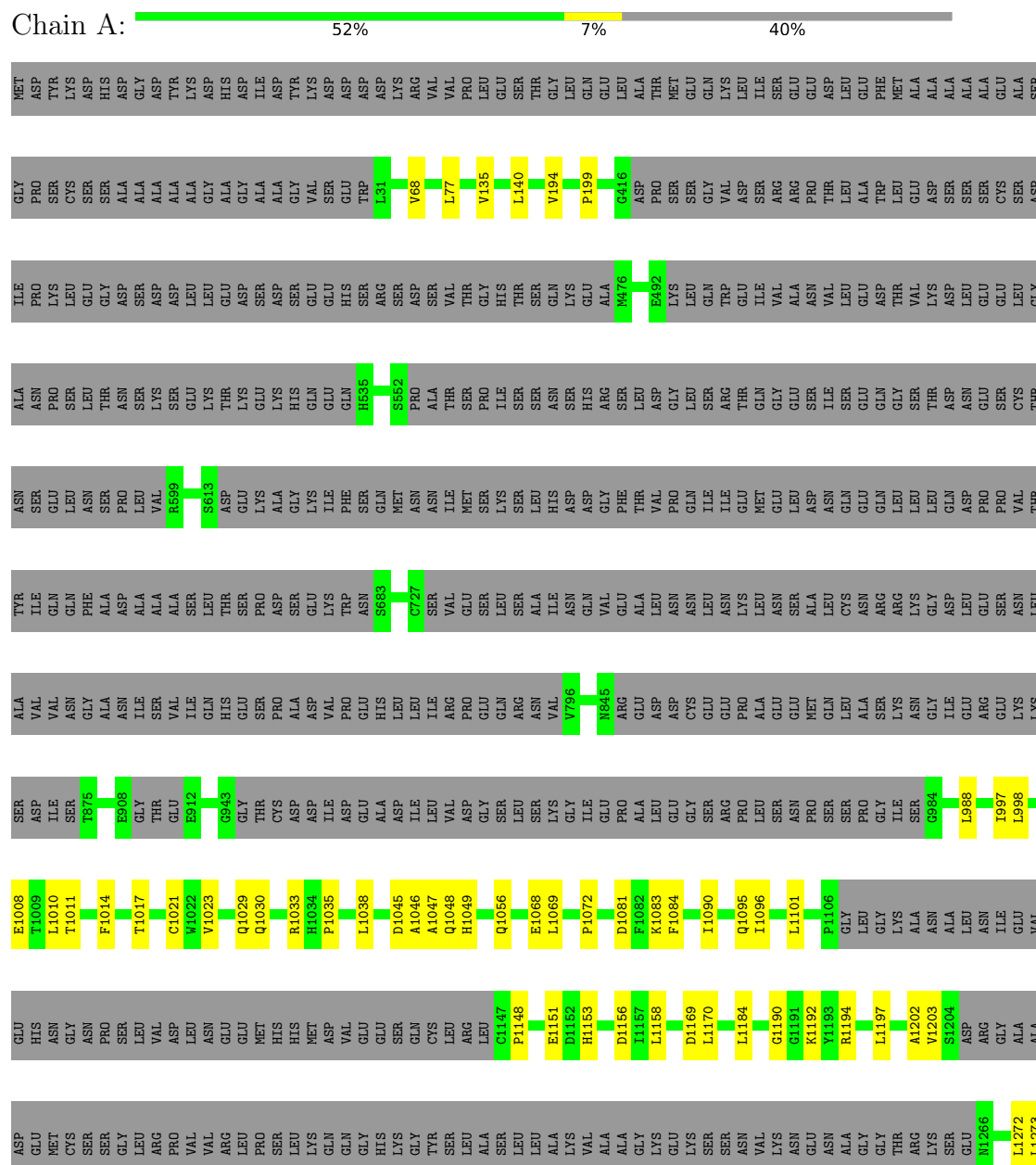
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	PHE	-	expression tag	UNP O88738
B	178	ILE	THR	conflict	UNP O88738
B	690	THR	ALA	conflict	UNP O88738
B	2079	ARG	GLY	conflict	UNP O88738
B	2418	GLY	CYS	conflict	UNP O88738
B	2959	ILE	THR	conflict	UNP 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



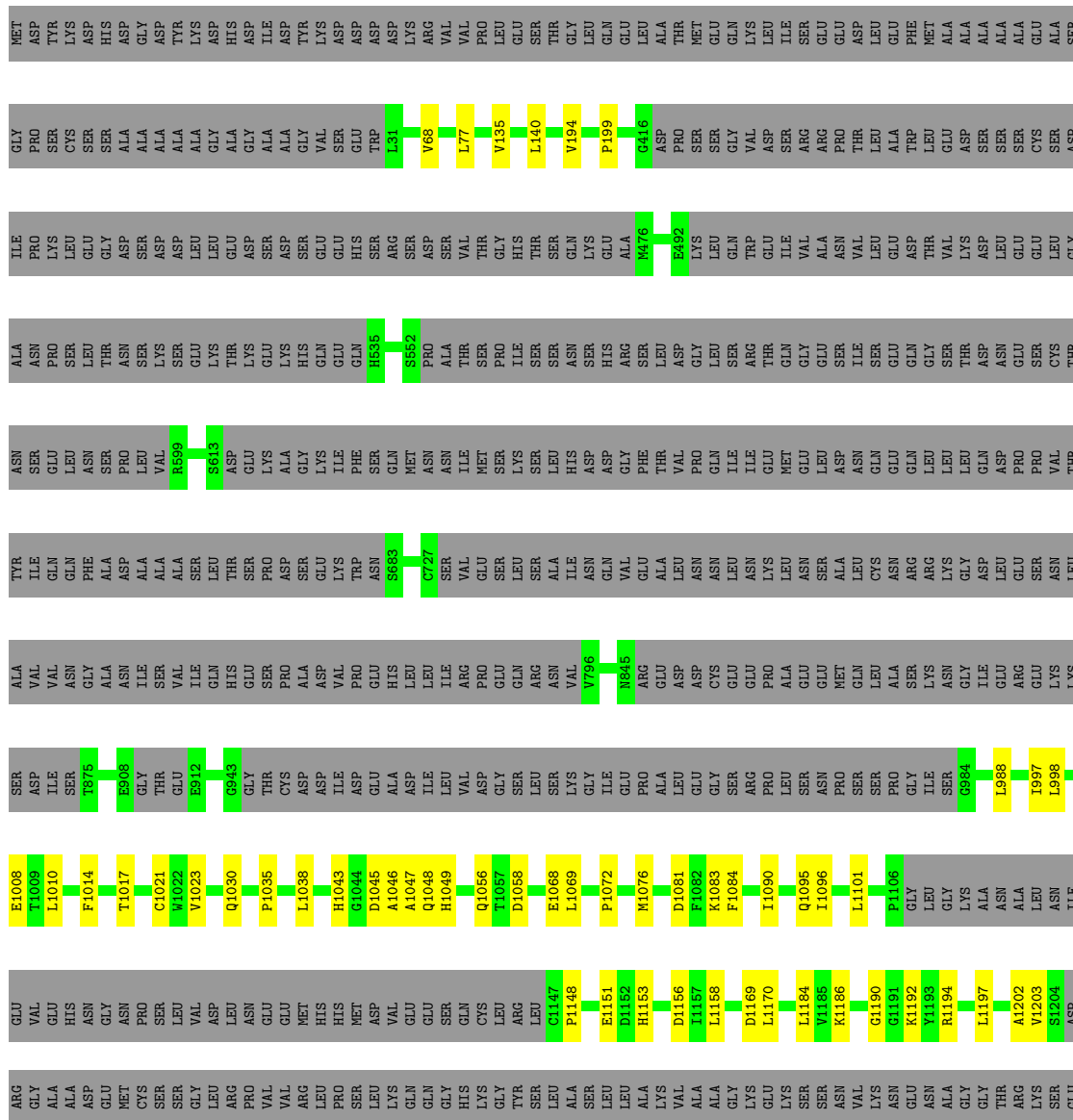


WORLDWIDE
PDB
PROTEIN DATA BANK

CYS	PRO	GLU	GLY	LEU	ASP	ASP	ILE	GLU	ASP	ALA	SER	PRO	VAL	CYS	ARG	ALA	THR	ALA	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
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 1: Isoform 2 of Baculoviral IAP repeat-containing protein 6

Chain B:  52% 8% 40%



LYS	VAL	S2711	GLN	TRP	LEU	R2352	GLN	ARG	L2062	HIS	SER	PRO	GLN	R1447
VAL	SER	L2712	SER	GLY	THR	R2352	ALA	SER	L2062	ASP	ARG	ASP	GLU	SER
SER	THR	T2713	PRO	ALA	HIS	L2355	LEU	SER	L2062	PRO	MET	LYS	LYS	VAL
GLY	THR	T2716	THR	ASP	GLY	I2355	LEU	LYS	L2062	LEU	ASN	ASN	GLN	GLN
GLY	THR	N2717	GLY	TYR	ILE	I2360	LYS	GLY	V2085	PRO	PRO	PRO	GLN	ALA
ASP	ASP	N2721	ASP	THR	GLY	R2368	ALA	SER	I2097	GLY	GLY	THR	LEU	SER
GLY	SER	SER	SER	TYR	THR	I2368	THR	SER	D2101	GLY	SER	THR	LEU	THR
SER	SER	GLY	LEU	ASN	PRO	I2370	SER	LEU	D2101	GLY	GLY	LYS	THR	PHE
SER	LEU	GLY	LEU	ASN	PRO	L2373	HIS	ARG	L2107	ALA	ALA	THR	GLN	VAL
ALA	ASN	SER	GLY	PRO	SER	V2374	PHE	TYR	L2107	LEU	LEU	THR	GLN	SER
LEU	LEU	SER	LEU	ILE	LEU	G2375	ASP	SER	I2110	ALA	ILE	LEU	LYS	PHE
GLN	GLN	GLY	ILE	GLY	GLU	R2380	LEU	ARG	L2125	D1909	SER	PHE	ALA	GLY
ALA	ALA	ILE	ILE	LEU	LYS	L2407	ILE	ILE	L2125	HIS	MET	VAL	VAL	GLY
CYS	ALA	Q2731	SER	GLY	ASP	ALA	ARG	LYS	D2129	Q1911	PRO	PRO	ALA	S1483
PHE	ASN	V2739	ASN	PRO	ILE	PRO	ARG	GLN	P2137	C1912	PRO	LEU	ALA	TRP
GLY	GLY	T2755	SER	VAL	ASP	VAL	THR	LEU	GLU	R1913	LEU	THR	VAL	LYS
LEU	GLN	T2761	LEU	GLY	LEU	ALA	ALA	VAL	LEU	M1915	PRO	GLY	GLY	VAL
ALA	MET	N2762	LEU	LYS	GLU	ALA	GLU	HIS	SER	L1916	PRO	GLN	LEU	TYR
ASN	ILE	H2763	PRO	ASN	LEU	ALA	TRP	LYS	MET	L1924	GLY	THR	SER	SER
LEU	ILE	Q2618	SER	GLY	GLN	MET	ARG	GLN	HIS	L1324	ALA	ALA	SER	SER
LEU	ASN	L2632	ASN	VAL	ASP	GLU	ARG	GLN	ARG	S1927	VAL	THR	THR	THR
ILE	ASN	V2641	GLN	GLY	LEU	GLY	THR	ASN	G2147	L1930	VAL	ALA	GLY	VAL
GLY	GLY	L2649	ASN	GLY	LEU	GLY	SER	LEU	M2153	L1935	VAL	ALA	GLY	VAL
ASN	GLY	Q2650	SER	ASN	ILE	GLY	VAL	LEU	ASP	Q1967	ILE	ALA	ALA	GLN
PRO	GLY	L2651	THR	GLN	ASP	VAL	THR	GLY	M2159	L1968	ALA	ALA	ALA	GLY
GLY	ASN	L2655	VAL	VAL	VAL	THR	GLY	LEU	GLY	L1970	ASN	GLN	ALA	ASN
GLY	GLY	S2658	SER	SER	ILE	THR	GLU	LEU	ASP	N1971	LEU	LEU	ALA	GLY
SER	SER	V2547	SER	VAL	ASP	THR	GLY	VAL	ASP	L1991	PHE	ALA	ALA	ASN
SER	GLY	Q2551	SER	GLY	ILE	ASP	SER	GLY	GLY	L2001	GLY	ALA	ALA	GLY
GLY	ASN	L2552	GLY	ASN	LEU	GLY	PRO	GLN	ALA	Q2002	PRO	ALA	ALA	ARG
LYS	ASN	L2553	LYS	LYS	GLY	ASP	GLY	MET	ALA	L2009	SER	PRO	ALA	VAL
GLY	GLY	D2554	ILE	ASP	ASP	ASP	ILE	GLY	LYS	L2009	VAL	ASN	ALA	VAL
ASN	ASN	L2557	PRO	PRO	ASP	SER	PRO	LYS	PRO	T2003	ASN	ASN	GLY	GLY
GLY	GLY	E2562	ALA	ALA	LEU	LEU	P2306	LYS	LEU	S2004	LEU	ALA	ALA	SER
ASP	ASP	Q2563	LYS	ALA	GLN	GLN	T2307	ILE	ASN	L2021	ALA	ALA	ALA	ALA
THR	THR	Q2564	VAL	SER	SER	SER	T2308	GLN	G2184	L2034	ALA	ALA	ALA	GLY
THR	THR	Q2565	PHE	PRO	LYS	ALA	L2309	ASN	N2185	A2034	VAL	ASN	ALA	GLY
ASN	ASN	E2566	LYS	ALA	LYS	ALA	H2311	LYS	S2188	L2034	ASN	ALA	ALA	THR
THR	THR	L2567	PRO	GLN	ILE	LEU	R2313	SER	N2193	S2038	LEU	ALA	ALA	GLY
ASP	ASP	L2584	ILE	LEU	SER	LEU	R2313	THR	LEU	L2049	GLY	GLN	ALA	GLY
THR	THR	Q2588	THR	GLY	SER	GLY	V2317	TYR	HIS	F2049	ASN	GLY	GLN	GLY
THR	THR	PRO	TRP	THR	THR	ILE	V2318	LYS	THR	K2050	LEU	LYS	GLY	PHE
THR	THR	PHE	TYR	THR	THR	ASP	V2322	LEU	GLN	H2051	LYS	ASN	GLY	PHE
SER	SER	SER	TYR	THR	THR	GLY	V2344	VAL	ASN	L2055	LEU	SER	GLY	ILE
						PRO	L2344	GLY	ASN	S2055	MET	LYS	LEU	LEU



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

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

5.1 Standard geometry

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.

All (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
1	B	4305	GLU	CA-CB-CG	5.22	124.54	114.10
1	A	4162	LEU	CB-CG-CD2	-5.06	95.51	110.70
1	B	4162	LEU	CB-CG-CD2	-5.05	95.53	110.70
1	A	2638	VAL	N-CA-CB	-5.02	106.51	112.39

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.

All (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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:4420:SER:N	1:B:4423:THR:HG1	2.04	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:A:4420:SER:N	1:A:4423:THR:HG1	2.04	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:3550:MET:HE2	1:A:3599:LEU:HG	1.92	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3550:MET:HE2	1:B:3599:LEU:HG	1.92	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:1924:LEU:O	1:A:1927:SER:OG	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1327:SER:HG	1:B:1380:LYS:HZ2	1.59	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:A:2153:MET:HE3	1:A:2153:MET:HB3	1.70	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:2034:ALA:O	1:B:2038:SER:OG	2.32	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:B:1298:MET:HE3	1:B:1298:MET:HB2	1.76	0.45
1:A:1298:MET:HE3	1:A:1298:MET:HB2	1.76	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
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:A:4360:MET:HE1	1:A:4386:LEU:HD21	2.00	0.44
1:B:2153:MET:HE3	1:B:2153:MET:HB3	1.70	0.44
1:B:2557:LEU:HD21	1:B:2566:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:3359:MET:HE2	1:B:3364:ILE:HD13	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:3359:MET:HE2	1:A:3364:ILE:HD13	1.99	0.43
1:B:3754:LEU:O	1:B:3758:SER:OG	2.34	0.43
1:A:2632:LEU:HD22	1:A:2641:VAL:HG11	2.00	0.43
1:B:1771:SER:OG	1:B:1849:ARG:O	2.33	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
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:3110:SER:OG	1:B:3111:MET:N	2.46	0.43
1:B:4360:MET:HE1	1:B:4386:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1510:ASP:N	1:A:1510:ASP:OD1	2.43	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: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:B:3116:MET:HB2	1:B:3116:MET:HE2	1.68	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:B:1479:PRO:O	1:B:1914:TYR:OH	2.34	0.42
1:A:1515:LEU:HD11	1:A:2062:LEU:HD21	2.00	0.42
1:B:1924:LEU:O	1:B:1927:SER:OG	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:3318:ARG:HG2	1:A:3359:MET:SD	2.61	0.41
1:A:3757:ILE:HD13	1:A:3767:MET:HE2	2.03	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
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:B:1433:ASN:HA	1:B:1436:LYS:HZ3	1.85	0.41
1:B:3685:MET:HE2	1:B:3685:MET:HB2	1.99	0.41
1:A:4357:ILE:HA	1:A:4360:MET:HG3	2.03	0.41
1:B:2854:HIS:O	1:B:2858:THR:OG1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3112:VAL:HG13	1:B:2159:MET:HE2	2.02	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:1186:LYS:C	1:B:1292:ARG:HH22	2.29	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
1:B:3757:ILE:HD13	1:B:3767:MET:HE2	2.03	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%)	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. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1040	GLN
1	A	1056	GLN
1	A	1305	HIS
1	A	1961	GLN
1	A	2136	GLN
1	A	2311	HIS
1	A	2399	GLN
1	A	2975	GLN
1	A	3041	GLN
1	A	3147	HIS
1	A	3428	GLN
1	A	3513	ASN
1	A	3660	ASN
1	A	3747	ASN
1	A	3962	GLN
1	A	4169	GLN

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Mol	Chain	Res	Type
1	B	1040	GLN
1	B	1056	GLN
1	B	1305	HIS
1	B	1961	GLN
1	B	2037	GLN
1	B	2311	HIS
1	B	2399	GLN
1	B	2975	GLN
1	B	3095	ASN
1	B	3147	HIS
1	B	3428	GLN
1	B	3513	ASN
1	B	3660	ASN
1	B	4169	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 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.