Full wwPDB EM Validation Report ⓘ

May 25, 2025 – 12:16 AM JST

PDB ID	:	9L43 / pdb_00009l43
EMDB ID	:	EMD-62804
Title	:	ATR Spiral -ATRIP bound with VE-822
Authors	:	Wang, G.
Deposited on	:	2024-12-19
Resolution	:	3.83 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:

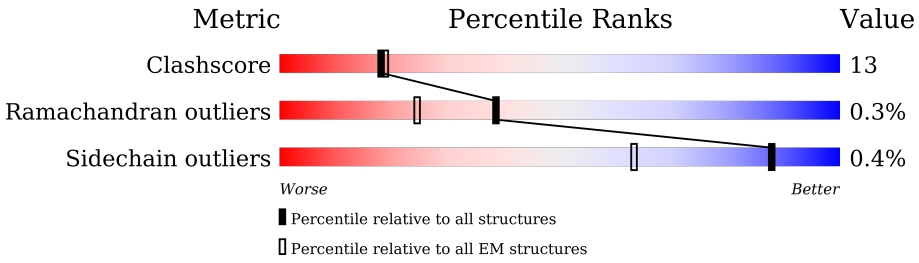
EMDB validation analysis	:	FAILED
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.83 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 <=5%

Mol	Chain	Length	Quality of chain
1	A	2644	23% 8% 69%
1	B	2644	24% 8% 68%
2	C	791	37% 9% 53%
2	D	791	36% 10% 54%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	C	801	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33261 atoms, of which 15995 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 Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	827	Total	C	H	N	O	S	0	0
			11843	3902	5783	1011	1107	40		
1	B	853	Total	C	H	N	O	S	0	0
			11860	3970	5696	1023	1129	42		

- Molecule 2 is a protein called ATR-interacting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	366	Total	C	H	N	O	S	0	0
			4754	1582	2252	439	464	17		
2	C	369	Total	C	H	N	O	S	0	0
			4802	1604	2264	442	470	22		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

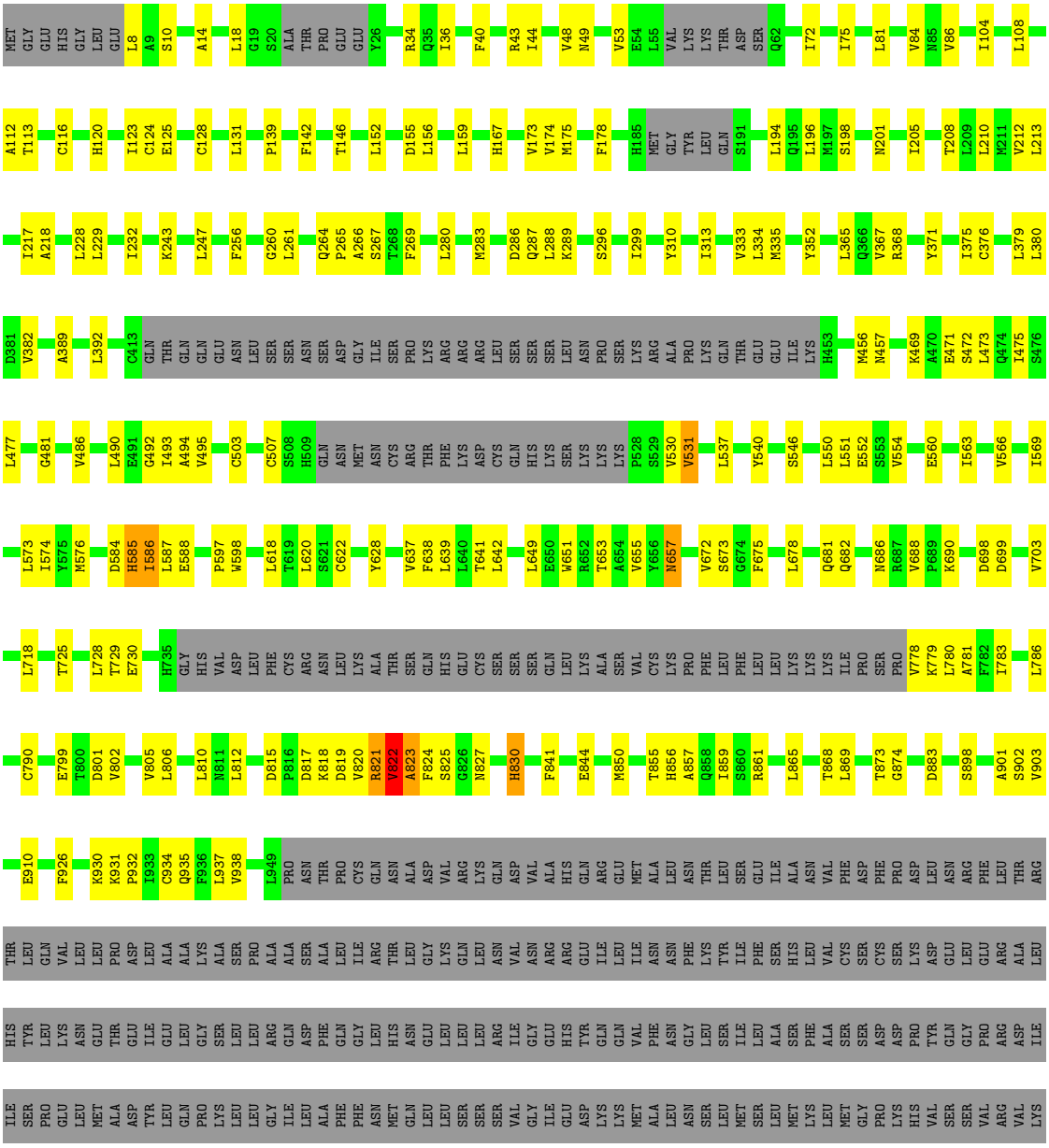
Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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: Serine/threonine-protein kinase ATR

Chain A: 23% 8% 69%



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

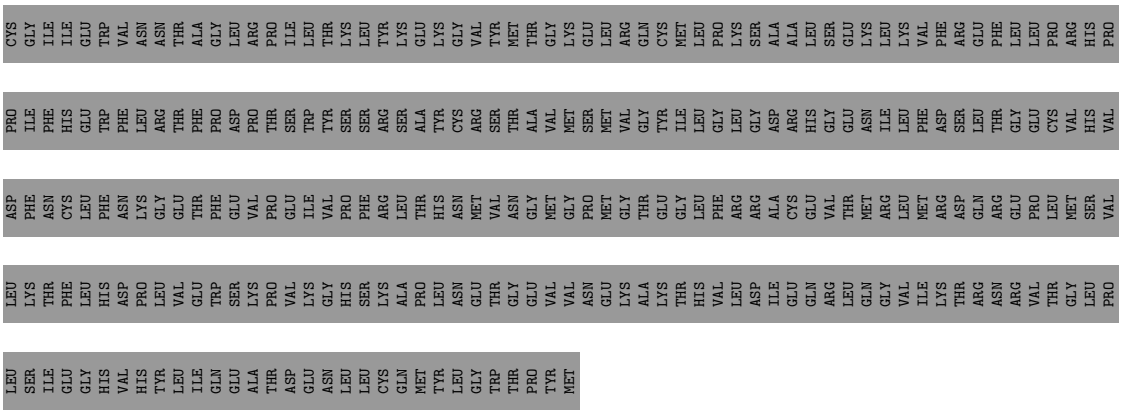
ARG SER LEU GLN TYR GLY ASN GLN PHE ILE TYR GLN SER MET PRO ARG MET LEU THR LEU TRP LEU ASP TYR GLY THR LYS ALA TYR GLU TRP GLU LYS ALA GLY ARG SER ASP ARG VAL GLN MET ARG ASN ASP LEU GLY LYS ILE ASN LYS VAL ILE THR GLU HIS THR ASN TYR LEU

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

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

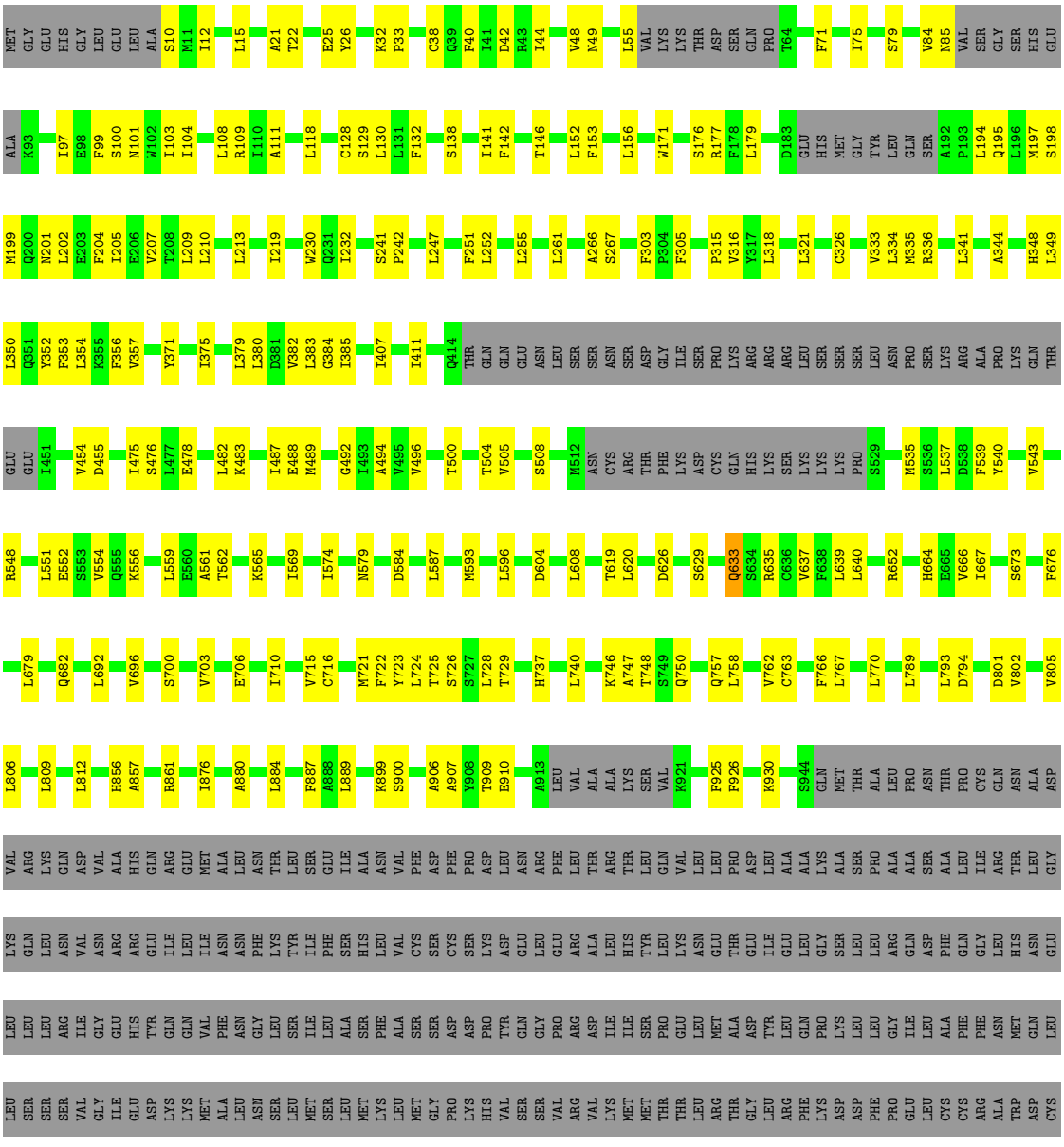
THR PHE SER GLU ILE LEU ILE PRO LEU GLN SER VAL MET ILE PRO THR LEU PRO SER ILE LEU GLY THR HIS ALA ASN HIS ALA SER HIS GLU PRO PHE PRO GLY HIS TRP ALA TYR ILE ALA GLY PHE ASP ASP MET VAL GLU ILE LEU ALA SER LEU GLN LYS PRO LYS LYS ILE SER

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



• Molecule 1: Serine/threonine-protein kinase ATR

Chain B:



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

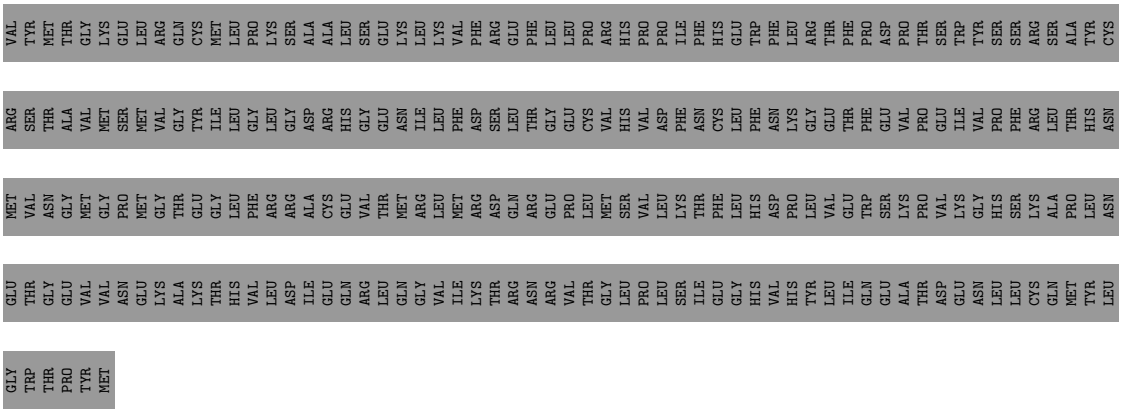
THR LYS ALA TYR GLU TRP GLU LYS ALA GLY ARG SER ASP ARG VAL GLN MET ARG ASN ASP LEU GLY LYS ILE ASN LYS VAL ILE THR GLU HIS THR ASN TYR LEU ALA PRO TYR GLN PHE LEU THR ALA PHE SER GLN LEU ILE SER ARG ILE CYS HIS SER HIS ASP GLU VAL PHE VAL

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

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

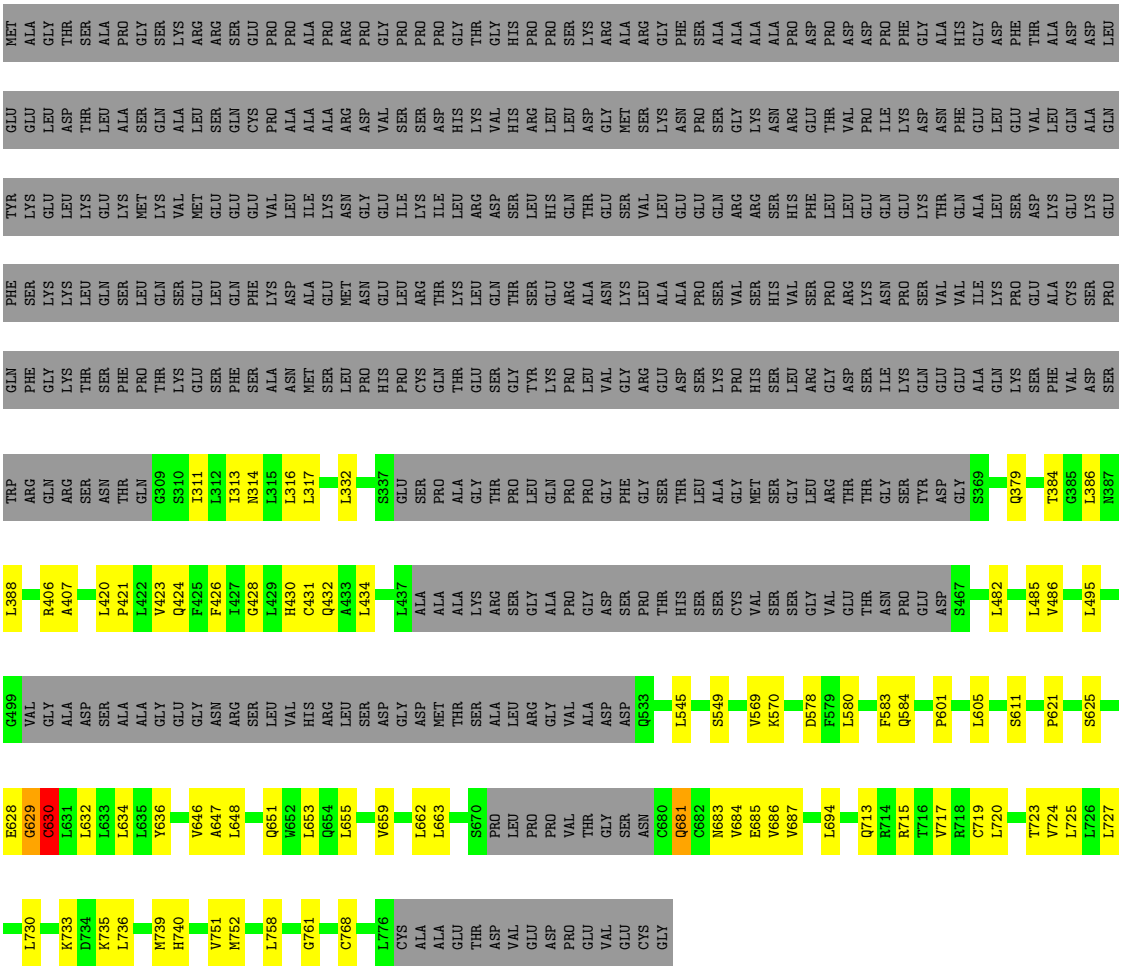
ASN HIS ALA SER HIS GLU PRO PHE PRO GLY HIS TRP ALA TYR ILE ALA GLY PHE ASP ASP MET VAL GLU ILE LEU ALA SER LEU GLN LYS PRO LYS LYS ILE SER LEU LYS GLY SER ASP GLY LYS PHE TYR ILE MET MET CYS LYS PRO LYS ASP ASP LEU ARG LYS ASP CYS ARG LEU

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



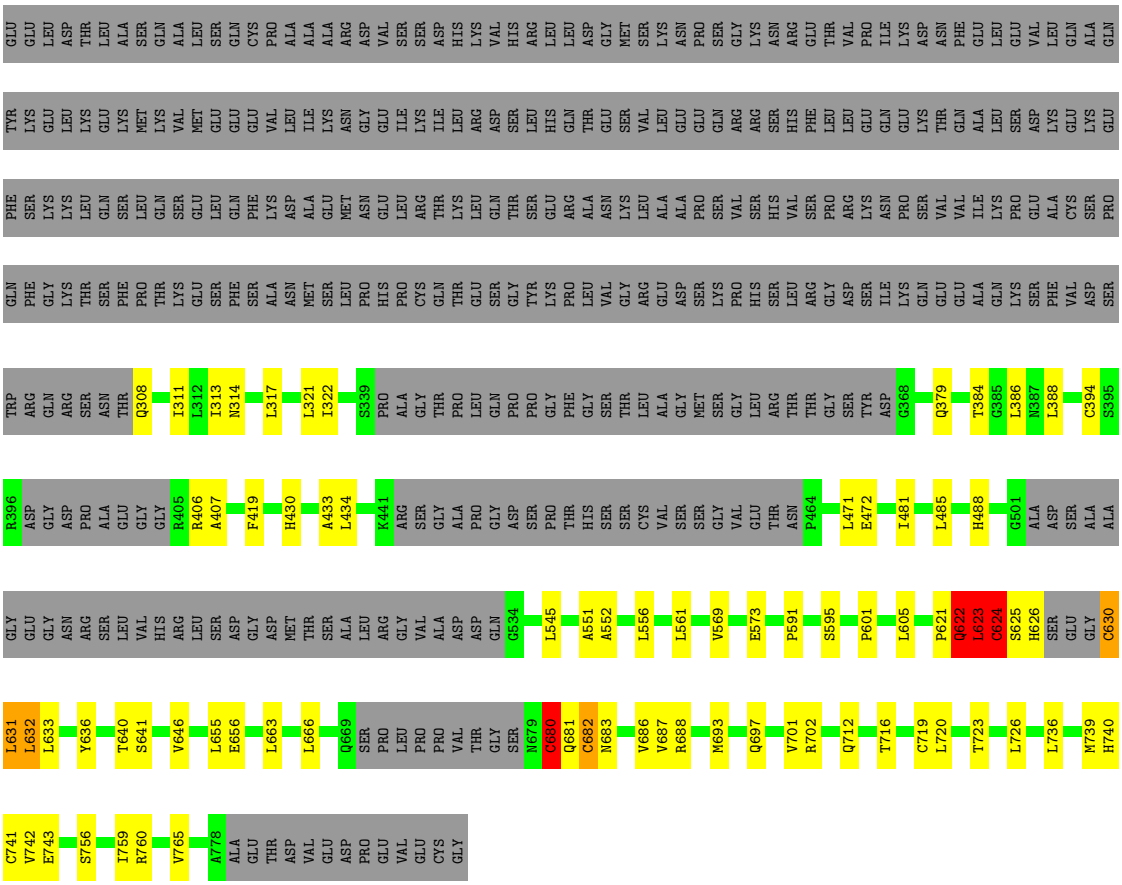
• Molecule 2: ATR-interacting protein

Chain D:



• Molecule 2: ATR-interacting protein

Chain C:


GLU GLU LEU ASP THR LEU ALA SER GLN ALA LEU SER GLN CYS PRO ALA ALA ALA ARG ASP VAL SER SER ASP HIS LYS VAL HIS ARG LEU LEU ASP GLY MET SER LYS ASN PRO SER GLY LYS ASN ARG GLU THR VAL PRO ILE LYS ASP ASN PHE GLU LEU GLU VAL LEU GLN LEU GLU
TYR LYS GLU LEU LYS GLU LYS MET LYS VAL MET GLU GLU GLU VAL LEU LYS ASN GLY GLU ILE LYS ILE LEU ARG ASP SER LEU HIS GLN THR GLU SER VAL LEU GLU GLN ARG SER HIS PHE LEU LEU GLU GLN GLU LYS THR GLN ALA LEU SER ASP LYS GLU LYS GLU
PHE SER LYS LYS LEU GLN SER LEU GLN SER GLU LEU GLN PHE LYS ASP ALA GLU MET ASN GLU LEU THR SER GLU ARG THR LYS LEU GLN THR SER VAL SER HIS VAL SER PRO ARG LYS ASN PRO SER GLU LEU ALA ILE LYS PRO GLU ALA CYS SER PRO
GLN PHE GLY LYS THR SER PHE PRO THR LYS GLU SER PHE SER ALA ASN MET SER LEU PRO HIS PRO CYS GLN THR GLU SER GLY TYR LYS PRO LEU VAL GLY ARG GLU ASP SER LYS PRO HIS SER LEU ARG GLY ASP SER ILE LYS GLN GLU GLU ALA GLN LYS SER PHE VAL ASP SER
TRP ARG GLN ARG SER ASN THR Q308 I311 L312 I313 N314 L317 L321 I322 S339 PRO ALA GLY THR PRO LEU GLN PRO PRO GLY PHE GLY SER THR LEU ALA GLY MET SER GLY LEU ARG THR THR GLY SER TYR ASP G368 Q379 T384 G385 L386 N387 L388 C394 S396
R396 ASP GLY ASP PRO ALA GLU GLY GLY R405 R406 A407 F419 H430 A433 L434 K441 ARG SER GLY ALA PRO GLY ASP SER PRO THR HIS SER SER CYS VAL SER SER GLY VAL GLU THR ASN P464 L471 E472 I481 L485 H488 G501 ALA ASP SER ALA ALA
GLY GLU GLY ASN ARG SER LEU VAL HIS ARG LEU SER ASP GLY ASP MET THR SER ALA LEU ARG GLY VAL ALA ASP ASP GLN G534 L545 A551 A552 L556 L561 V569 E573 P591 S595 P601 L605 P621 Q622 L623 C624 S625 H626 SER GLU GLY C630
L631 L632 L633 V636 T640 S641 V646 L655 E656 L663 L666 Q669 SER PRO LEU PRO PRO VAL THR GLY SER N679 C680 Q681 C682 N683 V686 V687 R688 M693 Q697 V701 R702 Q712 T716 C719 L720 T723 L726 L736 M739 H740
C741 V742 E743 S756 I759 R760 V765 A778 ALA GLU THR ASP VAL GLU ASP PRO GLU VAL GLU CYS GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66141	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.32	5/6156 (0.1%)	0.58	14/8371 (0.2%)
1	B	0.24	2/6271 (0.0%)	0.40	2/8533 (0.0%)
2	C	0.51	7/2574 (0.3%)	0.90	19/3510 (0.5%)
2	D	0.29	1/2539 (0.0%)	0.54	4/3473 (0.1%)
All	All	0.32	15/17540 (0.1%)	0.58	39/23887 (0.2%)

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
2	C	0	3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	623	LEU	CA-C	12.36	1.69	1.52
2	C	624	CYS	C-N	-5.84	1.25	1.33
2	C	624	CYS	CA-C	-5.66	1.45	1.52
2	C	631	LEU	N-CA	5.25	1.52	1.46
2	C	488	HIS	ND1-CE1	5.24	1.37	1.32
1	A	856	HIS	ND1-CE1	5.24	1.37	1.32
1	A	830	HIS	ND1-CE1	5.24	1.37	1.32
2	C	623	LEU	N-CA	5.22	1.52	1.46
1	A	167	HIS	ND1-CE1	5.21	1.37	1.32
1	B	856	HIS	ND1-CE1	5.19	1.37	1.32
2	D	379	GLN	CD-OE1	5.09	1.33	1.23
2	C	379	GLN	CD-OE1	5.09	1.33	1.23
1	A	657	ASN	CG-OD1	5.08	1.33	1.23
1	B	633	GLN	CD-OE1	5.08	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	681	GLN	CD-OE1	5.01	1.33	1.23

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	622	GLN	O-C-N	-24.42	90.11	122.59
1	A	822	VAL	N-CA-CB	-22.01	83.74	112.36
2	C	624	CYS	CB-CA-C	-14.47	86.61	110.77
2	C	624	CYS	N-CA-CB	13.88	132.15	109.94
2	C	681	GLN	N-CA-C	-11.41	98.58	111.71
2	C	624	CYS	CA-CB-SG	-10.36	90.57	114.40
1	A	821	ARG	CB-CA-C	-9.13	95.63	110.79
2	C	626	HIS	CB-CA-C	8.41	126.09	110.10
2	D	681	GLN	N-CA-C	-8.24	102.30	111.28
2	C	630	CYS	CB-CA-C	8.14	125.57	110.10
1	A	822	VAL	CB-CA-C	7.96	119.68	110.93
1	A	824	PHE	N-CA-C	-7.56	103.04	111.28
1	A	824	PHE	CA-C-O	-7.39	112.71	120.55
1	A	823	ALA	N-CA-C	-7.33	103.90	112.92
2	C	623	LEU	CA-C-O	-6.92	110.61	120.51
1	A	167	HIS	CB-CG-CD2	-6.64	122.56	131.20
1	A	856	HIS	CB-CG-CD2	-6.64	122.56	131.20
1	B	856	HIS	CB-CG-CD2	-6.59	122.63	131.20
2	C	488	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	A	830	HIS	CB-CG-CD2	-6.45	122.81	131.20
2	D	630	CYS	N-CA-CB	-6.40	101.54	113.89
2	C	623	LEU	CA-C-N	-6.27	112.64	121.99
2	C	623	LEU	C-N-CA	-6.27	112.64	121.99
2	C	682	CYS	CA-C-O	-6.25	113.92	120.55
1	A	34	ARG	CB-CA-C	6.19	121.06	110.79
2	D	630	CYS	CB-CA-C	6.07	124.00	110.76
2	C	622	GLN	CA-C-N	5.89	132.79	121.54
2	C	622	GLN	C-N-CA	5.89	132.79	121.54
1	A	856	HIS	CB-CG-ND1	5.75	131.32	122.70
1	A	167	HIS	CB-CG-ND1	5.75	131.32	122.70
2	C	625	SER	N-CA-C	-5.71	104.51	112.45
1	B	856	HIS	CB-CG-ND1	5.70	131.25	122.70
2	C	488	HIS	CB-CG-ND1	5.63	131.15	122.70
1	A	830	HIS	CB-CG-ND1	5.57	131.05	122.70
2	C	680	CYS	CB-CA-C	5.45	119.20	110.16
2	D	629	GLY	N-CA-C	-5.21	100.83	113.18
2	C	631	LEU	CA-C-N	5.20	131.48	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	631	LEU	C-N-CA	5.20	131.48	121.54
1	A	34	ARG	N-CA-CB	-5.03	102.72	110.12

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	622	GLN	Mainchain,Peptide
2	C	624	CYS	Mainchain

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	6060	5783	5794	153	0
1	B	6164	5696	5700	150	0
2	C	2538	2264	2271	74	0
2	D	2502	2252	2257	55	0
3	C	1	0	0	3	0
3	D	1	0	0	0	0
All	All	17266	15995	16022	430	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 13.

All (430) 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)
2:C:630:CYS:CB	2:C:680:CYS:SG	2.38	1.12
2:C:680:CYS:SG	3:C:801:ZN:ZN	1.39	1.08
1:A:822:VAL:HB	1:A:868:THR:HB	1.33	1.05
2:C:430:HIS:HA	2:C:433:ALA:HB3	1.36	1.04
2:C:308:GLN:N	2:C:394:CYS:SG	2.40	0.94
1:A:818:LYS:O	1:A:822:VAL:HG23	1.73	0.89
2:C:624:CYS:HG	3:C:801:ZN:ZN	0.82	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:HIS:O	1:A:587:LEU:N	2.07	0.87
1:A:124:CYS:SG	1:A:212:VAL:HG22	2.19	0.83
1:A:379:LEU:O	1:A:382:VAL:HG12	1.80	0.81
1:B:857:ALA:O	1:B:861:ARG:N	2.13	0.80
2:C:630:CYS:HB2	2:C:680:CYS:SG	2.21	0.80
1:B:926:PHE:O	1:B:930:LYS:N	2.15	0.80
2:C:621:PRO:O	2:C:623:LEU:N	2.14	0.80
2:C:630:CYS:HB3	2:C:680:CYS:SG	2.22	0.77
1:A:806:LEU:O	1:A:810:LEU:HD23	1.85	0.76
1:A:857:ALA:O	1:A:861:ARG:N	2.19	0.75
1:A:551:LEU:HD11	1:A:620:LEU:HD21	1.67	0.74
1:B:715:VAL:HG11	1:B:789:LEU:HD13	1.69	0.74
1:B:633:GLN:O	1:B:637:VAL:HG23	1.87	0.74
2:D:428:GLY:O	2:D:432:GLN:N	2.18	0.74
1:B:38:CYS:O	1:B:42:ASP:N	2.20	0.74
1:B:721:MET:O	1:B:750:GLN:N	2.20	0.74
1:A:819:ASP:O	1:A:823:ALA:HB3	1.89	0.73
2:D:621:PRO:O	2:D:625:SER:N	2.22	0.73
1:B:40:PHE:O	1:B:44:ILE:HD12	1.88	0.72
2:C:624:CYS:HA	2:C:630:CYS:HA	1.72	0.72
1:B:371:TYR:O	1:B:375:ILE:HD12	1.90	0.71
1:A:49:ASN:O	1:A:53:VAL:HG23	1.91	0.71
2:C:430:HIS:N	2:C:471:LEU:HD21	2.06	0.70
1:A:371:TYR:O	1:A:375:ILE:HD12	1.92	0.70
1:A:174:VAL:HG23	1:A:194:LEU:O	1.92	0.69
1:B:55:LEU:C	1:B:118:LEU:HD12	2.16	0.69
1:A:822:VAL:HB	1:A:868:THR:CB	2.16	0.69
2:C:656:GLU:HB3	2:C:693:MET:HE3	1.74	0.69
1:B:635:ARG:CB	1:B:740:LEU:HD11	2.23	0.69
1:A:213:LEU:HD21	1:A:229:LEU:HD22	1.73	0.69
1:B:692:LEU:O	1:B:696:VAL:HG12	1.92	0.69
1:A:550:LEU:O	1:A:554:VAL:HG23	1.94	0.68
1:B:723:TYR:N	1:B:748:THR:O	2.20	0.68
1:A:228:LEU:O	1:A:232:ILE:HD12	1.93	0.68
1:B:596:LEU:HD11	1:B:620:LEU:CD2	2.24	0.67
1:A:120:HIS:HA	1:A:123:ILE:HD12	1.75	0.67
1:A:822:VAL:CB	1:A:868:THR:HB	2.19	0.67
1:B:476:SER:OG	1:B:489:MET:HE1	1.95	0.66
1:B:596:LEU:HD11	1:B:620:LEU:HD22	1.77	0.65
2:C:308:GLN:N	2:C:394:CYS:O	2.30	0.65
1:B:664:HIS:ND1	1:B:667:ILE:HD12	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:LEU:HB2	1:A:820:VAL:HG22	1.78	0.65
2:C:430:HIS:HA	2:C:433:ALA:CB	2.22	0.64
2:D:632:LEU:C	2:D:634:LEU:H	2.06	0.64
2:D:719:CYS:O	2:D:723:THR:HG23	1.98	0.63
1:B:715:VAL:HG11	1:B:789:LEU:CD1	2.28	0.63
2:C:624:CYS:SG	2:C:630:CYS:CB	2.87	0.63
1:B:722:PHE:HA	1:B:748:THR:O	1.98	0.63
1:B:326:CYS:HB2	1:B:375:ILE:HD11	1.80	0.62
1:B:21:ALA:HB1	1:B:26:TYR:HA	1.82	0.62
1:A:546:SER:O	1:A:550:LEU:HD23	2.00	0.62
1:A:574:ILE:HG13	1:A:639:LEU:HD12	1.80	0.62
1:A:139:PRO:O	1:A:142:PHE:N	2.33	0.62
1:A:540:TYR:OH	1:A:576:MET:HE1	2.00	0.62
1:B:492:GLY:O	1:B:496:VAL:HG23	1.99	0.61
2:C:719:CYS:O	2:C:723:THR:HG23	2.00	0.61
1:B:700:SER:O	1:B:703:VAL:HG12	2.00	0.61
1:A:376:CYS:HA	1:A:379:LEU:HD12	1.83	0.61
1:A:155:ASP:O	1:A:159:LEU:HD23	1.99	0.61
1:B:635:ARG:O	1:B:639:LEU:HD23	2.01	0.61
1:A:14:ALA:O	1:A:18:LEU:HD23	2.00	0.61
1:B:209:LEU:O	1:B:213:LEU:HD23	2.00	0.61
1:B:99:PHE:CE2	1:B:103:ILE:HD11	2.36	0.60
1:A:786:LEU:O	1:A:790:CYS:N	2.35	0.60
1:A:156:LEU:HD21	1:A:175:MET:HE3	1.83	0.60
1:A:8:LEU:HD13	1:A:40:PHE:CD2	2.37	0.60
2:D:430:HIS:O	2:D:434:LEU:HD23	2.01	0.60
1:A:530:VAL:O	1:A:531:VAL:HG13	2.03	0.59
1:B:561:ALA:HB1	1:B:565:LYS:NZ	2.17	0.59
1:A:530:VAL:O	1:A:530:VAL:HG23	2.01	0.59
1:B:12:ILE:HA	1:B:15:LEU:HD12	1.84	0.59
1:B:230:TRP:CZ3	1:B:252:LEU:HD22	2.38	0.59
2:C:430:HIS:CA	2:C:433:ALA:HB3	2.22	0.59
1:B:71:PHE:O	1:B:75:ILE:HG22	2.02	0.59
1:B:142:PHE:O	1:B:146:THR:HG23	2.03	0.59
2:D:580:LEU:O	2:D:583:PHE:N	2.36	0.59
1:A:801:ASP:O	1:A:805:VAL:HG23	2.03	0.59
1:B:907:ALA:O	1:B:910:GLU:N	2.35	0.59
2:D:611:SER:OG	2:D:662:LEU:HD13	2.03	0.58
1:B:565:LYS:O	1:B:569:ILE:HD12	2.03	0.58
2:D:636:TYR:CZ	2:D:686:VAL:HG23	2.38	0.58
1:A:124:CYS:O	1:A:128:CYS:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:624:CYS:SG	2:C:630:CYS:HB2	2.44	0.58
2:D:545:LEU:C	2:D:545:LEU:HD23	2.29	0.58
1:A:72:ILE:HA	1:A:75:ILE:HG22	1.86	0.58
1:B:10:SER:N	1:B:15:LEU:HD11	2.19	0.57
1:A:725:THR:HG21	1:A:728:LEU:HB2	1.85	0.57
1:B:640:LEU:HD21	1:B:652:ARG:HA	1.86	0.57
1:B:84:VAL:HG22	1:B:85:ASN:N	2.19	0.57
2:C:632:LEU:HD12	2:C:632:LEU:H	1.69	0.57
1:A:243:LYS:O	1:A:247:LEU:HD23	2.05	0.57
1:A:815:ASP:HB3	1:A:821:ARG:CB	2.35	0.57
1:A:104:ILE:O	1:A:108:LEU:HD23	2.05	0.57
1:A:560:GLU:OE1	1:A:560:GLU:N	2.35	0.57
1:B:84:VAL:HG22	1:B:85:ASN:H	1.69	0.57
2:C:621:PRO:C	2:C:623:LEU:N	2.63	0.57
2:C:646:VAL:O	2:C:646:VAL:HG13	2.05	0.57
1:B:802:VAL:O	1:B:806:LEU:HD23	2.05	0.56
1:A:473:LEU:HB2	1:A:493:ILE:HD11	1.87	0.56
2:D:730:LEU:O	2:D:733:LYS:N	2.39	0.56
1:A:8:LEU:HD13	1:A:40:PHE:HD2	1.71	0.56
1:B:762:VAL:HG22	1:B:766:PHE:CE2	2.40	0.56
2:D:694:LEU:CD2	2:D:751:VAL:HG21	2.35	0.56
1:A:728:LEU:O	1:A:729:THR:HG23	2.04	0.56
2:D:428:GLY:O	2:D:431:CYS:N	2.39	0.56
2:D:736:LEU:O	2:D:739:MET:N	2.39	0.56
1:A:821:ARG:CB	1:A:822:VAL:HG22	2.36	0.56
2:D:659:VAL:O	2:D:663:LEU:HD23	2.06	0.56
1:B:251:PHE:CE2	1:B:255:LEU:HD11	2.41	0.55
1:B:635:ARG:HA	1:B:740:LEU:HD11	1.89	0.55
2:D:578:ASP:OD1	2:D:578:ASP:N	2.39	0.55
1:A:196:LEU:HD23	1:A:201:ASN:CG	2.31	0.55
1:B:763:CYS:SG	1:B:767:LEU:HD23	2.47	0.55
1:B:635:ARG:CA	1:B:740:LEU:HD11	2.37	0.55
1:B:475:ILE:O	1:B:478:GLU:N	2.40	0.54
2:C:624:CYS:HG	2:C:630:CYS:CB	2.19	0.54
1:A:380:LEU:O	1:A:380:LEU:HD23	2.06	0.54
1:B:757:GLN:HA	1:B:794:ASP:CB	2.37	0.54
2:D:628:GLU:O	2:D:630:CYS:N	2.39	0.54
2:D:725:LEU:HD22	2:D:768:CYS:HB3	1.87	0.54
2:C:632:LEU:HD23	2:C:636:TYR:OH	2.05	0.54
1:B:22:THR:O	1:B:26:TYR:N	2.33	0.54
2:C:656:GLU:CB	2:C:693:MET:HE3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:636:TYR:O	2:C:640:THR:HG22	2.07	0.54
1:A:469:LYS:O	1:A:472:SER:OG	2.22	0.54
1:A:638:PHE:O	1:A:641:THR:OG1	2.23	0.54
2:D:720:LEU:O	2:D:724:VAL:HG23	2.06	0.54
2:C:739:MET:O	2:C:742:VAL:HG22	2.08	0.54
1:A:104:ILE:HG21	1:A:178:PHE:HE2	1.73	0.53
2:C:545:LEU:HD23	2:C:545:LEU:C	2.33	0.53
1:A:210:LEU:HD23	1:A:247:LEU:HB3	1.91	0.53
1:B:380:LEU:HD23	1:B:380:LEU:C	2.33	0.53
1:A:477:LEU:O	1:A:481:GLY:N	2.42	0.53
2:D:648:LEU:O	2:D:651:GLN:N	2.42	0.53
2:C:656:GLU:HG2	2:C:693:MET:HE3	1.90	0.53
2:D:317:LEU:HD13	2:C:386:LEU:CD2	2.39	0.53
1:B:153:PHE:CD2	1:B:232:ILE:HD12	2.44	0.53
1:A:585:HIS:O	1:A:588:GLU:N	2.36	0.52
2:D:313:ILE:HG23	2:D:314:ASN:N	2.23	0.52
1:A:208:THR:O	1:A:212:VAL:HG23	2.09	0.52
2:D:482:LEU:O	2:D:486:VAL:HG23	2.10	0.52
2:C:701:VAL:HG13	2:C:702:ARG:N	2.25	0.52
1:A:108:LEU:HD12	1:A:205:ILE:HD11	1.92	0.52
1:A:131:LEU:HD12	1:A:142:PHE:CE1	2.44	0.52
1:B:48:VAL:HG23	1:B:49:ASN:N	2.25	0.52
1:B:357:VAL:O	1:B:357:VAL:HG13	2.09	0.52
2:C:321:LEU:O	2:C:322:ILE:HD13	2.10	0.52
2:C:430:HIS:O	2:C:434:LEU:HD23	2.09	0.52
2:D:723:THR:O	2:D:727:LEU:HD13	2.10	0.52
2:C:472:GLU:CB	2:C:556:LEU:HD23	2.40	0.52
1:B:198:SER:O	1:B:201:ASN:N	2.43	0.51
2:C:680:CYS:CB	2:C:682:CYS:SG	2.99	0.51
1:A:551:LEU:CD1	1:A:620:LEU:HD21	2.39	0.51
2:C:655:LEU:C	2:C:655:LEU:HD23	2.36	0.51
1:B:108:LEU:CD1	1:B:205:ILE:HD11	2.41	0.51
1:B:252:LEU:HD23	1:B:255:LEU:HD12	1.93	0.51
1:B:379:LEU:O	1:B:382:VAL:HG12	2.11	0.51
1:A:49:ASN:O	1:A:53:VAL:N	2.43	0.51
1:B:494:ALA:HB2	1:B:569:ILE:HD11	1.92	0.51
1:A:937:LEU:HD23	1:A:937:LEU:O	2.10	0.51
1:B:210:LEU:HD23	1:B:247:LEU:HB3	1.92	0.51
2:D:683:ASN:O	2:D:686:VAL:HG12	2.11	0.51
1:B:341:LEU:O	1:B:344:ALA:N	2.43	0.51
2:C:624:CYS:SG	3:C:801:ZN:ZN	1.81	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:VAL:HA	1:A:569:ILE:HG22	1.93	0.50
1:B:629:SER:O	1:B:633:GLN:N	2.34	0.50
2:D:386:LEU:HD13	2:C:317:LEU:HD13	1.93	0.50
2:D:751:VAL:HG13	2:D:752:MET:N	2.26	0.50
2:C:640:THR:HG23	2:C:641:SER:N	2.26	0.50
1:A:883:ASP:OD2	1:A:883:ASP:N	2.45	0.50
2:D:420:LEU:O	2:D:423:VAL:N	2.45	0.50
2:D:684:VAL:HG23	2:D:740:HIS:ND1	2.27	0.49
1:B:639:LEU:CD2	1:B:740:LEU:HD13	2.42	0.49
1:A:124:CYS:O	1:A:125:GLU:C	2.52	0.49
2:C:663:LEU:CB	2:C:726:LEU:HD21	2.43	0.49
1:B:407:ILE:O	1:B:411:ILE:HG22	2.13	0.49
1:A:551:LEU:HD12	1:A:552:GLU:N	2.28	0.49
1:B:341:LEU:O	1:B:344:ALA:HB3	2.13	0.49
1:A:173:VAL:HG22	1:A:174:VAL:N	2.28	0.49
2:D:601:PRO:O	2:D:605:LEU:HD23	2.13	0.49
1:B:111:ALA:HB3	1:B:205:ILE:HD12	1.95	0.48
1:B:725:THR:HG22	1:B:726:SER:N	2.28	0.48
1:A:379:LEU:HD22	1:A:392:LEU:HD12	1.95	0.48
1:B:505:VAL:HG22	1:B:579:ASN:ND2	2.27	0.48
2:D:655:LEU:HD23	2:D:655:LEU:C	2.38	0.48
1:A:926:PHE:O	1:A:930:LYS:N	2.45	0.48
1:B:724:LEU:O	1:B:725:THR:OG1	2.30	0.48
2:D:632:LEU:C	2:D:634:LEU:N	2.70	0.48
2:C:759:ILE:O	2:C:765:VAL:HG12	2.12	0.48
1:A:104:ILE:HG21	1:A:178:PHE:CE2	2.48	0.48
1:B:728:LEU:HD12	1:B:729:THR:N	2.28	0.48
1:A:486:VAL:O	1:A:490:LEU:HD13	2.14	0.48
1:A:653:THR:O	1:A:657:ASN:OD1	2.31	0.48
1:B:494:ALA:HB2	1:B:569:ILE:CD1	2.44	0.48
2:C:633:LEU:HD12	2:C:682:CYS:HB3	1.96	0.47
1:B:640:LEU:HD11	1:B:652:ARG:CB	2.43	0.47
1:B:706:GLU:O	1:B:710:ILE:HG23	2.14	0.47
2:C:683:ASN:O	2:C:686:VAL:HG12	2.14	0.47
2:C:712:GLN:O	2:C:716:THR:HG23	2.14	0.47
1:A:198:SER:O	1:A:201:ASN:N	2.46	0.47
1:A:585:HIS:C	1:A:587:LEU:N	2.73	0.47
1:B:153:PHE:CE2	1:B:232:ILE:HD12	2.49	0.47
1:B:593:MET:SD	1:B:593:MET:N	2.86	0.47
2:C:430:HIS:CA	2:C:471:LEU:HD21	2.44	0.47
1:B:333:VAL:O	1:B:336:ARG:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:LEU:O	1:A:873:THR:HG23	2.13	0.47
1:A:778:VAL:HG13	1:A:779:LYS:N	2.30	0.47
1:B:584:ASP:O	1:B:587:LEU:N	2.47	0.47
1:A:104:ILE:HG22	1:A:108:LEU:HD23	1.96	0.47
1:B:108:LEU:HD12	1:B:205:ILE:HD11	1.97	0.47
1:B:109:ARG:HG2	1:B:194:LEU:HD12	1.96	0.47
1:B:333:VAL:HG13	1:B:334:LEU:N	2.29	0.47
1:B:500:THR:O	1:B:504:THR:HG22	2.15	0.47
2:D:495:LEU:C	2:D:495:LEU:HD23	2.39	0.47
2:C:640:THR:HG23	2:C:641:SER:H	1.80	0.47
2:C:736:LEU:O	2:C:739:MET:N	2.48	0.47
2:D:758:LEU:O	2:D:761:GLY:N	2.48	0.47
1:A:113:THR:HG23	1:A:116:CYS:H	1.80	0.47
1:A:698:ASP:CB	1:A:703:VAL:HG22	2.44	0.47
1:A:855:THR:O	1:A:859:ILE:HD12	2.14	0.47
1:B:22:THR:OG1	1:B:25:GLU:N	2.43	0.47
2:C:666:LEU:HD23	2:C:666:LEU:C	2.39	0.46
1:B:152:LEU:CD2	1:B:156:LEU:HD11	2.46	0.46
1:B:710:ILE:O	1:B:746:LYS:NZ	2.46	0.46
1:B:357:VAL:O	1:B:357:VAL:CG1	2.64	0.46
2:C:311:ILE:HG22	2:C:311:ILE:O	2.14	0.46
1:A:86:VAL:HG23	1:A:86:VAL:O	2.16	0.46
1:A:779:LYS:HB2	1:A:820:VAL:HG21	1.97	0.46
1:A:817:ASP:O	1:A:822:VAL:HG22	2.16	0.46
1:A:818:LYS:HA	1:A:822:VAL:CG2	2.46	0.46
1:A:937:LEU:HD23	1:A:937:LEU:C	2.40	0.46
1:B:335:MET:HE2	1:B:382:VAL:HA	1.98	0.46
1:B:715:VAL:HG23	1:B:716:CYS:H	1.81	0.46
2:C:551:ALA:O	2:C:552:ALA:C	2.59	0.46
2:C:601:PRO:O	2:C:605:LEU:HD23	2.15	0.46
1:B:138:SER:OG	1:B:141:ILE:HD12	2.15	0.46
2:C:472:GLU:HB3	2:C:556:LEU:HD23	1.97	0.46
1:B:724:LEU:HD23	1:B:747:ALA:HB2	1.97	0.46
2:D:545:LEU:O	2:D:549:SER:N	2.47	0.46
2:C:591:PRO:O	2:C:595:SER:N	2.49	0.46
1:A:10:SER:HB2	1:A:36:ILE:HD12	1.98	0.45
1:A:651:TRP:O	1:A:655:VAL:HG23	2.16	0.45
1:A:81:LEU:HA	1:A:84:VAL:O	2.16	0.45
2:C:313:ILE:HG23	2:C:314:ASN:N	2.32	0.45
1:B:385:ILE:HG22	1:B:385:ILE:O	2.15	0.45
2:C:624:CYS:CB	2:C:630:CYS:HB2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:386:LEU:HD13	2:C:419:PHE:HZ	1.82	0.45
2:D:420:LEU:O	2:D:421:PRO:C	2.59	0.45
1:B:315:PRO:O	1:B:318:LEU:N	2.50	0.45
1:B:535:MET:HE2	1:B:539:PHE:CD2	2.51	0.45
1:A:818:LYS:HA	1:A:822:VAL:HG21	1.98	0.45
1:B:715:VAL:HG23	1:B:716:CYS:N	2.32	0.45
2:C:621:PRO:C	2:C:623:LEU:H	2.24	0.45
1:A:686:ASN:C	1:A:718:LEU:HD12	2.42	0.45
1:A:678:LEU:C	1:A:678:LEU:HD23	2.41	0.45
1:A:778:VAL:O	1:A:781:ALA:HB3	2.17	0.45
1:B:801:ASP:O	1:B:805:VAL:HG23	2.17	0.45
1:A:649:LEU:HD11	1:A:682:GLN:OE1	2.16	0.44
2:D:311:ILE:O	2:D:311:ILE:HG22	2.16	0.44
2:D:482:LEU:HD12	2:D:486:VAL:HG23	1.99	0.44
1:B:104:ILE:HG22	1:B:108:LEU:HD23	1.97	0.44
1:B:197:MET:N	1:B:201:ASN:OD1	2.51	0.44
1:B:204:PHE:O	1:B:207:VAL:HG12	2.18	0.44
2:C:680:CYS:HB3	2:C:683:ASN:H	1.82	0.44
1:A:40:PHE:HA	1:A:43:ARG:HG2	1.99	0.44
2:C:384:THR:O	2:C:388:LEU:HD23	2.17	0.44
1:B:383:LEU:HD12	1:B:384:GLY:N	2.32	0.44
1:A:597:PRO:HA	1:A:628:TYR:CE2	2.52	0.44
1:B:100:SER:HA	1:B:103:ILE:HD12	1.99	0.44
1:B:261:LEU:HD23	1:B:261:LEU:H	1.83	0.44
1:B:352:TYR:HD1	1:B:356:PHE:HB2	1.82	0.44
2:D:694:LEU:HD22	2:D:751:VAL:HG21	2.00	0.44
2:C:739:MET:HE3	2:C:740:HIS:CE1	2.52	0.44
1:A:333:VAL:HG13	1:A:334:LEU:N	2.33	0.44
1:A:367:VAL:HG22	1:A:371:TYR:CE1	2.52	0.44
1:A:503:CYS:O	1:A:507:CYS:HB2	2.17	0.44
2:D:384:THR:O	2:D:388:LEU:HD23	2.18	0.44
2:D:406:ARG:O	2:D:407:ALA:C	2.61	0.44
1:A:934:CYS:O	1:A:938:VAL:HG13	2.17	0.44
1:B:266:ALA:O	1:B:267:SER:C	2.60	0.44
1:B:504:THR:O	1:B:508:SER:OG	2.24	0.44
1:B:770:LEU:HD13	1:B:812:LEU:HD11	2.00	0.44
1:A:112:ALA:HB1	1:A:201:ASN:CG	2.43	0.43
1:A:699:ASP:N	1:A:699:ASP:OD1	2.50	0.43
1:A:931:LYS:CB	1:A:932:PRO:HD3	2.48	0.43
1:B:321:LEU:HD11	1:B:349:LEU:HD21	2.00	0.43
1:B:679:LEU:O	1:B:682:GLN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:CYS:O	1:A:128:CYS:CB	2.66	0.43
1:B:97:ILE:O	1:B:101:ASN:ND2	2.44	0.43
2:C:481:ILE:O	2:C:485:LEU:HG	2.17	0.43
1:B:152:LEU:HD12	1:B:177:ARG:HB2	2.01	0.43
1:B:176:SER:HB3	1:B:179:LEU:HD21	2.00	0.43
1:B:556:LYS:C	1:B:559:LEU:HD22	2.43	0.43
1:A:783:ILE:O	1:A:786:LEU:HD23	2.17	0.43
1:B:619:THR:HG23	1:B:620:LEU:N	2.31	0.43
1:B:767:LEU:HD12	1:B:767:LEU:C	2.42	0.43
1:A:266:ALA:O	1:A:267:SER:C	2.62	0.43
1:A:898:SER:CB	1:A:903:VAL:HG21	2.48	0.43
1:B:604:ASP:N	1:B:608:LEU:HD21	2.33	0.43
2:C:656:GLU:CG	2:C:693:MET:HE3	2.47	0.43
1:A:296:SER:HA	1:A:299:ILE:HG22	2.00	0.43
2:C:472:GLU:HB2	2:C:556:LEU:HD23	2.00	0.43
1:A:264:GLN:HB2	1:A:265:PRO:HD3	2.01	0.43
1:B:574:ILE:HD12	1:B:639:LEU:HD12	2.00	0.43
2:C:697:GLN:CB	2:C:720:LEU:HD21	2.49	0.43
1:A:456:MET:O	1:A:457:ASN:C	2.61	0.43
1:A:142:PHE:O	1:A:146:THR:HG23	2.19	0.43
1:A:584:ASP:O	1:A:588:GLU:CB	2.67	0.43
1:B:104:ILE:HG22	1:B:108:LEU:CD2	2.48	0.43
1:B:199:MET:HE2	1:B:199:MET:HA	2.00	0.43
1:B:350:LEU:O	1:B:354:LEU:HD13	2.19	0.43
1:A:280:LEU:O	1:A:283:MET:N	2.49	0.42
1:A:382:VAL:O	1:A:382:VAL:HG22	2.18	0.42
1:A:672:VAL:HG23	1:A:673:SER:N	2.34	0.42
1:A:779:LYS:HB3	1:A:820:VAL:HG11	2.01	0.42
1:A:310:TYR:HB3	1:A:352:TYR:OH	2.19	0.42
1:A:931:LYS:O	1:A:935:GLN:HG3	2.19	0.42
1:B:640:LEU:HD12	1:B:640:LEU:O	2.19	0.42
2:C:666:LEU:HD23	2:C:666:LEU:O	2.19	0.42
1:A:379:LEU:HB3	1:A:392:LEU:HD11	1.99	0.42
1:A:389:ALA:O	1:A:392:LEU:HB3	2.19	0.42
1:A:569:ILE:O	1:A:573:LEU:HD13	2.19	0.42
1:A:730:GLU:OE1	1:A:730:GLU:HA	2.19	0.42
1:B:884:LEU:O	1:B:887:PHE:N	2.52	0.42
2:C:686:VAL:HG13	2:C:687:VAL:N	2.33	0.42
1:A:286:ASP:OD1	1:A:287:GLN:N	2.50	0.42
1:A:288:LEU:O	1:A:289:LYS:C	2.62	0.42
1:A:618:LEU:HD23	1:A:622:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:CB	1:A:822:VAL:HG13	2.49	0.42
1:A:850:MET:HE3	1:A:869:LEU:HD22	2.01	0.42
1:B:32:LYS:HB2	1:B:33:PRO:HD3	2.01	0.42
1:B:626:ASP:OD1	1:B:626:ASP:N	2.49	0.42
1:B:758:LEU:CB	1:B:793:LEU:HA	2.50	0.42
1:A:43:ARG:NH2	1:A:44:ILE:HD11	2.35	0.42
1:A:598:TRP:CH2	1:A:637:VAL:HG13	2.54	0.42
1:B:129:SER:HA	1:B:132:PHE:HB2	2.00	0.42
1:B:454:VAL:HG12	1:B:455:ASP:N	2.34	0.42
1:A:194:LEU:O	1:A:194:LEU:HG	2.19	0.42
1:B:666:VAL:HG23	1:B:667:ILE:N	2.34	0.42
1:B:673:SER:O	1:B:676:PHE:CE1	2.72	0.42
2:D:580:LEU:HD23	2:D:583:PHE:CD2	2.55	0.42
1:A:688:VAL:O	1:A:690:LYS:NZ	2.34	0.42
1:A:799:GLU:O	1:A:802:VAL:HG12	2.19	0.42
2:C:741:CYS:O	2:C:742:VAL:C	2.62	0.42
1:A:380:LEU:HD23	1:A:380:LEU:C	2.45	0.42
1:B:321:LEU:HD12	1:B:321:LEU:O	2.20	0.42
1:B:349:LEU:HD11	1:B:353:PHE:HE2	1.85	0.42
2:D:713:GLN:O	2:D:717:VAL:HG23	2.19	0.42
1:B:104:ILE:O	1:B:108:LEU:HD23	2.20	0.42
1:B:540:TYR:O	1:B:543:VAL:HG22	2.20	0.42
2:C:569:VAL:O	2:C:573:GLU:HG3	2.20	0.42
2:C:701:VAL:O	2:C:702:ARG:C	2.62	0.42
1:A:256:PHE:CD1	1:A:260:GLY:HA2	2.55	0.42
1:B:482:LEU:HD12	1:B:483:LYS:N	2.34	0.42
2:D:646:VAL:O	2:D:647:ALA:C	2.63	0.42
1:B:537:LEU:HD12	1:B:537:LEU:N	2.35	0.41
1:B:551:LEU:HD21	1:B:562:THR:CB	2.50	0.41
2:D:684:VAL:HG13	2:D:685:GLU:N	2.35	0.41
2:C:321:LEU:C	2:C:322:ILE:HD13	2.45	0.41
1:B:737:HIS:O	1:B:737:HIS:ND1	2.53	0.41
2:D:686:VAL:HG13	2:D:687:VAL:N	2.35	0.41
1:A:173:VAL:HG22	1:A:174:VAL:H	1.86	0.41
1:A:471:GLU:O	1:A:475:ILE:HG12	2.20	0.41
1:B:152:LEU:O	1:B:156:LEU:HG	2.20	0.41
1:B:554:VAL:HG22	1:B:554:VAL:O	2.20	0.41
2:D:583:PHE:O	2:D:584:GLN:C	2.62	0.41
1:A:675:PHE:HA	1:A:678:LEU:HB3	2.01	0.41
1:B:241:SER:HB2	1:B:242:PRO:HD2	2.01	0.41
1:B:876:ILE:O	1:B:880:ALA:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:LEU:HD21	2:D:485:LEU:HD21	2.01	0.41
2:D:569:VAL:HG13	2:D:570:LYS:N	2.34	0.41
2:D:735:LYS:HD2	2:D:735:LYS:N	2.36	0.41
1:A:217:ILE:CG2	1:A:218:ALA:N	2.82	0.41
2:C:561:LEU:C	2:C:561:LEU:HD23	2.45	0.41
1:A:639:LEU:HD13	1:A:639:LEU:HA	1.93	0.41
1:A:901:ALA:O	1:A:902:SER:C	2.64	0.41
1:A:152:LEU:O	1:A:156:LEU:HG	2.21	0.41
1:B:142:PHE:CE2	1:B:219:ILE:HG22	2.56	0.41
1:B:202:LEU:O	1:B:205:ILE:HG22	2.21	0.41
1:A:585:HIS:O	1:A:586:ILE:C	2.62	0.41
1:B:305:PHE:CE1	1:B:348:HIS:CE1	3.09	0.41
2:D:421:PRO:HA	2:D:424:GLN:HG2	2.01	0.41
1:A:492:GLY:O	1:A:495:VAL:HG12	2.20	0.41
1:A:563:ILE:O	1:A:566:VAL:HG12	2.21	0.41
1:A:865:LEU:O	1:A:868:THR:OG1	2.33	0.41
1:B:171:TRP:CZ3	1:B:199:MET:HE3	2.55	0.41
1:B:198:SER:N	1:B:201:ASN:OD1	2.44	0.41
1:B:303:PHE:HB3	1:B:352:TYR:CD2	2.55	0.41
1:B:889:LEU:HD22	1:B:925:PHE:CZ	2.56	0.41
1:B:906:ALA:O	1:B:909:THR:OG1	2.37	0.41
2:C:406:ARG:O	2:C:407:ALA:HB3	2.20	0.41
2:C:756:SER:O	2:C:760:ARG:HD3	2.21	0.41
1:A:266:ALA:O	1:A:269:PHE:N	2.53	0.41
1:A:817:ASP:O	1:A:822:VAL:CG2	2.69	0.41
1:A:827:ASN:HA	1:A:830:HIS:HD2	1.86	0.41
1:A:874:GLY:HA3	1:A:910:GLU:CG	2.51	0.41
1:B:79:SER:O	1:B:79:SER:OG	2.34	0.41
1:A:812:LEU:O	1:A:821:ARG:CB	2.69	0.40
1:A:841:PHE:HA	1:A:844:GLU:CG	2.51	0.40
1:B:195:GLN:N	1:B:195:GLN:OE1	2.55	0.40
1:B:899:LYS:O	1:B:900:SER:C	2.65	0.40
2:D:730:LEU:O	2:D:733:LYS:O	2.39	0.40
2:C:742:VAL:HG23	2:C:743:GLU:N	2.36	0.40
1:A:261:LEU:HD21	1:A:313:ILE:CD1	2.51	0.40
1:A:779:LYS:H	1:A:779:LYS:HD2	1.87	0.40
2:C:430:HIS:H	2:C:471:LEU:HD21	1.83	0.40
2:C:687:VAL:HG13	2:C:688:ARG:N	2.36	0.40
1:B:487:ILE:HG13	1:B:488:GLU:N	2.35	0.40
2:D:681:GLN:O	2:D:684:VAL:HG12	2.20	0.40
1:A:48:VAL:HG23	1:A:49:ASN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ALA:HA	1:A:569:ILE:HD13	2.03	0.40
1:B:315:PRO:O	1:B:316:VAL:C	2.63	0.40
2:D:332:LEU:HD21	2:D:426:PHE:CE1	2.56	0.40
1:A:40:PHE:O	1:A:44:ILE:HG12	2.21	0.40
1:A:335:MET:HB3	1:A:382:VAL:HG23	2.04	0.40
1:A:365:LEU:O	1:A:368:ARG:HB3	2.21	0.40
1:A:537:LEU:HA	1:A:540:TYR:CD2	2.57	0.40
1:B:128:CYS:C	1:B:130:LEU:H	2.29	0.40
1:B:548:ARG:O	1:B:552:GLU:N	2.47	0.40
1:B:673:SER:O	1:B:676:PHE:CD1	2.75	0.40
1:B:809:LEU:O	1:B:812:LEU:HD13	2.21	0.40
2:D:653:LEU:HD21	2:D:715:ARG:CB	2.51	0.40
2:D:751:VAL:O	2:D:752:MET:C	2.65	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	813/2644 (31%)	756 (93%)	54 (7%)	3 (0%)	30	65
1	B	839/2644 (32%)	769 (92%)	70 (8%)	0	100	100
2	C	355/791 (45%)	324 (91%)	28 (8%)	3 (1%)	16	51
2	D	356/791 (45%)	312 (88%)	43 (12%)	1 (0%)	37	70
All	All	2363/6870 (34%)	2161 (92%)	195 (8%)	7 (0%)	38	70

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	586	ILE
2	C	622	GLN

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Mol	Chain	Res	Type
2	C	623	LEU
1	A	825	SER
2	C	632	LEU
1	A	585	HIS
2	D	629	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	599/2363 (25%)	596 (100%)	3 (0%)	86 90
1	B	585/2363 (25%)	585 (100%)	0	100 100
2	C	231/678 (34%)	229 (99%)	2 (1%)	75 83
2	D	228/678 (34%)	227 (100%)	1 (0%)	89 91
All	All	1643/6082 (27%)	1637 (100%)	6 (0%)	88 91

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

Mol	Chain	Res	Type
1	A	531	VAL
1	A	642	LEU
1	A	822	VAL
2	D	630	CYS
2	C	631	LEU
2	C	680	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	74	HIS
1	A	85	ASN
1	A	633	GLN
1	A	683	ASN

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Mol	Chain	Res	Type
1	A	830	HIS
2	C	683	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.