

May 4, 2024 – 12:23 pm BST

PDB ID	:	6100
EMDB ID	:	EMD-0320
Title	:	Cryo-EM informed directed evolution of Nitrilase 4 leads to a change in qua-
		ternary structure.
Authors	:	Mulelu, A.E.; Woodward, J.D.
Deposited on	:	2018-10-24
Resolution	:	3.40 Å(reported)
This is	аI	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 (i) 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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.



Motria	Whole archive	EM structures
Metric	$(\# { m Entries})$	$(\# {\rm Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	А	361	69%	9%	•	20%								
1	В	361	66%	14%		20%								
1	С	361	68%	11%	·	20%								
1	D	361	66%	14%	·	20%								
1	Е	361	66%	12%	·	20%								
1	F	361	66%	13%		20%								
1	G	361	66%	12%	·	20%								
1	Н	361	66%	13%		20%								
1	Ι	361	66%	12%	•	20%								



Mol	Chain	Length	Quality of chain											
1	J	361	66%	13%	20%									
1	K	361	66%	12%	• 20%									
1	L	361	66%	13%	20%									



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 26712 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	Bifunctional	nitrilase	/nitrile ł	ivdratase	NIT4.
-	morecome r	10 00	protonn	ounou	Diranouonai	11101110000	11101110 1	i ai a case	T T T T

Mol	Chain	Residues		At	AltConf	Trace				
1	I	289	Total	С	Ν	0	S	0	0	
	0	200	2226	1425	381	407	13	0	0	
1	т	280	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	
1	T	205	2226	1425	381	407	13	0	0	
1	н	280	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	
L L	11	209	2226	1425	381	407	13	0	0	
1	C	280	Total	С	Ν	0	\mathbf{S}	0	0	
1	G	289	2226	1425	381	407	13	0	0	
1	F	280	Total	С	Ν	0	\mathbf{S}	0	0	
1	Г	209	2226	1425	381	407	13	0	0	
1	F	280	Total	С	Ν	0	\mathbf{S}	0	0	
1	Ľ	289	2226	1425	381	407	13	0	0	
1	П	280	Total	С	Ν	0	\mathbf{S}	0	0	
1	D	289	2226	1425	381	407	13	0	0	
1	С	280	Total	С	Ν	0	\mathbf{S}	0	0	
1		289	2226	1425	381	407	13	0	0	
1	В	280	Total	С	Ν	0	S	0	0	
1	D	289	2226	1425	381	407	13	0	0	
1	Δ	280	Total	С	Ν	0	S	0	0	
1	A	209	2226	1425	381	407	13	0	0	
1	т	280	Total	С	Ν	0	S	0	0	
1		209	2226	1425	381	407	13	0	0	
1	K	280	Total	С	Ν	0	S	0	0	
	IX	209	2226	1425	381	407	13	U	U	

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference					
J	356	HIS	-	expression tag	UNP P46011					
J	357	HIS	-	expression tag	UNP P46011					
J	358	HIS	-	expression tag	UNP P46011					
J	359	HIS	-	expression tag	UNP P46011					
J	360	HIS	-	expression tag	UNP P46011					
J	361	HIS	-	expression tag	UNP P46011					



Continu	iea from pre	vious page			
Chain	Residue	Modelled	Actual	Comment	Reference
Ι	356	HIS	-	expression tag	UNP P46011
Ι	357	HIS	-	expression tag	UNP P46011
Ι	358	HIS	-	expression tag	UNP P46011
Ι	359	HIS	-	expression tag	UNP P46011
Ι	360	HIS	-	expression tag	UNP P46011
Ι	361	HIS	-	expression tag	UNP P46011
Н	356	HIS	-	expression tag	UNP P46011
Н	357	HIS	-	expression tag	UNP P46011
Н	358	HIS	-	expression tag	UNP P46011
Н	359	HIS	-	expression tag	UNP P46011
Н	360	HIS	-	expression tag	UNP P46011
Н	361	HIS	-	expression tag	UNP P46011
G	356	HIS	-	expression tag	UNP P46011
G	357	HIS	-	expression tag	UNP P46011
G	358	HIS	-	expression tag	UNP P46011
G	359	HIS	-	expression tag	UNP P46011
G	360	HIS	-	expression tag	UNP P46011
G	361	HIS	-	expression tag	UNP P46011
F	356	HIS	-	expression tag	UNP P46011
F	357	HIS	-	expression tag	UNP P46011
F	358	HIS	-	expression tag	UNP P46011
F	359	HIS	-	expression tag	UNP P46011
F	360	HIS	-	expression tag	UNP P46011
F	361	HIS	-	expression tag	UNP P46011
Е	356	HIS	-	expression tag	UNP P46011
Е	357	HIS	-	expression tag	UNP P46011
Е	358	HIS	-	expression tag	UNP P46011
Е	359	HIS	-	expression tag	UNP P46011
E	360	HIS	-	expression tag	UNP P46011
Е	361	HIS	-	expression tag	UNP P46011
D	356	HIS	-	expression tag	UNP P46011
D	357	HIS	-	expression tag	UNP P46011
D	358	HIS	-	expression tag	UNP P46011
D	359	HIS	-	expression tag	UNP P46011
D	360	HIS	-	expression tag	UNP P46011
D	361	HIS	-	expression tag	UNP P46011
С	356	HIS	-	expression tag	UNP P46011
С	357	HIS	-	expression tag	UNP P46011
С	358	HIS	-	expression tag	UNP P46011
С	359	HIS	-	expression tag	UNP P46011
С	360	HIS	-	expression tag	UNP P46011
С	361	HIS	-	expression tag	UNP P46011

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Chain	Residue	Modelled	Actual	Comment	Reference						
В	356	HIS	-	expression tag	UNP P46011						
В	357	HIS	-	expression tag	UNP P46011						
В	358	HIS	-	expression tag	UNP P46011						
В	359	HIS	-	expression tag	UNP P46011						
В	360	HIS	-	expression tag	UNP P46011						
В	361	HIS	-	expression tag	UNP P46011						
А	356	HIS	-	expression tag	UNP P46011						
А	357	HIS	-	expression tag	UNP P46011						
А	358	HIS	-	expression tag	UNP P46011						
A	359	HIS	-	expression tag	UNP P46011						
А	360	HIS	-	expression tag	UNP P46011						
A	361	HIS	-	expression tag	UNP P46011						
L	356	HIS	-	expression tag	UNP P46011						
L	357	HIS	-	expression tag	UNP P46011						
L	358	HIS	-	expression tag	UNP P46011						
L	359	HIS	-	expression tag	UNP P46011						
L	360	HIS	-	expression tag	UNP P46011						
L	361	HIS	-	expression tag	UNP P46011						
K	356	HIS	-	expression tag	UNP P46011						
K	357	HIS	-	expression tag	UNP P46011						
K	358	HIS	-	expression tag	UNP P46011						
K	359	HIS	-	expression tag	UNP P46011						
K	360	HIS	-	expression tag	UNP P46011						
K	361	HIS	-	expression tag	UNP P46011						

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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: Bifunctional nitrilase/nitrile hydratase NIT4



• Molecule 1: Bifunctional nitrilase/nitrile hydratase NIT4

Chain C:	68%	11% •	20%
MET MET MET MET GLN GLN GLN GLN GLN HIS HIS MET THR	PALA PALA CLN CLN ASP ASP CLN ASP CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	V36 V40 V41 Q42 V46 T53 L61	V73 R84 R87 187 192 R95 R95 R100 R100 R100
R104 R120 Y128 V130 W130 M165 L169	V184 P186 P186 T187 T187 T188 C197 C197 C197 C197 C197 C197 C197 C197	ARG LYR LYR ASP PRO PRO PRO GLU GLU MFT MFT	PHE SER GLY SER CLU GLU GLU SER HR PRO ASP SER VAL
V276 G279 1283 1283 1283 1283 1283 1287 1287 1311	F318 0322 V320 V321 6322 632 8331 F326 F326 F326 F326 F326 F326 F326 F326	STH SIH HIS	
• Molecule 1: Bi	functional nitrilase/nitrile hydra	atase NIT4	
Chain B:	66%	14%	20%
MET MET MET MET GLN GLN GLN CLU CLU CLU THR MET MET MET	PALA PALA CLN CLN ALN ALN ALA ALA ALA CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	42 42 153 153 161	179 (800 184 187 192 192 192 192
R100 R120 L123 L123 T137 T147 V148	H161 H163 L169 L169 F181 F181 F185 T185 T185 T185 T185 T185 T185 T185 T	T227 T227 L237 L237 L237 AR5 L237 AR5 L237 AR5 L237 AR5 L78 AR5	SER PRO PRO CIV CIV CIV SER SER SER SER SER SER
LEU THR PRO ASP ASP ASP VAL VAL C277 C277 C277 C277 C277 C277 C277 C27	A292 1311 1311 1311 1311 1311 1322 1322 1	GLU SER VAL HIS HIS HIS HIS HIS	
• Molecule 1: Bi	functional nitrilase/nitrile hydra	atase NIT4	
Chain A:	69%	9% •	20%
MET MET MET MET GLN GLN GLN GLN GLN GLN HIS MET MET MET	PALA PALA PINE ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	V40 V41 Q42 V46 T53 T53 L61	H104 H104 H120 H120 V128 V128 V128 V128 V128
M165 L169 L169 A195 A195 A195 C196 C196	N200 R201 1214 E2115 7217 7227 1226 1227 1227 1227 1227 1227	TTT MET PHE SER GLV GLV GLU LEU THEU	PR0 ASP ASP VAL VZT6 C279 C279 C279 A304 A304 A304 A304 1311
F318 D319 V320 V321 C322 H323 H326 S331 S331	A335 Strain L1YS VAL MET ASP CLU ASP ALD ASP ALD H1S H1S H1S H1S H1S		
• Molecule 1: Bi	functional nitrilase/nitrile hydra	atase NIT4	
Chain L:	66%	13%	20%
MET MET SER GLN GLN GLN GLN THR FTHR HIS THR THR MET	PALA PALA THR THR THR GLV GLV GLV CLLN GLN GLN GLN ASP SER SER SER SER	v36 q42 T53 A57 L61	179 680 192 192 R95 R100 R100



• Molecule 1: Bifunctional nitrilase/nitrile hydratase NIT4

С	ha	air	ı I	K :	-											(56°	%														12	2%		•				20	2%	5							
MET	SER	GLN	GLN GLN	THR	SER	HIS	THR	ALA	PRO	GLN	THR	ASN	SIH	GLN	ILE	PHE	UHU CI II	TLE	ASP	MET	SER	ALA GLY	ASP	SER	SER	SER. 135	0	V40	V41	Q42	V46		T53		L61	17.2		P83	R84		T87	A91	192		R95		N1 NO	
	R104	R120	1102	0217	Y128	K129 V130		H161	M165		L169	1212 1	7,170	T181		V184	F185	0017	A195	I196	C197	N200	R201		1214	E215 1216	Y217		T227	t 00 ,	r.23/	L244		R251	ARG	LYS	TYR	PRO	SER	PRO	PRO CTT	TYR	MET	PHE	SER	GLY	HES	



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-72.98°, rise=17.48 Å, ax-	Depositor
	ial sym=C1	
Number of segments used	133106	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	45.5	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k 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		B	ond angles
	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.43	0/2276	0.79	0/3081
1	В	0.54	1/2276~(0.0%)	0.86	4/3081~(0.1%)
1	С	0.44	0/2276	0.79	1/3081~(0.0%)
1	D	0.57	1/2276~(0.0%)	0.84	1/3081~(0.0%)
1	Е	0.44	0/2276	0.79	0/3081
1	F	0.46	0/2276	0.85	3/3081~(0.1%)
1	G	0.44	0/2276	0.80	1/3081~(0.0%)
1	Н	0.51	1/2276~(0.0%)	0.85	1/3081~(0.0%)
1	Ι	0.44	0/2276	0.81	1/3081~(0.0%)
1	J	0.46	1/2276~(0.0%)	0.84	4/3081~(0.1%)
1	Κ	0.44	0/2276	0.80	1/3081~(0.0%)
1	Ĺ	0.47	2/2276~(0.1%)	0.84	3/3081~(0.1%)
All	All	0.47	6/27312~(0.0%)	0.82	$20/\overline{36972}~(0.1\%)$

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	А	0	3
1	С	0	3
1	D	0	1
1	Е	0	3
1	G	0	3
1	Ι	0	3
1	Κ	0	3
1	L	0	1
All	All	0	20

All (6) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	D	251	ARG	C-O	16.22	1.54	1.23
1	В	251	ARG	C-O	13.75	1.49	1.23
1	Н	251	ARG	C-O	10.87	1.44	1.23
1	L	251	ARG	C-O	6.64	1.35	1.23
1	J	251	ARG	C-O	5.64	1.34	1.23
1	L	204	SER	CA-CB	-5.00	1.45	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	251	ARG	CA-C-O	7.85	136.59	120.10
1	В	206	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	207	THR	OG1-CB-CG2	-6.03	96.14	110.00
1	L	206	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	F	207	THR	OG1-CB-CG2	-5.95	96.31	110.00
1	Н	207	THR	OG1-CB-CG2	-5.90	96.43	110.00
1	J	326	ARG	CG-CD-NE	5.88	124.14	111.80
1	G	326	ARG	CG-CD-NE	5.70	123.76	111.80
1	В	207	THR	OG1-CB-CG2	-5.66	96.98	110.00
1	J	207	THR	OG1-CB-CG2	-5.65	97.01	110.00
1	J	326	ARG	CB-CG-CD	5.62	126.23	111.60
1	F	206	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	J	206	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	L	207	THR	OG1-CB-CG2	-5.51	97.32	110.00
1	L	326	ARG	CB-CG-CD	5.48	125.85	111.60
1	F	326	ARG	CB-CG-CD	5.43	125.72	111.60
1	Ι	326	ARG	CG-CD-NE	5.12	122.54	111.80
1	С	326	ARG	CG-CD-NE	5.06	122.42	111.80
1	К	201	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	В	326	ARG	CB-CG-CD	5.02	124.66	111.60

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	201	ARG	Sidechain
1	А	320	VAL	Peptide
1	А	326	ARG	Sidechain
1	С	201	ARG	Sidechain
1	С	320	VAL	Peptide
1	С	326	ARG	Sidechain
1	D	201	ARG	Sidechain



Mol	Chain	Res	Type	Group
1	Е	201	ARG	Sidechain
1	Е	320	VAL	Peptide
1	Е	326	ARG	Sidechain
1	G	201	ARG	Sidechain
1	G	320	VAL	Peptide
1	G	326	ARG	Sidechain
1	Ι	201	ARG	Sidechain
1	Ι	320	VAL	Peptide
1	Ι	326	ARG	Sidechain
1	Κ	201	ARG	Sidechain
1	Κ	320	VAL	Peptide
1	Κ	326	ARG	Sidechain
1	L	100	ARG	Sidechain

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	А	2226	0	2224	27	0
1	В	2226	0	2224	41	0
1	С	2226	0	2224	35	0
1	D	2226	0	2224	42	0
1	Е	2226	0	2224	40	0
1	F	2226	0	2224	40	0
1	G	2226	0	2224	39	0
1	Н	2226	0	2224	43	0
1	Ι	2226	0	2224	42	0
1	J	2226	0	2224	40	0
1	Κ	2226	0	2224	40	0
1	L	2226	0	2224	34	0
All	All	26712	0	26688	362	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 7.

All (362) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic	Clash
	At0111-2	distance (Å)	overlap (Å)
1:J:168:ALA:HB2	1:K:95:ARG:HH21	1.29	0.97
1:J:168:ALA:HB2	1:K:95:ARG:NH2	1.91	0.84
1:D:196:ILE:HG22	1:D:197:CYS:H	1.42	0.84
1:H:196:ILE:HG22	1:H:197:CYS:H	1.43	0.84
1:J:92:ILE:HG21	1:K:84:ARG:HA	1.60	0.84
1:L:320:VAL:HG22	1:L:321:VAL:H	1.42	0.83
1:L:196:ILE:HG22	1:L:197:CYS:H	1.43	0.83
1:E:84:ARG:HA	1:D:92:ILE:HG21	1.60	0.83
1:B:320:VAL:HG22	1:B:321:VAL:H	1.44	0.82
1:J:196:ILE:HG22	1:J:197:CYS:H	1.44	0.82
1:B:196:ILE:HG22	1:B:197:CYS:H	1.43	0.82
1:F:196:ILE:HG22	1:F:197:CYS:H	1.44	0.81
1:C:84:ARG:HA	1:B:92:ILE:HG21	1.61	0.81
1:H:320:VAL:HG22	1:H:321:VAL:H	1.45	0.81
1:G:84:ARG:HA	1:F:92:ILE:HG21	1.61	0.79
1:D:320:VAL:HG22	1:D:321:VAL:H	1.48	0.79
1:I:84:ARG:HA	1:H:92:ILE:HG21	1.64	0.77
1:F:320:VAL:HG22	1:F:321:VAL:H	1.50	0.76
1:B:184:VAL:HG23	1:B:185:PHE:H	1.50	0.76
1:I:196:ILE:HG22	1:I:197:CYS:H	1.50	0.76
1:E:196:ILE:HG22	1:E:197:CYS:H	1.51	0.75
1:L:184:VAL:HG23	1:L:185:PHE:H	1.50	0.75
1:H:184:VAL:HG23	1:H:185:PHE:H	1.50	0.75
1:J:184:VAL:HG23	1:J:185:PHE:H	1.50	0.74
1:F:184:VAL:HG23	1:F:185:PHE:H	1.52	0.74
1:C:318:PHE:HE2	1:C:320:VAL:HG22	1.53	0.74
1:G:196:ILE:HG22	1:G:197:CYS:H	1.53	0.74
1:A:196:ILE:HG22	1:A:197:CYS:H	1.53	0.73
1:I:184:VAL:HG12	1:I:214:ILE:HD11	1.70	0.73
1:G:184:VAL:HG12	1:G:214:ILE:HD11	1.68	0.73
1:E:184:VAL:HG12	1:E:214:ILE:HD11	1.71	0.73
1:K:196:ILE:HG22	1:K:197:CYS:H	1.53	0.72
1:G:318:PHE:CE2	1:G:320:VAL:HG22	2.25	0.71
1:C:318:PHE:CE2	1:C:320:VAL:HG22	2.24	0.71
1:D:184:VAL:HG23	1:D:185:PHE:H	1.52	0.71
1:I:318:PHE:HE2	1:I:320:VAL:HG22	1.54	0.71
1:C:196:ILE:HG22	1:C:197:CYS:H	1.54	0.71
1:L:324:TYR:HA	1:K:165:MET:HE1	1.73	0.70
1:E:318:PHE:HE2	1:E:320:VAL:HG22	1.55	0.70
1:G:95:ARG:HH21	1:F:168:ALA:HB2	1.56	0.69
1:A:318:PHE:HE2	1:A:320:VAL:HG22	1.55	0.69
1:F:324:TYR:HA	1:E:165:MET:HE1	1.74	0.69



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:324:TYR:HA	1:A:165:MET:HE1	1.76	0.68
1:I:318:PHE:CE2	1:I:320:VAL:HG22	2.29	0.68
1:C:95:ARG:HH21	1:B:168:ALA:HB2	1.59	0.68
1:I:95:ARG:HH21	1:H:168:ALA:HB2	1.59	0.67
1:G:318:PHE:HE2	1:G:320:VAL:HG22	1.57	0.67
1:K:318:PHE:HE2	1:K:320:VAL:HG22	1.59	0.67
1:A:318:PHE:CE2	1:A:320:VAL:HG22	2.30	0.67
1:L:237:LEU:HD11	1:K:227:THR:HG21	1.77	0.65
1:J:324:TYR:HA	1:I:165:MET:HE1	1.79	0.65
1:E:318:PHE:CE2	1:E:320:VAL:HG22	2.32	0.65
1:E:95:ARG:HH21	1:D:168:ALA:HB2	1.63	0.64
1:K:318:PHE:CE2	1:K:320:VAL:HG22	2.33	0.64
1:J:283:ILE:HG22	1:J:292:ALA:HB3	1.79	0.63
1:B:237:LEU:HD11	1:A:227:THR:HG21	1.79	0.63
1:J:91:ALA:HA	1:K:87:THR:HG22	1.81	0.62
1:L:335:ARG:HH22	1:K:331:SER:HB3	1.63	0.62
1:F:92:ILE:HG23	1:F:92:ILE:O	1.99	0.62
1:C:184:VAL:HG12	1:C:214:ILE:HD11	1.81	0.61
1:H:324:TYR:HA	1:G:165:MET:HE1	1.80	0.61
1:D:324:TYR:HA	1:C:165:MET:HE1	1.82	0.61
1:A:46:VAL:HG22	1:A:53:THR:HB	1.83	0.61
1:E:46:VAL:HG22	1:E:53:THR:HB	1.83	0.61
1:K:46:VAL:HG22	1:K:53:THR:HB	1.83	0.61
1:K:184:VAL:HG12	1:K:214:ILE:HD11	1.82	0.61
1:F:237:LEU:HD11	1:E:227:THR:HG21	1.82	0.60
1:K:215:GLU:HB2	1:K:311:ILE:HD13	1.82	0.60
1:A:184:VAL:HG12	1:A:214:ILE:HD11	1.84	0.60
1:I:46:VAL:HG22	1:I:53:THR:HB	1.84	0.60
1:H:237:LEU:HD11	1:G:227:THR:HG21	1.83	0.59
1:A:215:GLU:HB2	1:A:311:ILE:HD13	1.83	0.59
1:B:46:VAL:HG22	1:B:53:THR:HB	1.85	0.59
1:B:92:ILE:O	1:B:92:ILE:HG23	2.02	0.59
1:D:79:ILE:HG13	1:D:136:VAL:HG12	1.84	0.59
1:D:237:LEU:HD11	1:C:227:THR:HG21	1.83	0.59
1:L:46:VAL:HG22	1:L:53:THR:HB	1.85	0.59
1:J:92:ILE:HG23	1:J:92:ILE:O	2.02	0.59
1:C:46:VAL:HG22	1:C:53:THR:HB	1.85	0.58
1:F:46:VAL:HG22	1:F:53:THR:HB	1.85	0.58
1:L:42:GLN:NE2	1:L:279:GLY:O	2.37	0.58
1:H:92:ILE:HG23	1:H:92:ILE:O	2.02	0.58
1:B:215:GLU:HB2	1:B:311:ILE:HD13	1.85	0.58



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	A	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:46:VAL:HG22	1:D:53:THR:HB	1.86	0.58
1:B:42:GLN:NE2	1:B:279:GLY:O	2.37	0.58
1:F:215:GLU:HB2	1:F:311:ILE:HD13	1.85	0.58
1:E:215:GLU:HB2	1:E:311:ILE:HD13	1.84	0.58
1:H:215:GLU:HB2	1:H:311:ILE:HD13	1.86	0.58
1:J:42:GLN:NE2	1:J:279:GLY:O	2.37	0.58
1:G:46:VAL:HG22	1:G:53:THR:HB	1.85	0.57
1:F:283:ILE:HG22	1:F:292:ALA:HB3	1.86	0.57
1:H:46:VAL:HG22	1:H:53:THR:HB	1.86	0.57
1:I:321:VAL:HG21	1:K:341:ALA:HB3	1.86	0.57
1:F:42:GLN:NE2	1:F:279:GLY:O	2.37	0.57
1:H:313:ARG:HB2	1:F:100:ARG:HB3	1.87	0.57
1:F:79:ILE:HG13	1:F:136:VAL:HG12	1.86	0.57
1:B:320:VAL:HG22	1:B:321:VAL:N	2.18	0.56
1:B:331:SER:HB3	1:A:335:ARG:HH22	1.68	0.56
1:D:92:ILE:HG23	1:D:92:ILE:O	2.05	0.56
1:J:46:VAL:HG22	1:J:53:THR:HB	1.88	0.56
1:H:42:GLN:NE2	1:H:279:GLY:O	2.39	0.56
1:D:42:GLN:NE2	1:D:279:GLY:O	2.38	0.56
1:L:215:GLU:HB2	1:L:311:ILE:HD13	1.86	0.56
1:G:215:GLU:HB2	1:G:311:ILE:HD13	1.87	0.56
1:H:283:ILE:HG22	1:H:292:ALA:HB3	1.88	0.56
1:I:215:GLU:HB2	1:I:311:ILE:HD13	1.88	0.56
1:J:215:GLU:HB2	1:J:311:ILE:HD13	1.88	0.55
1:J:100:ARG:HB3	1:L:313:ARG:HB2	1.88	0.55
1:D:84:ARG:NH1	1:D:277:CYS:SG	2.79	0.55
1:B:283:ILE:HG22	1:B:292:ALA:HB3	1.87	0.55
1:D:215:GLU:HB2	1:D:311:ILE:HD13	1.88	0.55
1:B:123:LEU:HD11	1:K:123:LEU:HD11	1.87	0.55
1:C:244:LEU:HD13	1:C:283:ILE:HD12	1.89	0.55
1:K:244:LEU:HD13	1:K:283:ILE:HD12	1.88	0.55
1:H:84:ARG:NH1	1:H:277:CYS:SG	2.80	0.54
1:B:184:VAL:HG12	1:B:212:LYS:HD3	1.90	0.54
1:L:320:VAL:HG22	1:L:321:VAL:N	2.18	0.54
1:K:42:GLN:NE2	1:K:279:GLY:O	2.40	0.54
1:J:87:THR:HG22	1:K:91:ALA:HA	1.90	0.54
1:D:283:ILE:CG2	1:D:292:ALA:HB3	2.37	0.54
1:L:335:ARG:HH22	1:K:331:SER:CB	2.21	0.54
1:C:91:ALA:HA	1:B:87:THR:HG22	1.90	0.54
1:J:320:VAL:HG22	1:J:321:VAL:H	1.73	0.54
1:G:42:GLN:NE2	1:G:279:GLY:O	2.40	0.54



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	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:42:GLN:NE2	1:A:279:GLY:O	2.40	0.54
1:L:283:ILE:HG22	1:L:292:ALA:HB3	1.88	0.54
1:C:42:GLN:NE2	1:C:279:GLY:O	2.39	0.54
1:C:215:GLU:HB2	1:C:311:ILE:HD13	1.89	0.54
1:I:87:THR:HG22	1:H:91:ALA:HA	1.89	0.54
1:F:184:VAL:HG12	1:F:212:LYS:HD3	1.90	0.54
1:L:36:VAL:HG11	1:L:189:ILE:HB	1.90	0.53
1:J:84:ARG:NH1	1:J:277:CYS:SG	2.80	0.53
1:E:42:GLN:NE2	1:E:279:GLY:O	2.41	0.53
1:F:36:VAL:HG11	1:F:189:ILE:HB	1.89	0.53
1:B:36:VAL:HG11	1:B:189:ILE:HB	1.91	0.53
1:B:84:ARG:NH1	1:B:277:CYS:SG	2.80	0.53
1:D:196:ILE:HG22	1:D:197:CYS:N	2.19	0.53
1:L:84:ARG:NH1	1:L:277:CYS:SG	2.81	0.53
1:I:91:ALA:HA	1:H:87:THR:HG22	1.91	0.53
1:B:195:ALA:HB3	1:B:200:ASN:HD21	1.74	0.53
1:F:283:ILE:CG2	1:F:292:ALA:HB3	2.38	0.53
1:G:87:THR:HG22	1:F:91:ALA:HA	1.91	0.53
1:G:244:LEU:HD13	1:G:283:ILE:HD12	1.89	0.53
1:E:244:LEU:HD13	1:E:283:ILE:HD12	1.91	0.53
1:H:196:ILE:HG22	1:H:197:CYS:N	2.19	0.52
1:J:184:VAL:HG12	1:J:212:LYS:HD3	1.92	0.52
1:D:313:ARG:HB2	1:B:100:ARG:HB3	1.92	0.52
1:L:184:VAL:HG12	1:L:212:LYS:HD3	1.91	0.52
1:H:184:VAL:HG12	1:H:212:LYS:HD3	1.92	0.52
1:L:79:ILE:HG13	1:L:136:VAL:HG12	1.92	0.52
1:I:42:GLN:NE2	1:I:279:GLY:O	2.42	0.52
1:H:320:VAL:HG22	1:H:321:VAL:N	2.20	0.52
1:B:79:ILE:HG13	1:B:136:VAL:HG12	1.91	0.52
1:A:101:ASP:HA	1:A:104:ARG:HG2	1.92	0.52
1:C:87:THR:HG22	1:B:91:ALA:HA	1.92	0.52
1:E:61:LEU:HD11	1:E:128:TYR:OH	2.10	0.52
1:B:196:ILE:HG22	1:B:197:CYS:N	2.20	0.52
1:J:79:ILE:HG13	1:J:136:VAL:HG12	1.92	0.52
1:J:83:PRO:O	1:K:92:ILE:HG12	2.10	0.52
1:H:79:ILE:HG13	1:H:136:VAL:HG12	1.91	0.52
1:L:237:LEU:HD11	1:K:227:THR:CG2	2.40	0.52
1:J:36:VAL:HG11	1:J:189:ILE:HB	1.93	0.51
1:G:61:LEU:HD11	1:G:128:TYR:OH	2.09	0.51
1:D:184:VAL:HG12	1:D:212:LYS:HD3	1.92	0.51
1:I:321:VAL:CG2	1:K:341:ALA:HB3	2.41	0.51



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	i agem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:91:ALA:HA	1:D:87:THR:HG22	1.93	0.51
1:D:324:TYR:HA	1:C:165:MET:CE	2.40	0.51
1:D:283:ILE:HG22	1:D:292:ALA:HB3	1.91	0.51
1:F:84:ARG:NH1	1:F:277:CYS:SG	2.84	0.51
1:L:196:ILE:HG22	1:L:197:CYS:N	2.20	0.51
1:K:61:LEU:HD11	1:K:128:TYR:OH	2.10	0.51
1:C:61:LEU:HD11	1:C:128:TYR:OH	2.10	0.51
1:D:36:VAL:HG11	1:D:189:ILE:HB	1.93	0.51
1:D:79:ILE:CG1	1:D:136:VAL:HG12	2.40	0.51
1:E:87:THR:HG22	1:D:91:ALA:HA	1.92	0.51
1:L:195:ALA:HB3	1:L:200:ASN:HD21	1.75	0.51
1:B:184:VAL:CG1	1:B:212:LYS:HD3	2.42	0.50
1:K:101:ASP:HA	1:K:104:ARG:HG2	1.93	0.50
1:H:36:VAL:HG11	1:H:189:ILE:HB	1.93	0.50
1:F:196:ILE:HG22	1:F:197:CYS:N	2.20	0.50
1:H:335:ARG:HH22	1:G:331:SER:HB3	1.77	0.50
1:B:283:ILE:CG2	1:B:292:ALA:HB3	2.41	0.50
1:C:40:VAL:HG12	1:C:73:VAL:HB	1.93	0.50
1:A:61:LEU:HD11	1:A:128:TYR:OH	2.11	0.50
1:E:184:VAL:HG12	1:E:214:ILE:CD1	2.42	0.49
1:I:341:ALA:HB3	1:G:321:VAL:HG21	1.93	0.49
1:F:320:VAL:HG22	1:F:321:VAL:N	2.23	0.49
1:H:283:ILE:CG2	1:H:292:ALA:HB3	2.42	0.49
1:G:40:VAL:HG12	1:G:73:VAL:HB	1.94	0.49
1:D:320:VAL:HG22	1:D:321:VAL:N	2.22	0.49
1:A:244:LEU:HD13	1:A:283:ILE:HD12	1.94	0.49
1:K:195:ALA:HB3	1:K:200:ASN:HD21	1.78	0.49
1:A:195:ALA:HB3	1:A:200:ASN:HD21	1.77	0.49
1:L:324:TYR:HA	1:K:165:MET:CE	2.42	0.49
1:J:237:LEU:HD11	1:I:227:THR:HG21	1.95	0.49
1:B:335:ARG:HH22	1:A:331:SER:HB3	1.77	0.49
1:L:184:VAL:CG1	1:L:212:LYS:HD3	2.43	0.49
1:J:313:ARG:HB2	1:H:100:ARG:HB3	1.95	0.49
1:F:313:ARG:HB2	1:D:100:ARG:HB3	1.95	0.49
1:B:324:TYR:HA	1:A:165:MET:CE	2.42	0.49
1:E:101:ASP:HA	1:E:104:ARG:HG2	1.94	0.49
1:B:237:LEU:HD11	1:A:227:THR:CG2	2.42	0.49
1:J:196:ILE:HG22	1:J:197:CYS:N	2.20	0.48
1:D:195:ALA:HB3	1:D:200:ASN:HD21	1.78	0.48
1:I:61:LEU:HD11	1:I:128:TYR:OH	2.12	0.48
1:I:244:LEU:HD13	1:I:283:ILE:HD12	1.94	0.48



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	io ao pagoini	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:195:ALA:HB3	1:F:200:ASN:HD21	1.78	0.48
1:H:324:TYR:HA	1:G:165:MET:CE	2.41	0.48
1:D:227:THR:HG23	1:C:237:LEU:HD13	1.96	0.48
1:C:341:ALA:HB3	1:A:321:VAL:HG21	1.94	0.48
1:F:335:ARG:HH22	1:E:331:SER:HB3	1.78	0.48
1:C:101:ASP:HA	1:C:104:ARG:HG2	1.96	0.48
1:I:40:VAL:HG12	1:I:73:VAL:HB	1.95	0.48
1:G:91:ALA:HA	1:F:87:THR:HG22	1.96	0.48
1:B:79:ILE:CG1	1:B:136:VAL:HG12	2.44	0.48
1:L:79:ILE:CG1	1:L:136:VAL:HG12	2.44	0.48
1:L:283:ILE:CG2	1:L:292:ALA:HB3	2.43	0.48
1:H:195:ALA:HB3	1:H:200:ASN:HD21	1.78	0.48
1:F:184:VAL:CG1	1:F:212:LYS:HD3	2.44	0.48
1:J:227:THR:HG23	1:I:237:LEU:HD13	1.95	0.48
1:I:101:ASP:HA	1:I:104:ARG:HG2	1.95	0.48
1:G:195:ALA:HB3	1:G:200:ASN:HD21	1.79	0.48
1:G:92:ILE:HG12	1:F:83:PRO:O	2.13	0.47
1:D:335:ARG:HH22	1:C:331:SER:HB3	1.80	0.47
1:J:195:ALA:HB3	1:J:200:ASN:HD21	1.79	0.47
1:K:200:ASN:ND2	1:K:217:TYR:OH	2.47	0.47
1:H:227:THR:HG23	1:G:237:LEU:HD13	1.96	0.47
1:C:92:ILE:HG12	1:B:83:PRO:O	2.15	0.47
1:A:161:HIS:HA	1:A:181:THR:HG22	1.97	0.47
1:K:161:HIS:HA	1:K:181:THR:HG22	1.97	0.46
1:J:283:ILE:CG2	1:J:292:ALA:HB3	2.45	0.46
1:I:161:HIS:HA	1:I:181:THR:HG22	1.97	0.46
1:H:80:GLY:HA3	1:H:137:ILE:HB	1.96	0.46
1:E:40:VAL:HG12	1:E:73:VAL:HB	1.96	0.46
1:J:79:ILE:CG1	1:J:136:VAL:HG12	2.46	0.46
1:I:92:ILE:HG12	1:H:83:PRO:O	2.16	0.46
1:F:237:LEU:HD11	1:E:227:THR:CG2	2.44	0.46
1:D:333:ASN:HB3	1:B:343:SER:HB2	1.97	0.46
1:I:244:LEU:CD1	1:I:283:ILE:HD12	2.46	0.46
1:F:79:ILE:CG1	1:F:136:VAL:HG12	2.45	0.46
1:J:184:VAL:CG1	1:J:212:LYS:HD3	2.44	0.46
1:I:187:THR:OG1	1:I:190:GLY:O	2.29	0.46
1:A:200:ASN:ND2	1:A:217:TYR:OH	2.47	0.46
1:H:79:ILE:CG1	1:H:136:VAL:HG12	2.46	0.46
1:A:283:ILE:HD13	1:A:304:ALA:HB3	1.98	0.46
1:H:335:ARG:HH22	1:G:331:SER:CB	2.28	0.46
1:E:92:ILE:HG12	1:D:83:PRO:O	2.15	0.46



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	io ao pagoini	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:325:SER:OG	1:J:325:SER:O	2.33	0.45
1:G:101:ASP:HA	1:G:104:ARG:HG2	1.97	0.45
1:F:227:THR:HG23	1:E:237:LEU:HD13	1.97	0.45
1:F:80:GLY:HA3	1:F:137:ILE:HB	1.99	0.45
1:E:320:VAL:HG12	1:E:321:VAL:H	1.82	0.45
1:G:244:LEU:CD1	1:G:283:ILE:HD12	2.47	0.45
1:J:324:TYR:HA	1:I:165:MET:CE	2.46	0.45
1:F:287:LEU:HD11	1:D:100:ARG:HH12	1.81	0.45
1:F:324:TYR:HA	1:E:165:MET:CE	2.45	0.45
1:D:161:HIS:HA	1:D:181:THR:HG22	1.99	0.45
1:I:184:VAL:HG12	1:I:214:ILE:CD1	2.44	0.45
1:G:196:ILE:HG22	1:G:197:CYS:N	2.29	0.45
1:J:92:ILE:HG12	1:K:83:PRO:O	2.17	0.44
1:B:283:ILE:HD13	1:B:283:ILE:HG21	1.71	0.44
1:I:196:ILE:HG22	1:I:197:CYS:N	2.26	0.44
1:E:100:ARG:HH12	1:C:287:LEU:HD11	1.82	0.44
1:D:80:GLY:HA3	1:D:137:ILE:HB	1.99	0.44
1:J:343:SER:HB2	1:L:333:ASN:HB3	1.99	0.44
1:E:161:HIS:HA	1:E:181:THR:HG22	1.99	0.44
1:J:161:HIS:HA	1:J:181:THR:HG22	2.00	0.44
1:J:283:ILE:HD13	1:J:304:ALA:HB3	2.00	0.44
1:D:237:LEU:HD11	1:C:227:THR:CG2	2.46	0.44
1:E:196:ILE:HG22	1:E:197:CYS:N	2.27	0.44
1:C:320:VAL:HG12	1:C:321:VAL:H	1.82	0.44
1:C:95:ARG:HB3	1:C:100:ARG:HH21	1.82	0.44
1:J:320:VAL:O	1:J:322:GLY:N	2.45	0.44
1:E:165:MET:HE2	1:E:165:MET:HB2	1.86	0.43
1:B:335:ARG:HH22	1:A:331:SER:CB	2.31	0.43
1:K:244:LEU:CD1	1:K:283:ILE:HD12	2.47	0.43
1:E:55:ASP:OD1	1:E:120:ARG:NH2	2.50	0.43
1:D:283:ILE:HG21	1:D:283:ILE:HD13	1.71	0.43
1:I:95:ARG:HB3	1:I:100:ARG:HH21	1.83	0.43
1:I:320:VAL:HG12	1:I:321:VAL:H	1.84	0.43
1:H:283:ILE:HD13	1:H:283:ILE:HG21	1.70	0.43
1:H:333:ASN:HB3	1:F:343:SER:HB2	2.01	0.43
1:J:168:ALA:O	1:K:172:CYS:SG	2.73	0.43
1:I:287:LEU:HD11	1:K:100:ARG:HH12	1.84	0.43
1:H:184:VAL:CG1	1:H:212:LYS:HD3	2.49	0.43
1:F:333:ASN:HB3	1:D:343:SER:HB2	2.00	0.43
1:F:335:ARG:HH22	1:E:331:SER:CB	2.31	0.43
1:C:341:ALA:HB3	1:A:321:VAL:CG2	2.48	0.43



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	loue page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:341:ALA:HB3	1:E:321:VAL:HG21	2.00	0.43
1:F:57:ALA:O	1:F:61:LEU:HB2	2.18	0.43
1:E:200:ASN:ND2	1:E:217:TYR:OH	2.51	0.43
1:D:57:ALA:O	1:D:61:LEU:HB2	2.19	0.43
1:G:95:ARG:HB3	1:G:100:ARG:HH21	1.83	0.43
1:D:287:LEU:HD11	1:B:100:ARG:HH12	1.83	0.43
1:L:331:SER:HB3	1:K:335:ARG:HH22	1.82	0.43
1:H:237:LEU:HD11	1:G:227:THR:CG2	2.48	0.42
1:D:184:VAL:CG1	1:D:212:LYS:HD3	2.49	0.42
1:K:40:VAL:HG12	1:K:73:VAL:HB	2.01	0.42
1:K:322:GLY:HA2	1:K:323:HIS:HA	1.83	0.42
1:J:57:ALA:O	1:J:61:LEU:HB2	2.18	0.42
1:D:335:ARG:HH22	1:C:331:SER:CB	2.32	0.42
1:H:161:HIS:HA	1:H:181:THR:HG22	2.01	0.42
1:E:92:ILE:HD12	1:E:92:ILE:HA	1.95	0.42
1:J:335:ARG:HH22	1:I:331:SER:HB3	1.84	0.42
1:D:325:SER:OG	1:D:325:SER:O	2.36	0.42
1:I:313:ARG:HB2	1:K:100:ARG:HB3	2.01	0.42
1:H:39:THR:HG22	1:H:303:THR:HB	2.00	0.42
1:G:161:HIS:HA	1:G:181:THR:HG22	2.01	0.42
1:J:333:ASN:HB3	1:H:343:SER:HB2	2.01	0.42
1:I:195:ALA:HB3	1:I:200:ASN:HD21	1.84	0.42
1:A:40:VAL:HG12	1:A:73:VAL:HB	2.01	0.42
1:K:283:ILE:HD13	1:K:304:ALA:HB3	2.01	0.42
1:G:200:ASN:ND2	1:G:217:TYR:OH	2.53	0.42
1:E:341:ALA:HB3	1:C:321:VAL:HG21	2.00	0.42
1:B:57:ALA:O	1:B:61:LEU:HB2	2.19	0.42
1:B:331:SER:CB	1:A:335:ARG:HH22	2.31	0.42
1:E:187:THR:OG1	1:E:190:GLY:O	2.29	0.42
1:B:227:THR:HG23	1:A:237:LEU:HD13	2.02	0.41
1:L:227:THR:HG23	1:K:237:LEU:HD13	2.01	0.41
1:J:335:ARG:HH22	1:I:331:SER:CB	2.33	0.41
1:H:283:ILE:HD13	1:H:304:ALA:HB3	2.02	0.41
1:L:80:GLY:HA3	1:L:137:ILE:HB	2.01	0.41
1:I:61:LEU:HD11	1:I:128:TYR:CZ	2.56	0.41
1:L:57:ALA:O	1:L:61:LEU:HB2	2.19	0.41
1:L:147:THR:OG1	1:L:148:VAL:N	2.54	0.41
1:I:342:VAL:HG22	1:G:332:LEU:HD23	2.03	0.41
1:F:39:THR:HG22	1:F:303:THR:HB	2.01	0.41
1:C:36:VAL:HG11	1:C:189:ILE:HB	2.03	0.41
1:A:322:GLY:HA2	1:A:323:HIS:HA	1.83	0.41



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Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:I:341:ALA:HB3	1:G:321:VAL:CG2	2.50	0.41
1:H:196:ILE:CG2	1:H:197:CYS:H	2.24	0.41
1:H:287:LEU:HD11	1:F:100:ARG:HH12	1.85	0.41
1:H:325:SER:OG	1:H:325:SER:O	2.38	0.41
1:B:80:GLY:HA3	1:B:137:ILE:HB	2.02	0.41
1:L:161:HIS:HA	1:L:181:THR:HG22	2.03	0.41
1:I:100:ARG:HB3	1:G:313:ARG:HB2	2.03	0.41
1:I:100:ARG:HH12	1:G:287:LEU:HD11	1.86	0.41
1:G:204:SER:HA	1:G:207:THR:HG22	2.03	0.41
1:L:325:SER:OG	1:L:325:SER:O	2.39	0.41
1:G:165:MET:HB2	1:G:165:MET:HE2	1.77	0.41
1:E:39:THR:HG22	1:E:303:THR:HB	2.02	0.41
1:E:244:LEU:CD1	1:E:283:ILE:HD12	2.50	0.41
1:C:283:ILE:HD13	1:C:304:ALA:HB3	2.03	0.41
1:K:186:ASP:OD1	1:K:186:ASP:N	2.54	0.41
1:H:92:ILE:HD12	1:H:92:ILE:HA	1.97	0.41
1:E:322:GLY:HA2	1:E:323:HIS:HA	1.83	0.41
1:I:206:ARG:HH11	1:I:206:ARG:HD2	1.68	0.40
1:G:36:VAL:HG11	1:G:189:ILE:HB	2.03	0.40
1:G:283:ILE:HD13	1:G:304:ALA:HB3	2.02	0.40
1:C:187:THR:OG1	1:C:190:GLY:O	2.30	0.40
1:L:335:ARG:NH2	1:K:331:SER:HB3	2.34	0.40
1:I:283:ILE:HD13	1:I:304:ALA:HB3	2.03	0.40
1:D:39:THR:HG22	1:D:303:THR:HB	2.03	0.40
1:B:147:THR:OG1	1:B:148:VAL:N	2.53	0.40
1:F:283:ILE:HG21	1:F:283:ILE:HD13	1.73	0.40
1:C:244:LEU:CD1	1:C:283:ILE:HD12	2.51	0.40
1:B:161:HIS:HA	1:B:181:THR:HG22	2.03	0.40
1:L:92:ILE:O	1:L:92:ILE:HG23	2.19	0.40
1:E:283:ILE:HD13	1:E:304:ALA:HB3	2.03	0.40
1:C:186:ASP:N	1:C:186:ASP:OD1	2.55	0.40
1:E:195:ALA:HB3	1:E:200:ASN:HD21	1.87	0.40
1:C:92:ILE:HD12	1:C:92:ILE:HA	1.98	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	Perc	entiles
1	А	285/361~(79%)	236 (83%)	47 (16%)	2 (1%)	22	55
1	В	285/361~(79%)	238 (84%)	45 (16%)	2 (1%)	22	55
1	С	285/361~(79%)	238 (84%)	45 (16%)	2 (1%)	22	55
1	D	285/361~(79%)	236 (83%)	46 (16%)	3 (1%)	14	44
1	Е	285/361~(79%)	235 (82%)	48 (17%)	2 (1%)	22	55
1	F	285/361~(79%)	240 (84%)	43 (15%)	2 (1%)	22	55
1	G	285/361~(79%)	238 (84%)	45 (16%)	2 (1%)	22	55
1	Н	285/361~(79%)	236 (83%)	47 (16%)	2(1%)	22	55
1	Ι	285/361~(79%)	233 (82%)	50 (18%)	2 (1%)	22	55
1	J	285/361~(79%)	236 (83%)	47 (16%)	2 (1%)	22	55
1	K	285/361~(79%)	236 (83%)	47 (16%)	2 (1%)	22	55
1	L	285/361~(79%)	238 (84%)	45 (16%)	2 (1%)	22	55
All	All	3420/4332 (79%)	2840 (83%)	555 (16%)	25 (1%)	26	55

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	321	VAL
1	Ι	321	VAL
1	Н	321	VAL
1	G	321	VAL
1	F	321	VAL
1	Е	321	VAL
1	D	321	VAL
1	С	321	VAL
1	В	321	VAL
1	А	321	VAL
1	L	321	VAL
1	Κ	321	VAL



Mol	Chain	Res	Type
1	Ι	322	GLY
1	G	322	GLY
1	Е	322	GLY
1	С	322	GLY
1	А	322	GLY
1	K	322	GLY
1	J	92	ILE
1	F	92	ILE
1	D	92	ILE
1	D	197	CYS
1	L	92	ILE
1	Н	92	ILE
1	В	92	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
1	А	233/299~(78%)	226~(97%)	7 (3%)	41	68
1	В	233/299~(78%)	229~(98%)	4 (2%)	60	80
1	С	233/299~(78%)	226~(97%)	7 (3%)	41	68
1	D	233/299~(78%)	229~(98%)	4 (2%)	60	80
1	Ε	233/299~(78%)	226~(97%)	7 (3%)	41	68
1	F	233/299~(78%)	229~(98%)	4 (2%)	60	80
1	G	233/299~(78%)	225~(97%)	8 (3%)	37	65
1	Н	233/299~(78%)	229~(98%)	4 (2%)	60	80
1	Ι	233/299~(78%)	224 (96%)	9 (4%)	32	61
1	J	233/299~(78%)	229~(98%)	4 (2%)	60	80
1	K	233/299 (78%)	225 (97%)	8 (3%)	37	65
1	L	233/299~(78%)	229~(98%)	4 (2%)	60	80
All	All	2796/3588 (78%)	2726 (98%)	70 (2%)	50	72



Mol	Chain	Res	Type
1	J	95	ARG
1	J	120	ARG
1	J	169	LEU
1	J	321	VAL
1	Ι	61	LEU
1	Ι	95	ARG
1	Ι	120	ARG
1	Ι	130	VAL
1	Ι	169	LEU
1	Ι	184	VAL
1	Ι	227	THR
1	Ι	320	VAL
1	Ι	340	LYS
1	Н	95	ARG
1	Н	120	ARG
1	Н	169	LEU
1	Н	321	VAL
1	G	61	LEU
1	G	95	ARG
1	G	120	ARG
1	G	130	VAL
1	G	169	LEU
1	G	184	VAL
1	G	227	THR
1	G	320	VAL
1	F	95	ARG
1	F	120	ARG
1	F	169	LEU
1	F	321	VAL
1	Е	61	LEU
1	Е	95	ARG
1	Е	120	ARG
1	Е	130	VAL
1	Е	169	LEU
1	Е	184	VAL
1	Е	227	THR
1	D	95	ARG
1	D	120	ARG
1	D	169	LEU
1	D	321	VAL
1	С	61	LEU
1	С	95	ARG

All (70) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	С	120	ARG
1	С	130	VAL
1	С	169	LEU
1	С	184	VAL
1	С	227	THR
1	В	95	ARG
1	В	120	ARG
1	В	169	LEU
1	В	321	VAL
1	А	61	LEU
1	А	120	ARG
1	А	130	VAL
1	А	169	LEU
1	А	184	VAL
1	А	227	THR
1	А	320	VAL
1	L	95	ARG
1	L	120	ARG
1	L	169	LEU
1	L	321	VAL
1	K	61	LEU
1	К	95	ARG
1	K	120	ARG
1	К	130	VAL
1	К	169	LEU
1	K	184	VAL
1	К	227	THR
1	К	320	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	200	ASN
1	Ι	200	ASN
1	Н	200	ASN
1	Н	234	HIS
1	G	107	HIS
1	G	200	ASN
1	F	200	ASN
1	F	234	HIS
1	Е	200	ASN
1	D	200	ASN



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Mol	Chain	Res	Type
1	D	234	HIS
1	С	200	ASN
1	В	200	ASN
1	А	200	ASN
1	L	200	ASN
1	Κ	200	ASN

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 monosaccharides 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.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0320. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section was not generated.

