Full wwPDB EM Validation Report ⓘ

Jun 16, 2025 – 01:15 PM JST

PDB ID	:	9IVR / pdb_00009ivr
EMDB ID	:	EMD-60933
Title	:	Cryo-EM structure of the CHIKV nsP3 peptide in complex with the NTF2L domain of G3BP1 (Conformation II)
Authors	:	Wang, J.; Liu, Y.Z.; Lei, J.; Wang, K.T.
Deposited on	:	2024-07-24
Resolution	:	2.80 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:

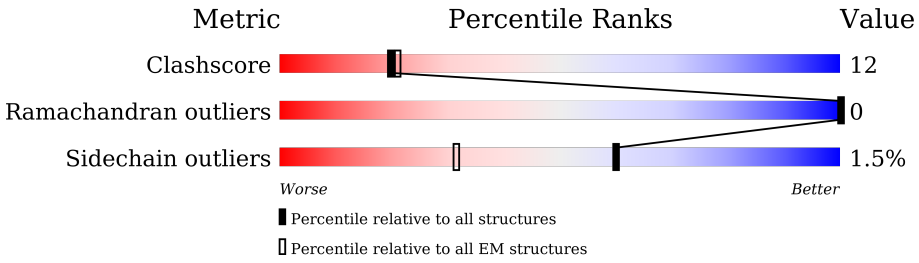
EMDB validation analysis	:	FAILED
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 2.80 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	141	74% 20% • 5%
1	B	141	68% 26% • 5%
1	C	141	66% 31% ••
1	D	141	65% 29% • 5%
1	E	141	70% 25% 5%
1	F	141	62% 33% • 5%
1	G	141	67% 31% •
1	H	141	62% 33% 5%
1	M	141	67% 26% • 5%

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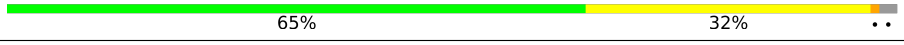
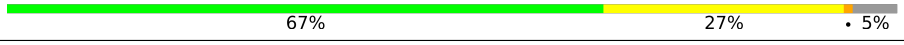
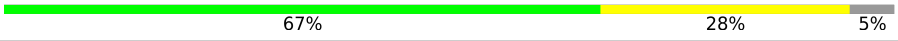
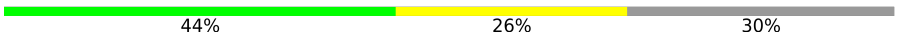
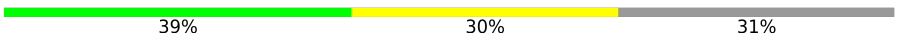
Mol	Chain	Length	Quality of chain
1	N	141	
1	O	141	
1	P	141	
1	Q	141	
1	R	141	
1	S	141	
1	T	141	
2	I	54	
2	J	54	
2	K	54	
2	L	54	
2	U	54	
2	V	54	
2	W	54	
2	X	54	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19758 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 Ras GTPase-activating protein-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	134	Total	C	N	O	S	0	0
			1082	684	198	195	5		
1	C	138	Total	C	N	O	S	0	0
			1114	704	202	201	7		
1	D	134	Total	C	N	O	S	0	0
			1082	684	198	195	5		
1	B	134	Total	C	N	O	S	0	0
			1082	684	198	195	5		
1	P	134	Total	C	N	O	S	0	0
			1082	684	198	195	5		
1	N	138	Total	C	N	O	S	0	0
			1114	704	202	201	7		
1	M	134	Total	C	N	O	S	0	0
			1082	684	198	195	5		
1	O	134	Total	C	N	O	S	0	0
			1082	684	198	195	5		
1	T	134	Total	C	N	O	S	0	0
			1082	684	198	195	5		
1	R	138	Total	C	N	O	S	0	0
			1114	704	202	201	7		
1	Q	134	Total	C	N	O	S	0	0
			1082	684	198	195	5		
1	S	134	Total	C	N	O	S	0	0
			1082	684	198	195	5		
1	E	134	Total	C	N	O	S	1	0
			1088	687	199	196	6		
1	G	138	Total	C	N	O	S	0	0
			1114	704	202	201	7		
1	H	134	Total	C	N	O	S	0	0
			1082	684	198	195	5		
1	F	134	Total	C	N	O	S	0	0
			1082	684	198	195	5		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q13283
A	-1	ALA	-	expression tag	UNP Q13283
A	0	SER	-	expression tag	UNP Q13283
C	-2	GLY	-	expression tag	UNP Q13283
C	-1	ALA	-	expression tag	UNP Q13283
C	0	SER	-	expression tag	UNP Q13283
D	-2	GLY	-	expression tag	UNP Q13283
D	-1	ALA	-	expression tag	UNP Q13283
D	0	SER	-	expression tag	UNP Q13283
B	-2	GLY	-	expression tag	UNP Q13283
B	-1	ALA	-	expression tag	UNP Q13283
B	0	SER	-	expression tag	UNP Q13283
P	-2	GLY	-	expression tag	UNP Q13283
P	-1	ALA	-	expression tag	UNP Q13283
P	0	SER	-	expression tag	UNP Q13283
N	-2	GLY	-	expression tag	UNP Q13283
N	-1	ALA	-	expression tag	UNP Q13283
N	0	SER	-	expression tag	UNP Q13283
M	-2	GLY	-	expression tag	UNP Q13283
M	-1	ALA	-	expression tag	UNP Q13283
M	0	SER	-	expression tag	UNP Q13283
O	-2	GLY	-	expression tag	UNP Q13283
O	-1	ALA	-	expression tag	UNP Q13283
O	0	SER	-	expression tag	UNP Q13283
T	-2	GLY	-	expression tag	UNP Q13283
T	-1	ALA	-	expression tag	UNP Q13283
T	0	SER	-	expression tag	UNP Q13283
R	-2	GLY	-	expression tag	UNP Q13283
R	-1	ALA	-	expression tag	UNP Q13283
R	0	SER	-	expression tag	UNP Q13283
Q	-2	GLY	-	expression tag	UNP Q13283
Q	-1	ALA	-	expression tag	UNP Q13283
Q	0	SER	-	expression tag	UNP Q13283
S	-2	GLY	-	expression tag	UNP Q13283
S	-1	ALA	-	expression tag	UNP Q13283
S	0	SER	-	expression tag	UNP Q13283
E	-2	GLY	-	expression tag	UNP Q13283
E	-1	ALA	-	expression tag	UNP Q13283
E	0	SER	-	expression tag	UNP Q13283
G	-2	GLY	-	expression tag	UNP Q13283
G	-1	ALA	-	expression tag	UNP Q13283
G	0	SER	-	expression tag	UNP Q13283
H	-2	GLY	-	expression tag	UNP Q13283

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	ALA	-	expression tag	UNP Q13283
H	0	SER	-	expression tag	UNP Q13283
F	-2	GLY	-	expression tag	UNP Q13283
F	-1	ALA	-	expression tag	UNP Q13283
F	0	SER	-	expression tag	UNP Q13283

- Molecule 2 is a protein called Polyprotein P1234.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	L	37	Total	C	N	O	0	0
			282	177	38	67		
2	I	38	Total	C	N	O	0	0
			296	188	40	68		
2	V	37	Total	C	N	O	0	0
			282	177	38	67		
2	U	38	Total	C	N	O	0	0
			296	188	40	68		
2	X	37	Total	C	N	O	0	0
			282	177	38	67		
2	W	38	Total	C	N	O	0	0
			296	188	40	68		
2	J	37	Total	C	N	O	0	0
			282	177	38	67		
2	K	38	Total	C	N	O	0	0
			296	188	40	68		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	464	GLY	-	expression tag	UNP A0A0U5KFN5
L	465	PRO	-	expression tag	UNP A0A0U5KFN5
L	466	LEU	-	expression tag	UNP A0A0U5KFN5
L	467	GLY	-	expression tag	UNP A0A0U5KFN5
L	512	HIS	-	expression tag	UNP A0A0U5KFN5
L	513	HIS	-	expression tag	UNP A0A0U5KFN5
L	514	HIS	-	expression tag	UNP A0A0U5KFN5
L	515	HIS	-	expression tag	UNP A0A0U5KFN5
L	516	HIS	-	expression tag	UNP A0A0U5KFN5
L	517	HIS	-	expression tag	UNP A0A0U5KFN5
I	464	GLY	-	expression tag	UNP A0A0U5KFN5
I	465	PRO	-	expression tag	UNP A0A0U5KFN5
I	466	LEU	-	expression tag	UNP A0A0U5KFN5

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Chain	Residue	Modelled	Actual	Comment	Reference
I	467	GLY	-	expression tag	UNP A0A0U5KFN5
I	512	HIS	-	expression tag	UNP A0A0U5KFN5
I	513	HIS	-	expression tag	UNP A0A0U5KFN5
I	514	HIS	-	expression tag	UNP A0A0U5KFN5
I	515	HIS	-	expression tag	UNP A0A0U5KFN5
I	516	HIS	-	expression tag	UNP A0A0U5KFN5
I	517	HIS	-	expression tag	UNP A0A0U5KFN5
V	464	GLY	-	expression tag	UNP A0A0U5KFN5
V	465	PRO	-	expression tag	UNP A0A0U5KFN5
V	466	LEU	-	expression tag	UNP A0A0U5KFN5
V	467	GLY	-	expression tag	UNP A0A0U5KFN5
V	512	HIS	-	expression tag	UNP A0A0U5KFN5
V	513	HIS	-	expression tag	UNP A0A0U5KFN5
V	514	HIS	-	expression tag	UNP A0A0U5KFN5
V	515	HIS	-	expression tag	UNP A0A0U5KFN5
V	516	HIS	-	expression tag	UNP A0A0U5KFN5
V	517	HIS	-	expression tag	UNP A0A0U5KFN5
U	464	GLY	-	expression tag	UNP A0A0U5KFN5
U	465	PRO	-	expression tag	UNP A0A0U5KFN5
U	466	LEU	-	expression tag	UNP A0A0U5KFN5
U	467	GLY	-	expression tag	UNP A0A0U5KFN5
U	512	HIS	-	expression tag	UNP A0A0U5KFN5
U	513	HIS	-	expression tag	UNP A0A0U5KFN5
U	514	HIS	-	expression tag	UNP A0A0U5KFN5
U	515	HIS	-	expression tag	UNP A0A0U5KFN5
U	516	HIS	-	expression tag	UNP A0A0U5KFN5
U	517	HIS	-	expression tag	UNP A0A0U5KFN5
X	464	GLY	-	expression tag	UNP A0A0U5KFN5
X	465	PRO	-	expression tag	UNP A0A0U5KFN5
X	466	LEU	-	expression tag	UNP A0A0U5KFN5
X	467	GLY	-	expression tag	UNP A0A0U5KFN5
X	512	HIS	-	expression tag	UNP A0A0U5KFN5
X	513	HIS	-	expression tag	UNP A0A0U5KFN5
X	514	HIS	-	expression tag	UNP A0A0U5KFN5
X	515	HIS	-	expression tag	UNP A0A0U5KFN5
X	516	HIS	-	expression tag	UNP A0A0U5KFN5
X	517	HIS	-	expression tag	UNP A0A0U5KFN5
W	464	GLY	-	expression tag	UNP A0A0U5KFN5
W	465	PRO	-	expression tag	UNP A0A0U5KFN5
W	466	LEU	-	expression tag	UNP A0A0U5KFN5
W	467	GLY	-	expression tag	UNP A0A0U5KFN5
W	512	HIS	-	expression tag	UNP A0A0U5KFN5

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Chain	Residue	Modelled	Actual	Comment	Reference
W	513	HIS	-	expression tag	UNP A0A0U5KFN5
W	514	HIS	-	expression tag	UNP A0A0U5KFN5
W	515	HIS	-	expression tag	UNP A0A0U5KFN5
W	516	HIS	-	expression tag	UNP A0A0U5KFN5
W	517	HIS	-	expression tag	UNP A0A0U5KFN5
J	464	GLY	-	expression tag	UNP A0A0U5KFN5
J	465	PRO	-	expression tag	UNP A0A0U5KFN5
J	466	LEU	-	expression tag	UNP A0A0U5KFN5
J	467	GLY	-	expression tag	UNP A0A0U5KFN5
J	512	HIS	-	expression tag	UNP A0A0U5KFN5
J	513	HIS	-	expression tag	UNP A0A0U5KFN5
J	514	HIS	-	expression tag	UNP A0A0U5KFN5
J	515	HIS	-	expression tag	UNP A0A0U5KFN5
J	516	HIS	-	expression tag	UNP A0A0U5KFN5
J	517	HIS	-	expression tag	UNP A0A0U5KFN5
K	464	GLY	-	expression tag	UNP A0A0U5KFN5
K	465	PRO	-	expression tag	UNP A0A0U5KFN5
K	466	LEU	-	expression tag	UNP A0A0U5KFN5
K	467	GLY	-	expression tag	UNP A0A0U5KFN5
K	512	HIS	-	expression tag	UNP A0A0U5KFN5
K	513	HIS	-	expression tag	UNP A0A0U5KFN5
K	514	HIS	-	expression tag	UNP A0A0U5KFN5
K	515	HIS	-	expression tag	UNP A0A0U5KFN5
K	516	HIS	-	expression tag	UNP A0A0U5KFN5
K	517	HIS	-	expression tag	UNP A0A0U5KFN5

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: Ras GTPase-activating protein-binding protein 1

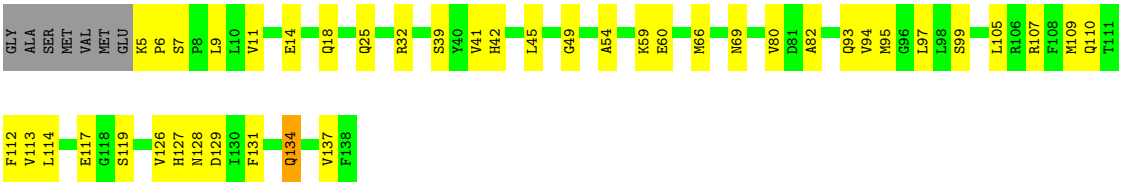
Chain A:

• Molecule 1: Ras GTPase-activating protein-binding protein 1

Chain C:

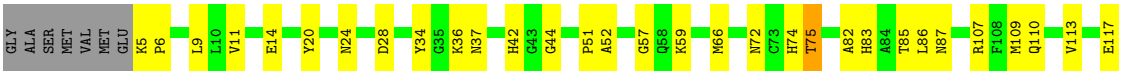
• Molecule 1: Ras GTPase-activating protein-binding protein 1

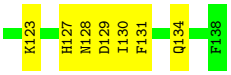
Chain D:



• Molecule 1: Ras GTPase-activating protein-binding protein 1

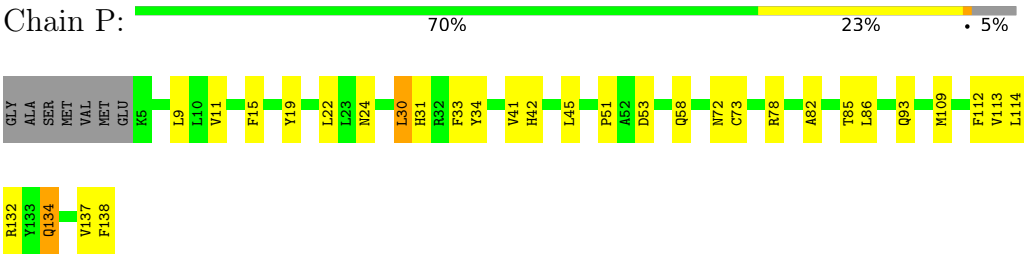
Chain B:





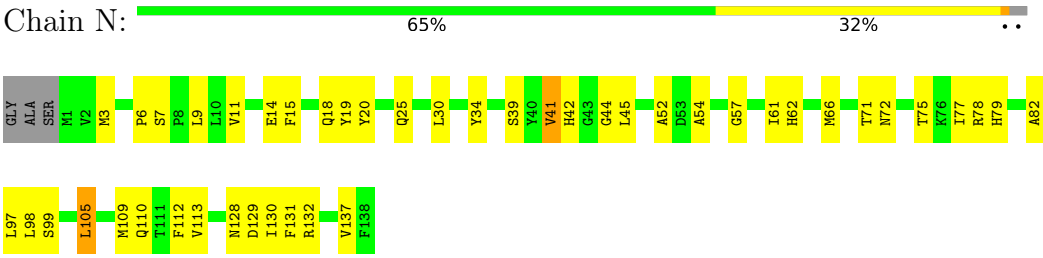
• Molecule 1: Ras GTPase-activating protein-binding protein 1

Chain P:



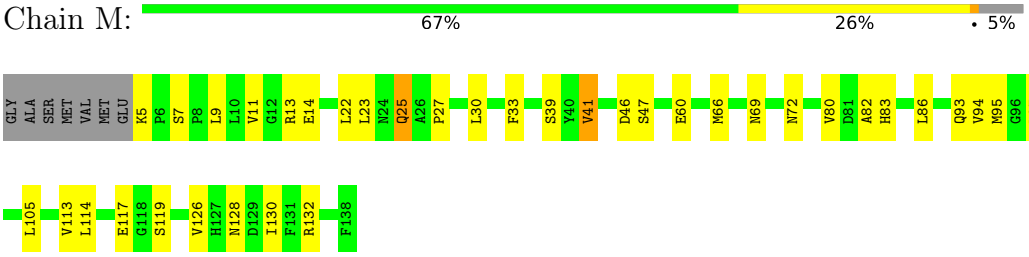
• Molecule 1: Ras GTPase-activating protein-binding protein 1

Chain N:



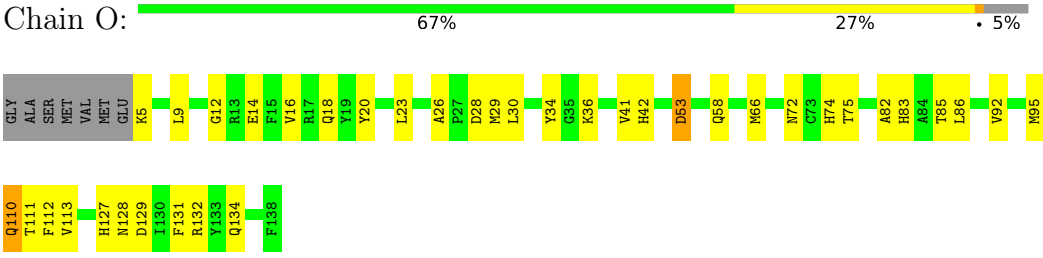
• Molecule 1: Ras GTPase-activating protein-binding protein 1

Chain M:



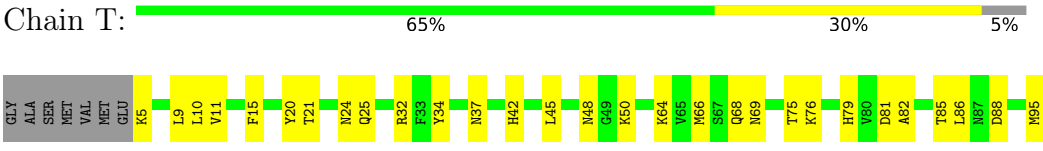
• Molecule 1: Ras GTPase-activating protein-binding protein 1

Chain O:



• Molecule 1: Ras GTPase-activating protein-binding protein 1

Chain T:

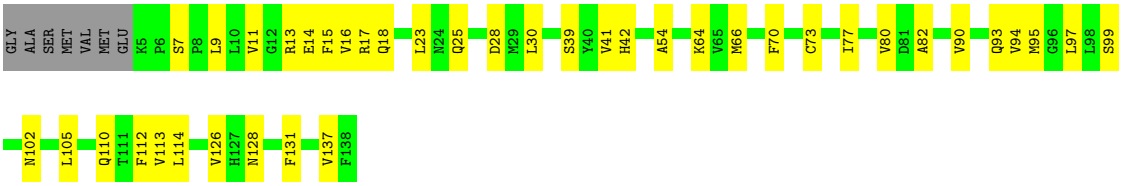


• Molecule 1: Ras GTPase-activating protein-binding protein 1

Chain R:

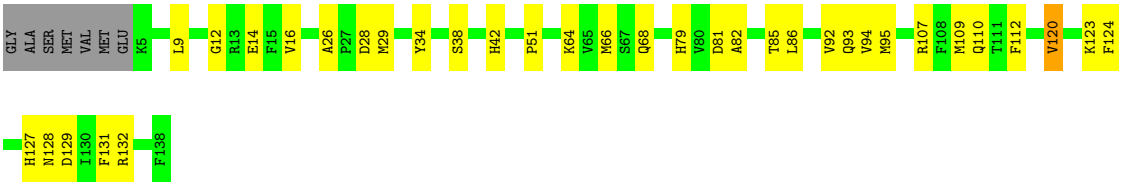
• Molecule 1: Ras GTPase-activating protein-binding protein 1

Chain Q:



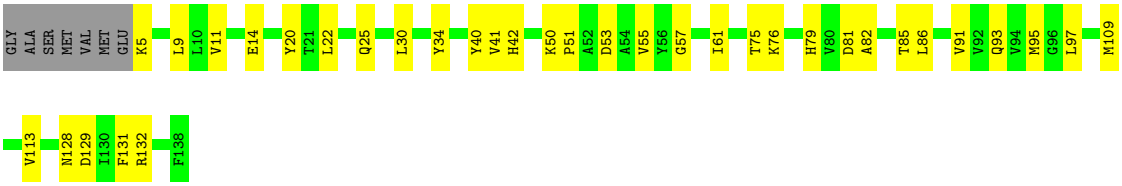
• Molecule 1: Ras GTPase-activating protein-binding protein 1

Chain S:



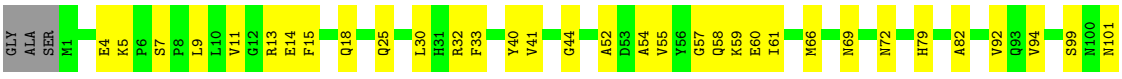
• Molecule 1: Ras GTPase-activating protein-binding protein 1

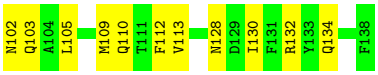
Chain E:



• Molecule 1: Ras GTPase-activating protein-binding protein 1

Chain G:



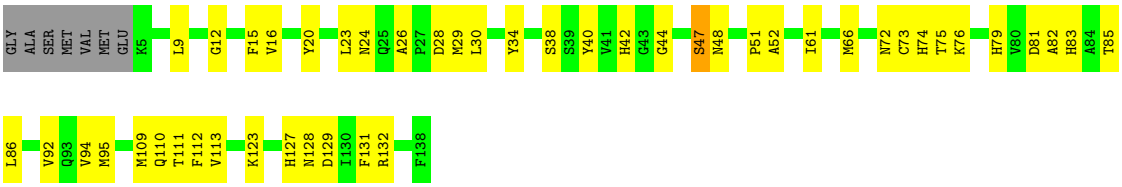


• Molecule 1: Ras GTPase-activating protein-binding protein 1

Chain H:

• Molecule 1: Ras GTPase-activating protein-binding protein 1

Chain F:



• Molecule 2: Polyprotein P1234

Chain L:

• Molecule 2: Polyprotein P1234

Chain I:

• Molecule 2: Polyprotein P1234

Chain V:

• Molecule 2: Polyprotein P1234

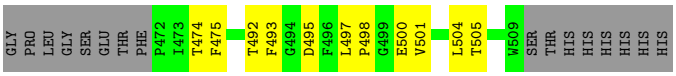
Chain U:

• Molecule 2: Polyprotein P1234

Chain X:

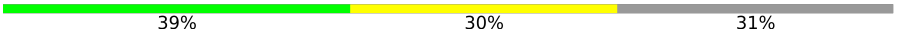
• Molecule 2: Polyprotein P1234

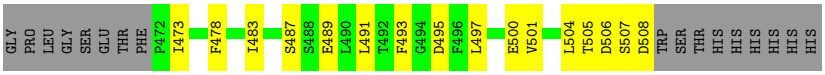
Chain W:



• Molecule 2: Polyprotein P1234

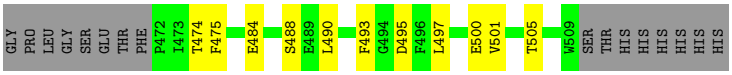
Chain J:





• Molecule 2: Polyprotein P1234

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	296402	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k 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	0.38	0/1108	0.56	0/1496
1	B	0.34	0/1108	0.59	0/1496
1	C	0.29	0/1140	0.52	0/1538
1	D	0.40	0/1108	0.63	0/1496
1	E	0.29	0/1114	0.56	0/1504
1	F	0.33	0/1108	0.59	1/1496 (0.1%)
1	G	0.30	0/1140	0.56	0/1538
1	H	0.29	0/1108	0.51	0/1496
1	M	0.31	0/1108	0.56	0/1496
1	N	0.30	0/1140	0.59	0/1538
1	O	0.33	0/1108	0.60	0/1496
1	P	0.31	0/1108	0.53	0/1496
1	Q	0.28	0/1108	0.50	0/1496
1	R	0.34	0/1140	0.57	0/1538
1	S	0.31	0/1108	0.56	0/1496
1	T	0.31	0/1108	0.50	0/1496
2	I	0.32	0/303	0.57	0/412
2	J	0.33	0/287	0.61	0/389
2	K	0.43	0/303	0.70	1/412 (0.2%)
2	L	0.37	0/287	0.61	0/389
2	U	0.36	0/303	0.59	0/412
2	V	0.28	0/287	0.49	0/389
2	W	0.51	0/303	0.77	0/412
2	X	0.25	0/287	0.49	0/389
All	All	0.33	0/20222	0.57	2/27316 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	497	LEU	N-CA-C	-5.68	102.03	110.20
1	F	47	SER	CB-CA-C	-5.23	110.11	117.23

There are no chirality outliers.

There are no planarity outliers.

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	1082	0	1053	21	0
1	B	1082	0	1053	31	0
1	C	1114	0	1089	37	0
1	D	1082	0	1053	32	0
1	E	1088	0	1057	27	0
1	F	1082	0	1053	39	0
1	G	1114	0	1089	36	0
1	H	1082	0	1053	34	0
1	M	1082	0	1053	28	0
1	N	1114	0	1089	34	0
1	O	1082	0	1053	30	0
1	P	1082	0	1053	25	0
1	Q	1082	0	1053	28	0
1	R	1114	0	1089	25	0
1	S	1082	0	1053	30	0
1	T	1082	0	1053	37	0
2	I	296	0	257	13	0
2	J	282	0	247	14	0
2	K	296	0	257	8	0
2	L	282	0	247	4	0
2	U	296	0	257	8	0
2	V	282	0	247	4	0
2	W	296	0	257	9	0
2	X	282	0	247	11	0
All	All	19758	0	19012	473	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 12.

All (473) 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:C:109:MET:HE1	1:D:109:MET:HB3	1.54	0.90
1:R:59:LYS:HE3	1:R:59:LYS:HA	1.62	0.82
1:C:79:HIS:HB2	1:D:137:VAL:HG11	1.62	0.81
1:D:18:GLN:HG2	2:J:483:ILE:HD11	1.63	0.80
1:B:85:THR:HG22	1:B:86:LEU:H	1.47	0.79
1:G:132:ARG:HB2	1:H:95:MET:HE1	1.63	0.79
1:R:132:ARG:HB2	1:Q:95:MET:HE1	1.63	0.79
1:T:113:VAL:HB	1:T:128:ASN:HB2	1.65	0.79
1:A:113:VAL:HB	1:A:128:ASN:HB2	1.66	0.77
1:G:59:LYS:HE3	1:G:59:LYS:HA	1.65	0.77
1:M:97:LEU:HB3	1:M:105:LEU:HD12	1.68	0.75
1:O:42:HIS:HA	1:O:131:PHE:HB3	1.67	0.75
1:Q:23:LEU:HD23	1:Q:30:LEU:HD11	1.69	0.75
1:N:132:ARG:HB2	1:M:95:MET:HE1	1.69	0.75
1:P:113:VAL:HB	1:P:128:ASN:HB2	1.69	0.75
1:G:113:VAL:HB	1:G:128:ASN:HB2	1.69	0.74
1:F:42:HIS:HA	1:F:131:PHE:HB3	1.69	0.74
1:C:134:GLN:HE22	1:D:134:GLN:HG3	1.52	0.74
1:A:45:LEU:HG	1:A:136:GLU:HG2	1.69	0.73
1:C:113:VAL:HB	1:C:128:ASN:HB2	1.69	0.73
1:C:132:ARG:HB2	1:D:95:MET:HE1	1.69	0.73
1:C:4:GLU:HA	1:B:24:ASN:HD21	1.53	0.72
1:E:113:VAL:HB	1:E:128:ASN:HB2	1.71	0.71
1:R:113:VAL:HB	1:R:128:ASN:HB2	1.73	0.71
1:G:32:ARG:NH2	2:K:500:GLU:OE1	2.24	0.71
1:T:107:ARG:HB2	1:T:134:GLN:HG2	1.71	0.70
1:G:66:MET:HE3	1:G:66:MET:HA	1.74	0.70
1:F:66:MET:HE3	1:F:66:MET:HA	1.72	0.70
1:S:123:LYS:NZ	2:W:474:THR:OG1	2.21	0.69
1:D:69:ASN:ND2	1:E:76:LYS:HD2	2.07	0.68
1:T:81:ASP:OD2	1:S:132:ARG:NH2	2.25	0.68
1:E:81:ASP:OD2	1:F:132:ARG:NH2	2.27	0.68
1:N:113:VAL:HB	1:N:128:ASN:HB2	1.75	0.67
1:M:39:SER:OG	1:M:128:ASN:ND2	2.27	0.67
1:G:109:MET:HB3	1:H:109:MET:HE3	1.75	0.67
1:S:127:HIS:ND1	1:S:128:ASN:OD1	2.29	0.66
1:H:113:VAL:HB	1:H:128:ASN:HB2	1.77	0.66
2:X:484:GLU:OE1	2:X:484:GLU:N	2.28	0.66
1:O:85:THR:HG22	1:O:86:LEU:H	1.61	0.65
1:G:9:LEU:HA	1:G:82:ALA:HB3	1.79	0.65
1:N:92:VAL:HB	1:N:112:PHE:HB2	1.77	0.65
1:G:92:VAL:HB	1:G:112:PHE:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:9:LEU:HA	1:N:82:ALA:HB3	1.79	0.64
1:T:25:GLN:HG3	2:X:505:THR:HB	1.79	0.64
1:H:39:SER:OG	1:H:128:ASN:ND2	2.29	0.64
1:S:14:GLU:HG3	2:W:475:PHE:HE2	1.62	0.64
1:S:42:HIS:HA	1:S:131:PHE:HB3	1.80	0.64
2:V:483:ILE:HD11	1:Q:18:GLN:HG2	1.80	0.64
1:B:20:TYR:OH	1:B:110:GLN:NE2	2.31	0.64
1:A:41:VAL:HG22	1:A:130:ILE:HA	1.79	0.64
1:R:24:ASN:OD1	1:R:25:GLN:NE2	2.31	0.64
1:F:26:ALA:HB1	1:F:29:MET:HG3	1.80	0.64
1:G:134:GLN:OE1	1:H:134:GLN:NE2	2.25	0.63
1:A:9:LEU:HA	1:A:82:ALA:HB3	1.79	0.63
1:C:92:VAL:HB	1:C:112:PHE:HB2	1.79	0.63
1:D:39:SER:OG	1:D:128:ASN:ND2	2.30	0.63
1:B:42:HIS:HA	1:B:131:PHE:HB3	1.78	0.63
1:F:127:HIS:ND1	1:F:128:ASN:OD1	2.30	0.63
1:P:31:HIS:O	1:P:58:GLN:NE2	2.32	0.63
1:O:127:HIS:ND1	1:O:128:ASN:OD1	2.31	0.63
1:Q:93:GLN:HE22	1:Q:95:MET:HE2	1.63	0.63
1:R:99:SER:HB3	1:R:105:LEU:HD23	1.80	0.63
1:M:113:VAL:HB	1:M:128:ASN:HB2	1.81	0.62
1:Q:39:SER:OG	1:Q:128:ASN:ND2	2.30	0.62
1:B:127:HIS:ND1	1:B:128:ASN:OD1	2.31	0.62
1:S:85:THR:HG22	1:S:86:LEU:HD12	1.81	0.62
1:R:29:MET:SD	1:R:32:ARG:NH1	2.73	0.62
1:R:92:VAL:HB	1:R:112:PHE:HB2	1.82	0.62
2:J:501:VAL:O	2:J:505:THR:HG23	2.00	0.62
1:Q:113:VAL:HB	1:Q:128:ASN:HB2	1.82	0.62
1:M:27:PRO:HA	1:M:30:LEU:HD23	1.82	0.61
1:T:5:LYS:NZ	1:T:88:ASP:OD2	2.34	0.61
1:R:123:LYS:NZ	2:W:492:THR:OG1	2.29	0.61
1:Q:28:ASP:N	1:Q:28:ASP:OD1	2.34	0.61
1:N:41:VAL:HG12	1:N:54:ALA:HA	1.83	0.61
1:E:41:VAL:HG21	1:F:83:HIS:CE1	2.36	0.61
1:R:32:ARG:NE	2:W:495:ASP:OD1	2.31	0.60
1:H:99:SER:HB3	1:H:105:LEU:HD23	1.83	0.60
2:W:501:VAL:O	2:W:505:THR:HG23	2.01	0.60
1:R:24:ASN:ND2	1:R:73:CYS:O	2.35	0.60
1:H:42:HIS:HA	1:H:131:PHE:HB3	1.83	0.60
2:I:501:VAL:O	2:I:505:THR:HG23	2.01	0.60
2:K:501:VAL:O	2:K:505:THR:HG23	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:34:TYR:OH	1:N:129:ASP:OD2	2.20	0.60
1:E:57:GLY:O	1:E:61:ILE:HD12	2.00	0.60
1:T:66:MET:HE3	1:T:66:MET:HA	1.83	0.60
1:H:9:LEU:HA	1:H:82:ALA:HB3	1.84	0.60
1:Q:9:LEU:HA	1:Q:82:ALA:HB3	1.84	0.59
1:P:9:LEU:HA	1:P:82:ALA:HB3	1.85	0.59
2:I:500:GLU:O	2:I:504:LEU:HD13	2.02	0.59
1:P:51:PRO:HB3	1:P:132:ARG:HH21	1.68	0.59
1:M:66:MET:HE2	1:M:66:MET:HA	1.85	0.59
1:D:66:MET:HE2	1:D:66:MET:HA	1.85	0.58
1:H:66:MET:HE2	1:H:66:MET:HA	1.85	0.58
1:T:9:LEU:HA	1:T:82:ALA:HB3	1.86	0.58
1:E:40:TYR:HB3	1:E:55:VAL:HG23	1.84	0.58
1:Q:90:VAL:HG23	1:Q:114:LEU:HB2	1.83	0.58
1:D:80:VAL:HG22	1:D:94:VAL:HG22	1.84	0.58
1:B:66:MET:HA	1:B:66:MET:HE3	1.86	0.58
1:S:79:HIS:HB3	1:S:95:MET:HB2	1.86	0.58
1:E:9:LEU:HA	1:E:82:ALA:HB3	1.85	0.58
1:D:97:LEU:HG	1:D:105:LEU:HD13	1.85	0.58
1:T:42:HIS:HA	1:T:131:PHE:HB3	1.84	0.58
1:E:95:MET:HE3	1:F:109:MET:HG3	1.86	0.58
1:T:107:ARG:HB2	1:T:134:GLN:CG	2.33	0.57
1:Q:114:LEU:HD23	1:Q:126:VAL:HA	1.84	0.57
1:G:72:ASN:ND2	1:G:102:ASN:OD1	2.35	0.57
1:C:9:LEU:HA	1:C:82:ALA:HB3	1.85	0.57
1:O:66:MET:HE3	1:O:66:MET:HA	1.86	0.57
1:R:57:GLY:O	1:R:60:GLU:HG2	2.05	0.57
1:M:9:LEU:HA	1:M:82:ALA:HB3	1.86	0.57
1:T:64:LYS:O	1:T:68:GLN:HG2	2.04	0.57
1:R:57:GLY:O	1:R:61:ILE:HG12	2.04	0.57
1:B:9:LEU:HA	1:B:82:ALA:HB3	1.87	0.57
1:F:9:LEU:HA	1:F:82:ALA:HB3	1.86	0.57
1:E:11:VAL:HG22	2:J:491:LEU:HD21	1.87	0.56
1:T:32:ARG:NH2	2:X:500:GLU:OE2	2.30	0.56
1:R:9:LEU:HA	1:R:82:ALA:HB3	1.88	0.56
1:A:22:LEU:HD23	1:A:30:LEU:HD12	1.87	0.56
1:C:97:LEU:HB3	1:C:105:LEU:HD22	1.87	0.56
1:G:57:GLY:O	1:G:61:ILE:HD12	2.06	0.56
2:L:490:LEU:H	2:L:490:LEU:HD23	1.70	0.56
1:C:7:SER:O	1:C:11:VAL:HG23	2.06	0.56
1:R:61:ILE:O	1:R:65:VAL:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:22:LEU:HD23	1:M:33:PHE:CE2	2.41	0.56
1:H:80:VAL:HG22	1:H:94:VAL:HG22	1.87	0.56
1:F:94:VAL:HB	1:F:110:GLN:HB3	1.88	0.56
1:M:23:LEU:HA	1:M:30:LEU:HD21	1.87	0.55
1:C:4:GLU:OE2	1:B:75:THR:N	2.38	0.55
1:C:109:MET:CE	1:D:109:MET:HB3	2.33	0.55
1:Q:97:LEU:HB3	1:Q:105:LEU:HD22	1.89	0.55
1:D:113:VAL:HB	1:D:128:ASN:HB2	1.86	0.55
1:S:94:VAL:HB	1:S:110:GLN:HB3	1.87	0.55
1:D:97:LEU:HB3	1:D:105:LEU:HD22	1.89	0.55
1:C:78:ARG:NH2	1:P:72:ASN:OD1	2.40	0.55
1:D:9:LEU:HA	1:D:82:ALA:HB3	1.88	0.54
1:Q:93:GLN:NE2	1:Q:95:MET:HE2	2.22	0.54
1:D:114:LEU:HD23	1:D:126:VAL:HA	1.90	0.54
1:B:72:ASN:OD1	1:B:74:HIS:NE2	2.40	0.54
1:O:34:TYR:O	1:O:58:GLN:NE2	2.40	0.54
1:M:80:VAL:HG22	1:M:94:VAL:HG22	1.90	0.54
1:D:117:GLU:OE2	1:D:119:SER:OG	2.25	0.54
1:P:41:VAL:HG22	1:P:130:ILE:HA	1.89	0.54
1:N:57:GLY:O	1:N:61:ILE:HG12	2.07	0.54
1:T:69:ASN:O	1:G:13:ARG:NH2	2.41	0.54
1:Q:9:LEU:O	1:Q:13:ARG:HG2	2.07	0.54
1:A:75:THR:O	1:H:101:ASN:ND2	2.40	0.54
1:E:79:HIS:NE2	1:F:51:PRO:HG2	2.21	0.54
1:G:5:LYS:H	1:F:24:ASN:HD21	1.55	0.54
1:P:34:TYR:OH	1:P:129:ASP:OD2	2.23	0.53
1:G:79:HIS:HB2	1:H:137:VAL:HG11	1.89	0.53
1:G:101:ASN:HB3	1:G:103:GLN:NE2	2.23	0.53
1:H:44:GLY:HA2	1:H:52:ALA:HB2	1.90	0.53
1:B:5:LYS:NZ	1:B:6:PRO:O	2.40	0.53
1:T:85:THR:OG1	1:T:86:LEU:N	2.41	0.53
1:T:76:LYS:HB3	1:T:97:LEU:HB2	1.89	0.53
1:F:20:TYR:OH	1:F:110:GLN:OE1	2.20	0.53
1:P:53:ASP:OD1	1:P:53:ASP:N	2.37	0.53
1:S:9:LEU:HA	1:S:82:ALA:HB3	1.90	0.53
1:M:25:GLN:NE2	2:X:487:SER:OG	2.39	0.53
1:T:34:TYR:OH	1:T:129:ASP:OD2	2.26	0.53
1:T:138:PHE:HB3	1:S:107:ARG:HH21	1.74	0.53
1:H:22:LEU:HD23	1:H:33:PHE:HE2	1.73	0.53
1:C:59:LYS:HE2	1:C:59:LYS:HA	1.91	0.53
1:Q:42:HIS:HA	1:Q:131:PHE:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:TYR:OH	1:E:129:ASP:OD2	2.25	0.53
2:L:483:ILE:HG22	2:L:486:LEU:HD13	1.90	0.53
1:E:20:TYR:HB3	1:E:75:THR:HG21	1.90	0.53
1:H:55:VAL:HB	1:H:60:GLU:HB3	1.91	0.53
1:S:85:THR:HG22	1:S:86:LEU:H	1.74	0.53
1:F:79:HIS:HB3	1:F:95:MET:HB2	1.89	0.53
1:N:41:VAL:HG22	1:N:130:ILE:HA	1.90	0.52
1:C:123:LYS:NZ	2:I:492:THR:OG1	2.37	0.52
2:U:484:GLU:O	2:U:488:SER:HB3	2.09	0.52
1:S:26:ALA:HB1	1:S:29:MET:HG3	1.91	0.52
1:P:41:VAL:HG11	1:O:83:HIS:NE2	2.25	0.52
1:P:24:ASN:ND2	1:Q:102:ASN:HB2	2.24	0.52
1:N:7:SER:O	1:N:11:VAL:HG23	2.10	0.52
1:B:85:THR:HG22	1:B:86:LEU:N	2.22	0.52
1:A:45:LEU:HB3	1:A:49:GLY:HA2	1.92	0.52
1:N:110:GLN:HA	1:N:130:ILE:O	2.09	0.52
1:F:113:VAL:HB	1:F:128:ASN:HB2	1.92	0.52
1:M:117:GLU:OE2	1:M:119:SER:OG	2.28	0.52
1:A:41:VAL:HG11	1:B:83:HIS:NE2	2.25	0.52
1:H:22:LEU:HD23	1:H:33:PHE:CE2	2.45	0.52
1:A:53:ASP:OD1	1:A:53:ASP:N	2.35	0.52
1:M:46:ASP:OD1	1:M:47:SER:N	2.41	0.52
1:T:20:TYR:HB3	1:T:75:THR:HG21	1.92	0.52
1:S:66:MET:HA	1:S:66:MET:HE3	1.91	0.52
1:E:25:GLN:HG3	2:J:505:THR:HB	1.92	0.52
1:H:9:LEU:O	1:H:13:ARG:HG2	2.10	0.52
1:A:71:THR:OG1	1:N:77:ILE:O	2.26	0.51
1:E:5:LYS:NZ	1:E:5:LYS:HB3	2.25	0.51
1:O:20:TYR:OH	1:O:110:GLN:NE2	2.44	0.51
1:H:114:LEU:HD23	1:H:126:VAL:HA	1.90	0.51
1:A:109:MET:HE3	1:B:109:MET:SD	2.49	0.51
1:N:25:GLN:HA	1:N:25:GLN:OE1	2.10	0.51
1:G:4:GLU:HG2	1:F:24:ASN:HD22	1.76	0.51
2:L:495:ASP:OD1	2:L:495:ASP:N	2.40	0.51
1:G:25:GLN:HA	1:G:25:GLN:OE1	2.11	0.51
1:M:41:VAL:HG13	1:M:130:ILE:HA	1.93	0.51
1:N:109:MET:HG3	1:M:95:MET:SD	2.51	0.51
1:T:109:MET:HE3	1:S:109:MET:SD	2.51	0.51
1:G:61:ILE:HD12	1:G:61:ILE:H	1.76	0.51
1:C:25:GLN:OE1	1:C:25:GLN:HA	2.11	0.51
1:Q:110:GLN:HG2	1:Q:112:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:34:TYR:OH	1:S:129:ASP:OD2	2.25	0.51
1:E:22:LEU:HD23	1:E:30:LEU:HD12	1.92	0.50
1:G:55:VAL:HB	1:G:60:GLU:CB	2.40	0.50
1:H:5:LYS:HD3	1:H:6:PRO:HD2	1.93	0.50
2:J:495:ASP:OD1	2:J:495:ASP:N	2.42	0.50
1:O:9:LEU:HA	1:O:82:ALA:HB3	1.94	0.50
1:C:98:LEU:HD12	1:C:99:SER:N	2.26	0.50
1:B:11:VAL:HG13	2:I:475:PHE:HE2	1.76	0.50
1:M:93:GLN:HE22	1:M:95:MET:HE2	1.75	0.50
1:O:72:ASN:OD1	1:O:74:HIS:NE2	2.44	0.50
1:S:92:VAL:HB	1:S:112:PHE:HB2	1.93	0.50
2:V:475:PHE:CE2	1:Q:15:PHE:HB2	2.47	0.50
1:C:44:GLY:HA3	1:C:52:ALA:HB3	1.94	0.49
1:S:120:VAL:HB	1:S:123:LYS:HB2	1.94	0.49
1:F:34:TYR:OH	1:F:129:ASP:OD2	2.28	0.49
1:M:22:LEU:HD23	1:M:33:PHE:HE2	1.76	0.49
1:O:26:ALA:HB1	1:O:29:MET:HG3	1.94	0.49
1:E:42:HIS:HA	1:E:131:PHE:HB3	1.94	0.49
1:C:30:LEU:HD22	1:C:33:PHE:HD2	1.77	0.49
1:R:78:ARG:HG2	1:R:96:GLY:HA2	1.94	0.49
1:D:42:HIS:HA	1:D:131:PHE:HB3	1.95	0.49
2:X:495:ASP:OD1	2:X:495:ASP:N	2.37	0.49
1:E:128:ASN:OD1	1:F:85:THR:OG1	2.27	0.49
1:O:20:TYR:HB3	1:O:75:THR:HG21	1.93	0.49
1:E:85:THR:OG1	1:E:86:LEU:N	2.45	0.49
1:G:99:SER:HB3	1:G:105:LEU:HD23	1.95	0.49
1:T:109:MET:SD	1:S:93:GLN:HG3	2.53	0.49
2:J:473:ILE:HD12	2:J:473:ILE:H	1.78	0.49
1:D:93:GLN:HE22	1:D:95:MET:HE2	1.77	0.48
1:G:7:SER:O	1:G:11:VAL:HG23	2.13	0.48
1:F:72:ASN:OD1	1:F:74:HIS:NE2	2.46	0.48
1:D:110:GLN:HG2	1:D:112:PHE:CZ	2.47	0.48
1:T:37:ASN:O	1:T:37:ASN:ND2	2.45	0.48
1:G:15:PHE:HB2	2:K:493:PHE:CE1	2.48	0.48
1:G:101:ASN:HB3	1:G:103:GLN:HE22	1.79	0.48
1:D:99:SER:OG	1:D:105:LEU:HD23	2.13	0.48
1:N:42:HIS:HA	1:N:131:PHE:HB3	1.95	0.48
1:T:48:ASN:HB2	1:T:50:LYS:HD2	1.95	0.48
1:F:123:LYS:HE2	2:K:474:THR:OG1	2.13	0.48
1:A:15:PHE:HE2	1:A:112:PHE:CG	2.32	0.48
1:C:3:MET:HG3	2:I:487:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:44:GLY:HA3	1:N:52:ALA:HB3	1.95	0.48
1:O:14:GLU:OE1	1:O:18:GLN:NE2	2.41	0.48
1:O:41:VAL:HG11	1:O:132:ARG:NH2	2.28	0.48
1:S:124:PHE:HB2	2:W:475:PHE:HD1	1.78	0.48
2:K:484:GLU:O	2:K:488:SER:HB3	2.13	0.48
1:A:37:ASN:O	1:A:37:ASN:ND2	2.47	0.48
1:P:134:GLN:HE21	1:P:134:GLN:HB3	1.51	0.48
1:Q:66:MET:HA	1:Q:66:MET:HE2	1.96	0.48
2:X:501:VAL:O	2:X:505:THR:HG23	2.13	0.48
1:P:93:GLN:OE1	1:O:111:THR:OG1	2.26	0.47
1:P:132:ARG:HH11	1:P:132:ARG:HG2	1.78	0.47
1:Q:7:SER:O	1:Q:11:VAL:HG12	2.14	0.47
1:G:55:VAL:HB	1:G:60:GLU:HB2	1.97	0.47
1:F:12:GLY:O	1:F:16:VAL:HG23	2.15	0.47
1:N:15:PHE:HB2	2:U:493:PHE:CZ	2.49	0.47
1:E:132:ARG:NH2	1:F:81:ASP:OD2	2.47	0.47
1:F:24:ASN:HB2	1:F:73:CYS:O	2.14	0.47
1:H:53:ASP:OD1	1:H:53:ASP:N	2.39	0.47
1:C:14:GLU:HG3	2:I:493:PHE:HE2	1.80	0.47
1:D:14:GLU:HA	1:D:14:GLU:OE2	2.14	0.47
1:B:110:GLN:HG3	1:B:130:ILE:O	2.14	0.47
1:F:47:SER:HG	1:F:48:ASN:N	2.11	0.47
1:C:39:SER:OG	1:C:128:ASN:OD1	2.28	0.47
1:T:97:LEU:HB3	1:T:105:LEU:HB3	1.97	0.47
1:R:19:TYR:CE1	1:R:30:LEU:HD21	2.50	0.47
1:S:12:GLY:O	1:S:16:VAL:HG23	2.14	0.47
1:N:3:MET:HA	1:N:3:MET:HE2	1.95	0.47
1:D:110:GLN:NE2	1:D:129:ASP:OD2	2.48	0.47
1:N:97:LEU:HB3	1:N:105:LEU:HG	1.97	0.47
1:T:95:MET:SD	1:S:109:MET:HG3	2.55	0.47
1:E:76:LYS:HB3	1:E:97:LEU:HB2	1.97	0.47
1:M:14:GLU:OE2	1:M:14:GLU:HA	2.15	0.46
1:A:97:LEU:HB3	1:A:105:LEU:HB3	1.97	0.46
1:B:117:GLU:HG2	1:B:123:LYS:HG2	1.97	0.46
1:D:7:SER:O	1:D:11:VAL:HG23	2.16	0.46
1:M:72:ASN:O	1:M:72:ASN:ND2	2.48	0.46
1:M:69:ASN:HD22	1:T:76:LYS:HE3	1.80	0.46
1:R:71:THR:O	1:R:72:ASN:C	2.59	0.46
1:M:7:SER:O	1:M:11:VAL:HG23	2.16	0.46
1:T:79:HIS:NE2	1:S:51:PRO:HG2	2.30	0.46
1:R:35:GLY:N	1:R:38:SER:OG	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:14:GLU:HG3	2:W:493:PHE:HE2	1.81	0.46
1:D:45:LEU:HA	1:D:49:GLY:HA2	1.98	0.46
1:N:19:TYR:CE1	1:N:30:LEU:HD21	2.50	0.46
1:D:93:GLN:NE2	1:D:95:MET:HE2	2.31	0.46
1:Q:80:VAL:HG22	1:Q:94:VAL:HG12	1.98	0.46
1:G:14:GLU:OE2	1:G:18:GLN:HG3	2.16	0.46
1:A:87:ASN:ND2	1:B:87:ASN:OD1	2.49	0.45
1:O:12:GLY:O	1:O:16:VAL:HG23	2.16	0.45
1:P:109:MET:HB2	1:O:109:MET:SD	2.57	0.45
1:T:45:LEU:HG	1:T:136:GLU:HG2	1.97	0.45
2:J:497:LEU:N	2:J:500:GLU:OE1	2.38	0.45
1:T:134:GLN:HE22	1:S:109:MET:CE	2.28	0.45
1:G:109:MET:HE3	1:H:109:MET:HE3	1.99	0.45
1:C:14:GLU:OE2	1:C:18:GLN:HG3	2.17	0.45
1:T:15:PHE:HE2	1:T:112:PHE:CG	2.35	0.45
1:Q:99:SER:OG	1:Q:105:LEU:HD23	2.15	0.45
1:A:81:ASP:O	1:A:92:VAL:HA	2.16	0.45
1:C:11:VAL:HG13	2:I:491:LEU:HD21	1.98	0.45
1:R:34:TYR:OH	1:R:129:ASP:OD2	2.34	0.45
1:G:30:LEU:HD22	1:G:33:PHE:HD2	1.82	0.45
1:F:44:GLY:O	1:F:52:ALA:N	2.45	0.45
1:F:38:SER:HA	1:F:127:HIS:O	2.16	0.45
1:H:78:ARG:HA	1:H:78:ARG:HD3	1.76	0.45
1:D:41:VAL:HG12	1:D:54:ALA:HA	1.98	0.44
1:S:64:LYS:NZ	1:S:68:GLN:OE1	2.48	0.44
1:B:44:GLY:O	1:B:52:ALA:N	2.43	0.44
1:P:11:VAL:HG22	2:V:491:LEU:HD21	1.99	0.44
1:O:113:VAL:HB	1:O:128:ASN:HB2	2.00	0.44
1:H:7:SER:O	1:H:11:VAL:HG12	2.16	0.44
2:J:473:ILE:HD12	2:J:473:ILE:N	2.32	0.44
2:J:487:SER:OG	2:J:489:GLU:OE1	2.35	0.44
2:J:508:ASP:OD1	2:J:508:ASP:N	2.50	0.44
1:H:14:GLU:OE2	1:H:14:GLU:HA	2.17	0.44
1:N:15:PHE:HB2	2:U:493:PHE:CE1	2.53	0.44
1:T:11:VAL:HG22	2:X:491:LEU:HD21	1.99	0.44
1:G:40:TYR:CD2	1:G:61:ILE:HG23	2.52	0.44
1:T:97:LEU:CD1	1:T:107:ARG:HG2	2.48	0.44
1:H:13:ARG:HA	1:H:16:VAL:HG12	2.00	0.44
1:C:62:HIS:O	1:C:65:VAL:HG12	2.17	0.44
1:M:102:ASN:HB2	1:T:24:ASN:ND2	2.33	0.44
2:X:500:GLU:O	2:X:504:LEU:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:VAL:HB	1:F:112:PHE:HB2	1.99	0.44
1:F:85:THR:HG22	1:F:86:LEU:N	2.33	0.44
1:N:66:MET:HE2	1:N:66:MET:HA	2.00	0.44
1:T:132:ARG:NH2	1:S:81:ASP:OD2	2.51	0.44
1:A:11:VAL:HG22	2:L:491:LEU:HD21	1.99	0.43
1:E:40:TYR:CG	1:E:61:ILE:HG23	2.52	0.43
1:C:98:LEU:HD23	1:C:131:PHE:CZ	2.54	0.43
1:C:109:MET:HG3	1:C:134:GLN:HG2	1.99	0.43
1:P:15:PHE:HE2	1:P:112:PHE:CG	2.36	0.43
1:S:29:MET:HE2	1:S:29:MET:HB3	1.95	0.43
1:C:34:TYR:OH	1:C:129:ASP:OD2	2.33	0.43
1:D:110:GLN:OE1	1:D:131:PHE:HD2	2.01	0.43
2:U:503:ASP:OD1	2:U:504:LEU:HD22	2.18	0.43
2:U:503:ASP:OD1	2:U:504:LEU:N	2.52	0.43
2:J:500:GLU:O	2:J:504:LEU:HG	2.18	0.43
1:E:57:GLY:C	1:E:61:ILE:HD12	2.44	0.43
1:F:47:SER:OG	1:F:48:ASN:N	2.51	0.43
1:F:76:LYS:HE3	1:F:76:LYS:HB2	1.77	0.43
1:C:32:ARG:HH21	2:I:495:ASP:C	2.27	0.43
1:T:10:LEU:HD21	2:X:488:SER:HB2	1.99	0.43
1:M:99:SER:OG	1:M:105:LEU:HD13	2.18	0.43
1:R:28:ASP:OD1	1:R:28:ASP:N	2.49	0.43
1:Q:9:LEU:HD11	1:Q:13:ARG:HH11	1.83	0.43
1:C:69:ASN:O	1:C:100:ASN:ND2	2.28	0.43
1:H:41:VAL:HB	1:H:54:ALA:HB2	2.01	0.43
1:C:6:PRO:HG3	2:I:491:LEU:HD22	2.01	0.43
1:N:20:TYR:CD1	1:N:75:THR:HG21	2.53	0.43
2:U:497:LEU:HD13	2:U:498:PRO:HD2	2.01	0.43
1:R:76:LYS:HB2	1:R:76:LYS:HE2	1.65	0.43
1:F:24:ASN:OD1	1:F:24:ASN:C	2.62	0.43
1:B:37:ASN:OD1	1:B:37:ASN:N	2.52	0.43
1:R:42:HIS:HA	1:R:131:PHE:HB3	2.00	0.43
1:Q:64:LYS:HD2	1:Q:64:LYS:HA	1.79	0.43
1:G:55:VAL:HB	1:G:60:GLU:HB3	2.01	0.43
1:H:17:ARG:NH1	1:H:17:ARG:HG2	2.34	0.43
2:J:506:ASP:OD1	2:J:507:SER:N	2.52	0.43
1:A:79:HIS:ND1	1:A:81:ASP:OD1	2.51	0.43
1:N:45:LEU:HD12	1:N:45:LEU:HA	1.88	0.43
1:O:34:TYR:OH	1:O:129:ASP:OD2	2.28	0.43
1:S:28:ASP:OD1	1:S:28:ASP:C	2.62	0.43
1:M:5:LYS:HE2	1:M:5:LYS:HB2	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:28:ASP:C	1:O:28:ASP:OD1	2.62	0.42
2:V:483:ILE:HA	2:V:486:LEU:HB3	2.01	0.42
1:E:50:LYS:HB2	1:E:51:PRO:HD3	2.01	0.42
1:G:94:VAL:HB	1:G:110:GLN:HB3	2.01	0.42
1:H:41:VAL:HG13	1:H:130:ILE:HA	2.01	0.42
1:P:42:HIS:HA	1:P:131:PHE:HB3	2.01	0.42
1:N:78:ARG:HG2	1:N:96:GLY:HA2	2.01	0.42
1:E:14:GLU:HG3	2:J:493:PHE:HE2	1.84	0.42
1:B:59:LYS:N	1:B:59:LYS:HD3	2.35	0.42
1:O:92:VAL:HB	1:O:112:PHE:HB2	2.01	0.42
1:H:110:GLN:HG2	1:H:112:PHE:CZ	2.54	0.42
1:B:129:ASP:OD1	1:B:129:ASP:C	2.63	0.42
1:N:6:PRO:HG3	2:U:491:LEU:HD12	2.00	0.42
1:Q:13:ARG:HA	1:Q:16:VAL:HG12	2.00	0.42
2:W:497:LEU:HD13	2:W:498:PRO:HD2	2.01	0.42
1:F:28:ASP:OD1	1:F:28:ASP:C	2.62	0.42
1:O:129:ASP:OD1	1:O:129:ASP:C	2.63	0.42
1:G:15:PHE:HB2	2:K:493:PHE:CZ	2.55	0.42
2:K:495:ASP:OD1	2:K:495:ASP:N	2.52	0.42
1:C:97:LEU:HG	1:C:105:LEU:HD13	2.01	0.42
1:D:59:LYS:NZ	1:D:59:LYS:HB3	2.35	0.42
1:P:19:TYR:HA	1:P:33:PHE:HE2	1.84	0.42
1:P:78:ARG:HA	1:P:78:ARG:HD2	1.87	0.42
1:N:71:THR:O	1:N:72:ASN:C	2.63	0.42
1:A:80:VAL:HG22	1:A:94:VAL:HG13	2.02	0.42
1:M:114:LEU:HD23	1:M:126:VAL:HA	2.02	0.42
1:T:131:PHE:O	1:T:132:ARG:HG2	2.20	0.42
1:C:40:TYR:HB3	1:C:55:VAL:HG23	2.02	0.42
1:C:60:GLU:OE1	1:C:60:GLU:N	2.50	0.42
1:B:113:VAL:HB	1:B:128:ASN:HB2	2.02	0.42
1:P:22:LEU:HD23	1:P:30:LEU:HD12	2.02	0.42
1:O:23:LEU:HD23	1:O:30:LEU:HD22	2.01	0.42
1:Q:70:PHE:HD1	1:Q:73:CYS:HG	1.68	0.42
2:X:483:ILE:HA	2:X:486:LEU:HB3	2.02	0.42
1:E:109:MET:HE3	1:F:109:MET:SD	2.59	0.42
1:H:63:ARG:HB2	1:H:63:ARG:CZ	2.49	0.42
1:F:47:SER:OG	1:F:48:ASN:OD1	2.37	0.42
1:S:129:ASP:OD1	1:S:129:ASP:C	2.62	0.42
2:W:500:GLU:O	2:W:504:LEU:HG	2.20	0.42
1:F:29:MET:HE2	1:F:29:MET:HB3	1.88	0.42
1:B:28:ASP:OD1	1:B:28:ASP:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:LEU:HB2	1:H:30:LEU:HD21	2.02	0.41
1:B:123:LYS:NZ	2:I:476:GLY:O	2.37	0.41
2:I:495:ASP:N	2:I:495:ASP:OD1	2.51	0.41
1:N:79:HIS:CE1	1:M:132:ARG:HE	2.36	0.41
1:N:105:LEU:HD12	1:N:105:LEU:HA	1.91	0.41
1:M:9:LEU:O	1:M:13:ARG:HG2	2.20	0.41
1:T:5:LYS:HE2	1:T:5:LYS:HB2	1.80	0.41
1:Q:14:GLU:OE1	1:Q:17:ARG:NH2	2.48	0.41
1:S:38:SER:HA	1:S:127:HIS:O	2.19	0.41
1:G:41:VAL:HB	1:G:54:ALA:HB2	2.02	0.41
1:G:110:GLN:HA	1:G:130:ILE:O	2.20	0.41
1:C:23:LEU:HD12	1:C:27:PRO:HB3	2.02	0.41
1:C:99:SER:OG	1:C:105:LEU:HD23	2.19	0.41
1:B:36:LYS:O	1:B:57:GLY:HA2	2.20	0.41
1:T:110:GLN:HG2	1:T:112:PHE:CZ	2.55	0.41
1:H:107:ARG:HB2	1:H:134:GLN:HB2	2.02	0.41
1:A:79:HIS:NE2	1:B:51:PRO:HG2	2.35	0.41
1:D:107:ARG:HB2	1:D:134:GLN:HB3	2.01	0.41
1:H:59:LYS:NZ	1:H:59:LYS:HB3	2.35	0.41
1:F:129:ASP:OD1	1:F:129:ASP:C	2.62	0.41
1:B:34:TYR:OH	1:B:129:ASP:OD2	2.29	0.41
1:G:57:GLY:O	1:G:58:GLN:C	2.64	0.41
1:F:40:TYR:HB2	1:F:61:ILE:HG12	2.01	0.41
1:N:25:GLN:HE21	2:U:508:ASP:HB2	1.86	0.41
1:P:19:TYR:HA	1:P:33:PHE:CE2	2.55	0.41
1:Q:77:ILE:HD13	1:Q:77:ILE:HA	1.91	0.41
1:S:85:THR:HG22	1:S:86:LEU:N	2.35	0.41
1:E:93:GLN:OE1	1:F:111:THR:OG1	2.28	0.41
1:A:99:SER:HB3	1:A:105:LEU:HD23	2.03	0.41
1:D:32:ARG:HB2	2:J:478:PHE:CZ	2.56	0.41
1:N:39:SER:OG	1:N:128:ASN:OD1	2.25	0.41
1:N:62:HIS:O	1:N:66:MET:HG2	2.20	0.41
1:O:5:LYS:HE2	1:O:5:LYS:HB2	1.84	0.41
1:P:138:PHE:CG	1:O:107:ARG:HD3	2.56	0.41
1:N:14:GLU:OE2	1:N:18:GLN:HG3	2.20	0.41
1:N:129:ASP:OD1	1:N:129:ASP:C	2.63	0.41
1:R:2:VAL:HG22	1:R:4:GLU:HG2	2.03	0.41
1:F:15:PHE:HB2	2:K:475:PHE:CE1	2.55	0.41
1:O:41:VAL:HG11	1:O:132:ARG:HH22	1.85	0.41
1:R:14:GLU:OE2	1:R:18:GLN:HG3	2.21	0.41
1:C:86:LEU:N	1:D:127:HIS:HE1	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:132:ARG:HB3	1:O:95:MET:HE2	2.03	0.40
1:T:21:THR:HG22	2:X:505:THR:HG21	2.02	0.40
1:G:44:GLY:HA3	1:G:52:ALA:HB3	2.02	0.40
1:H:22:LEU:HD11	1:H:29:MET:HB2	2.03	0.40
1:B:109:MET:HE3	1:B:134:GLN:NE2	2.36	0.40
1:P:85:THR:OG1	1:P:86:LEU:N	2.43	0.40
1:O:29:MET:HE2	1:O:29:MET:HB3	1.93	0.40
1:Q:41:VAL:HG12	1:Q:54:ALA:HA	2.02	0.40
1:E:53:ASP:OD1	1:E:53:ASP:N	2.41	0.40
1:D:5:LYS:HA	1:D:6:PRO:HD3	1.86	0.40
1:B:14:GLU:HG3	2:I:475:PHE:CE1	2.56	0.40
1:O:53:ASP:OD1	1:O:53:ASP:N	2.34	0.40
1:F:23:LEU:HD23	1:F:30:LEU:HD22	2.03	0.40
2:I:497:LEU:HD13	2:I:498:PRO:HD2	2.04	0.40
1:P:134:GLN:HG3	1:O:134:GLN:OE1	2.21	0.40
1:N:98:LEU:HD23	1:N:99:SER:N	2.36	0.40
1:B:36:LYS:HE2	1:B:36:LYS:HB2	1.93	0.40
1:B:107:ARG:HG2	1:B:134:GLN:NE2	2.36	0.40
1:M:82:ALA:O	1:M:83:HIS:ND1	2.54	0.40
1:O:36:LYS:HB2	1:O:36:LYS:HE2	1.91	0.40
1:G:69:ASN:OD1	1:G:69:ASN:N	2.54	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	132/141 (94%)	128 (97%)	4 (3%)	0	100	100
1	B	132/141 (94%)	129 (98%)	3 (2%)	0	100	100
1	C	136/141 (96%)	126 (93%)	10 (7%)	0	100	100
1	D	132/141 (94%)	124 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	133/141 (94%)	121 (91%)	12 (9%)	0	100	100
1	F	132/141 (94%)	124 (94%)	8 (6%)	0	100	100
1	G	136/141 (96%)	122 (90%)	14 (10%)	0	100	100
1	H	132/141 (94%)	126 (96%)	6 (4%)	0	100	100
1	M	132/141 (94%)	125 (95%)	7 (5%)	0	100	100
1	N	136/141 (96%)	128 (94%)	8 (6%)	0	100	100
1	O	132/141 (94%)	129 (98%)	3 (2%)	0	100	100
1	P	132/141 (94%)	124 (94%)	8 (6%)	0	100	100
1	Q	132/141 (94%)	127 (96%)	5 (4%)	0	100	100
1	R	136/141 (96%)	127 (93%)	9 (7%)	0	100	100
1	S	132/141 (94%)	127 (96%)	5 (4%)	0	100	100
1	T	132/141 (94%)	122 (92%)	10 (8%)	0	100	100
2	I	36/54 (67%)	36 (100%)	0	0	100	100
2	J	35/54 (65%)	34 (97%)	1 (3%)	0	100	100
2	K	36/54 (67%)	36 (100%)	0	0	100	100
2	L	35/54 (65%)	34 (97%)	1 (3%)	0	100	100
2	U	36/54 (67%)	35 (97%)	1 (3%)	0	100	100
2	V	35/54 (65%)	31 (89%)	4 (11%)	0	100	100
2	W	36/54 (67%)	36 (100%)	0	0	100	100
2	X	35/54 (65%)	35 (100%)	0	0	100	100
All	All	2413/2688 (90%)	2286 (95%)	127 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	117/122 (96%)	115 (98%)	2 (2%)	56	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	117/122 (96%)	116 (99%)	1 (1%)	75 92
1	C	121/122 (99%)	119 (98%)	2 (2%)	56 84
1	D	117/122 (96%)	114 (97%)	3 (3%)	41 75
1	E	118/122 (97%)	117 (99%)	1 (1%)	79 93
1	F	117/122 (96%)	116 (99%)	1 (1%)	75 92
1	G	121/122 (99%)	121 (100%)	0	100 100
1	H	117/122 (96%)	117 (100%)	0	100 100
1	M	117/122 (96%)	113 (97%)	4 (3%)	32 66
1	N	121/122 (99%)	118 (98%)	3 (2%)	42 75
1	O	117/122 (96%)	115 (98%)	2 (2%)	56 84
1	P	117/122 (96%)	111 (95%)	6 (5%)	20 51
1	Q	117/122 (96%)	115 (98%)	2 (2%)	56 84
1	R	121/122 (99%)	120 (99%)	1 (1%)	79 93
1	S	117/122 (96%)	116 (99%)	1 (1%)	75 92
1	T	117/122 (96%)	117 (100%)	0	100 100
2	I	34/48 (71%)	33 (97%)	1 (3%)	37 71
2	J	33/48 (69%)	33 (100%)	0	100 100
2	K	34/48 (71%)	33 (97%)	1 (3%)	37 71
2	L	33/48 (69%)	32 (97%)	1 (3%)	36 70
2	U	34/48 (71%)	34 (100%)	0	100 100
2	V	33/48 (69%)	32 (97%)	1 (3%)	36 70
2	W	34/48 (71%)	34 (100%)	0	100 100
2	X	33/48 (69%)	33 (100%)	0	100 100
All	All	2157/2336 (92%)	2124 (98%)	33 (2%)	60 86

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	73	CYS
1	C	24	ASN
1	C	86	LEU
1	D	25	GLN
1	D	60	GLU

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Mol	Chain	Res	Type
1	D	134	GLN
1	B	75	THR
2	L	473	ILE
2	I	473	ILE
1	P	30	LEU
1	P	45	LEU
1	P	73	CYS
1	P	114	LEU
1	P	134	GLN
1	P	137	VAL
1	N	41	VAL
1	N	105	LEU
1	N	137	VAL
1	M	25	GLN
1	M	41	VAL
1	M	60	GLU
1	M	86	LEU
1	O	53	ASP
1	O	110	GLN
2	V	497	LEU
1	R	117	GLU
1	Q	25	GLN
1	Q	137	VAL
1	S	120	VAL
1	E	91	VAL
1	F	75	THR
2	K	490	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	87	ASN
1	A	134	GLN
1	C	24	ASN
1	C	31	HIS
1	C	42	HIS
1	C	48	ASN
1	C	58	GLN
1	C	62	HIS
1	C	68	GLN
1	D	93	GLN

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Mol	Chain	Res	Type
1	D	127	HIS
1	D	134	GLN
1	B	87	ASN
1	B	93	GLN
1	B	110	GLN
1	B	122	ASN
1	P	128	ASN
1	N	62	HIS
1	N	74	HIS
1	N	102	ASN
1	M	24	ASN
1	M	93	GLN
1	M	101	ASN
1	O	48	ASN
1	O	110	GLN
1	T	128	ASN
1	R	58	GLN
1	R	62	HIS
1	R	127	HIS
1	Q	72	ASN
1	Q	101	ASN
1	Q	102	ASN
1	S	100	ASN
1	E	24	ASN
1	E	58	GLN
1	E	68	GLN
1	E	72	ASN
1	G	24	ASN
1	G	100	ASN
1	H	18	GLN
1	H	74	HIS
1	F	24	ASN
1	F	93	GLN
1	F	100	ASN
1	F	122	ASN

5.3.3 RNA

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.