



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:59 pm BST

PDB ID : 6AXF  
Title : Structure of RasGRP2 in complex with Rap1B  
Authors : Kondo, Y.; Iwig, J.S.; Kuriyan, J.  
Deposited on : 2017-09-06  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

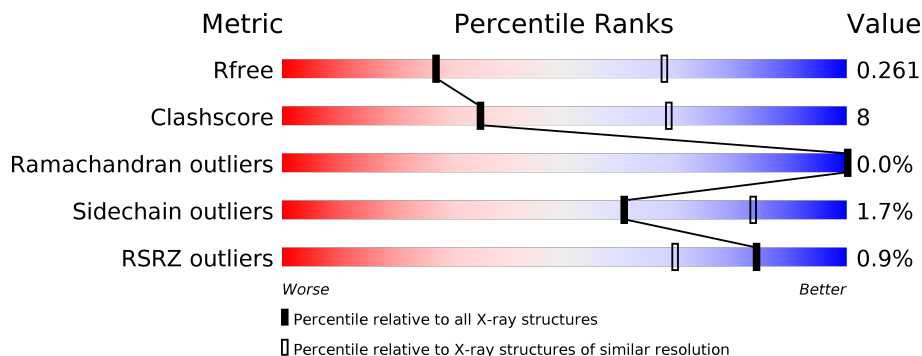
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	397	
1	C	397	
1	E	397	
1	G	397	
1	I	397	
1	K	397	

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Mol	Chain	Length	Quality of chain
1	M	397	 73% 21% • 6%
1	O	397	 2% 73% 20% • 7%
2	B	169	 80% 19% •
2	D	169	 82% 17% •
2	F	169	 79% 20% •
2	H	169	 79% 20% •
2	J	169	 78% 21% •
2	L	169	 80% 19% •
2	N	169	 78% 21% •
2	P	169	 79% 20% •

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 34903 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 guanyl-releasing protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	380	Total 3063	C 1958	N 534	O 556	S 6	Se 9	0	0	0
1	C	381	Total 3081	C 1970	N 539	O 557	S 6	Se 9	0	0	0
1	E	381	Total 3067	C 1961	N 534	O 557	S 6	Se 9	0	0	0
1	G	381	Total 3069	C 1964	N 533	O 557	S 6	Se 9	0	0	0
1	I	372	Total 2989	C 1912	N 517	O 545	S 6	Se 9	0	0	0
1	K	372	Total 2999	C 1920	N 519	O 545	S 6	Se 9	0	0	0
1	M	375	Total 3030	C 1939	N 526	O 550	S 6	Se 9	0	0	0
1	O	370	Total 2974	C 1905	N 512	O 542	S 6	Se 9	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q7LDG7
A	-1	ASN	-	expression tag	UNP Q7LDG7
A	0	ALA	-	expression tag	UNP Q7LDG7
C	-2	SER	-	expression tag	UNP Q7LDG7
C	-1	ASN	-	expression tag	UNP Q7LDG7
C	0	ALA	-	expression tag	UNP Q7LDG7
E	-2	SER	-	expression tag	UNP Q7LDG7
E	-1	ASN	-	expression tag	UNP Q7LDG7
E	0	ALA	-	expression tag	UNP Q7LDG7
G	-2	SER	-	expression tag	UNP Q7LDG7
G	-1	ASN	-	expression tag	UNP Q7LDG7
G	0	ALA	-	expression tag	UNP Q7LDG7
I	-2	SER	-	expression tag	UNP Q7LDG7

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	ASN	-	expression tag	UNP Q7LDG7
I	0	ALA	-	expression tag	UNP Q7LDG7
K	-2	SER	-	expression tag	UNP Q7LDG7
K	-1	ASN	-	expression tag	UNP Q7LDG7
K	0	ALA	-	expression tag	UNP Q7LDG7
M	-2	SER	-	expression tag	UNP Q7LDG7
M	-1	ASN	-	expression tag	UNP Q7LDG7
M	0	ALA	-	expression tag	UNP Q7LDG7
O	-2	SER	-	expression tag	UNP Q7LDG7
O	-1	ASN	-	expression tag	UNP Q7LDG7
O	0	ALA	-	expression tag	UNP Q7LDG7

- Molecule 2 is a protein called Ras-related protein Rap-1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	167	Total	C	N	O	S	0	0	0
			1325	827	228	262	8			
2	D	167	Total	C	N	O	S	0	0	0
			1331	833	228	262	8			
2	F	166	Total	C	N	O	S	0	0	0
			1320	827	224	261	8			
2	H	167	Total	C	N	O	S	0	0	0
			1331	833	228	262	8			
2	J	167	Total	C	N	O	S	0	0	0
			1331	833	228	262	8			
2	L	167	Total	C	N	O	S	0	0	0
			1331	833	228	262	8			
2	N	167	Total	C	N	O	S	0	0	0
			1331	833	228	262	8			
2	P	167	Total	C	N	O	S	0	0	0
			1331	833	228	262	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P61224
B	0	ALA	-	expression tag	UNP P61224
D	-1	GLY	-	expression tag	UNP P61224
D	0	ALA	-	expression tag	UNP P61224
F	-1	GLY	-	expression tag	UNP P61224
F	0	ALA	-	expression tag	UNP P61224
H	-1	GLY	-	expression tag	UNP P61224

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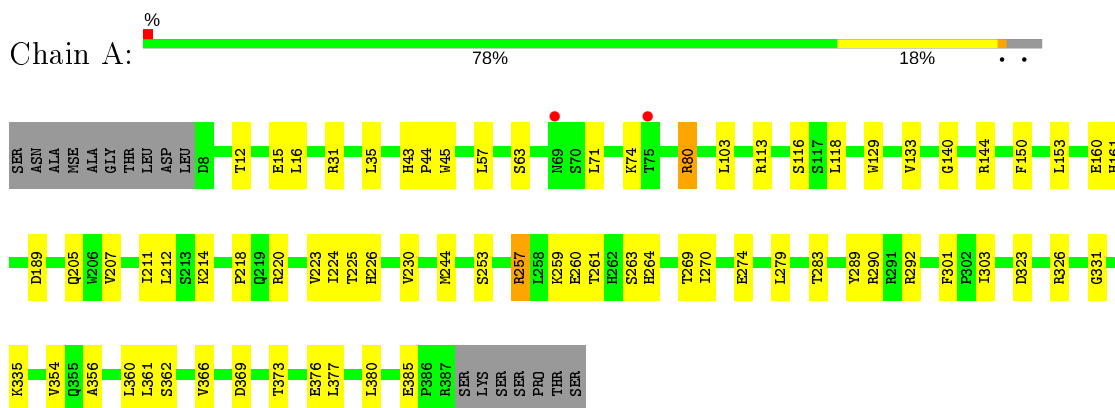
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<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
H	0	ALA	-	expression tag	UNP P61224
J	-1	GLY	-	expression tag	UNP P61224
J	0	ALA	-	expression tag	UNP P61224
L	-1	GLY	-	expression tag	UNP P61224
L	0	ALA	-	expression tag	UNP P61224
N	-1	GLY	-	expression tag	UNP P61224
N	0	ALA	-	expression tag	UNP P61224
P	-1	GLY	-	expression tag	UNP P61224
P	0	ALA	-	expression tag	UNP P61224

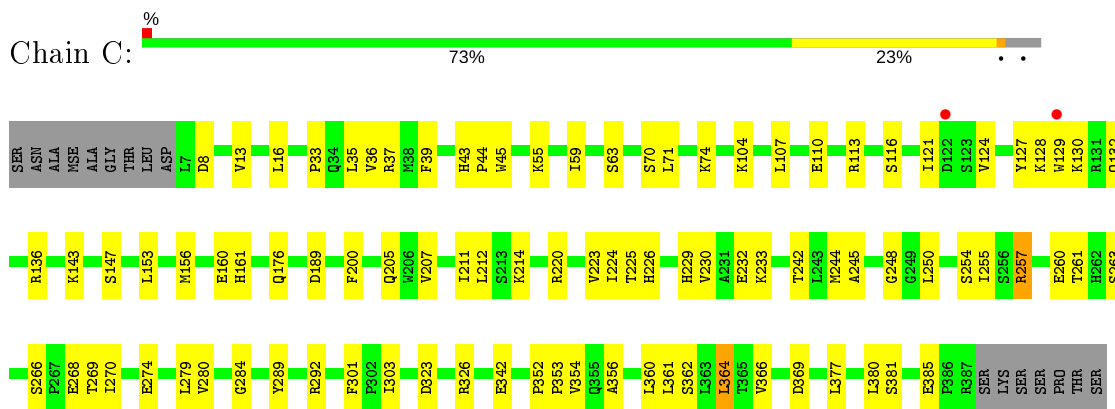
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

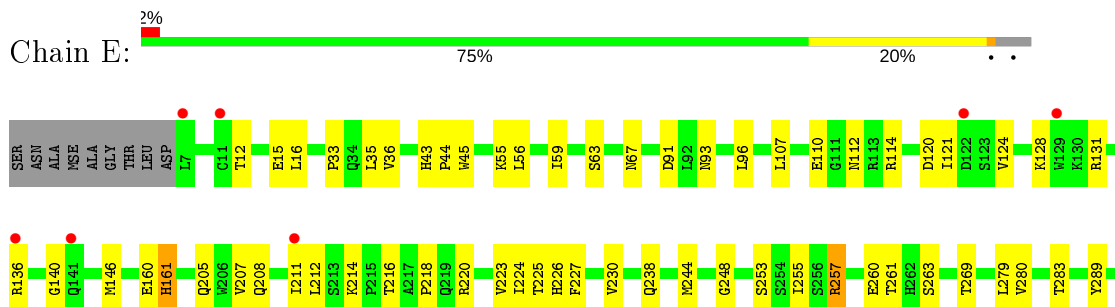
- Molecule 1: RAS guanyl-releasing protein 2



- Molecule 1: RAS guanyl-releasing protein 2

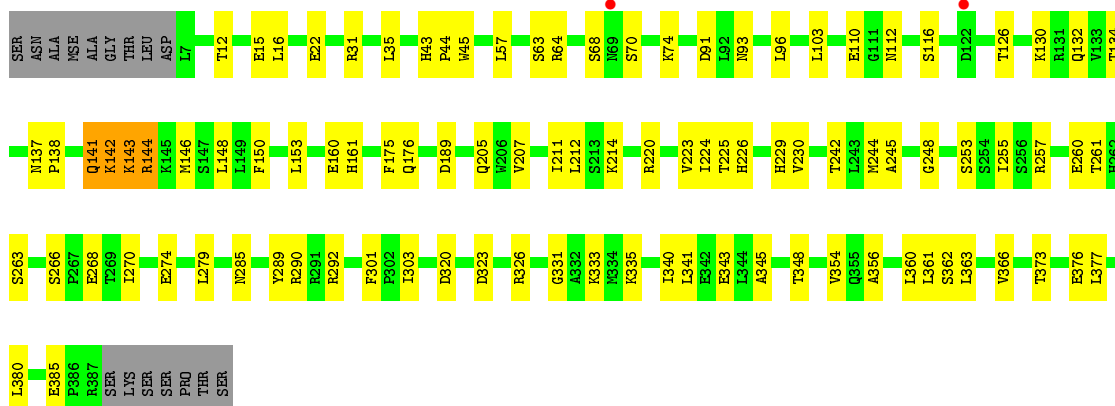


- Molecule 1: RAS guanyl-releasing protein 2

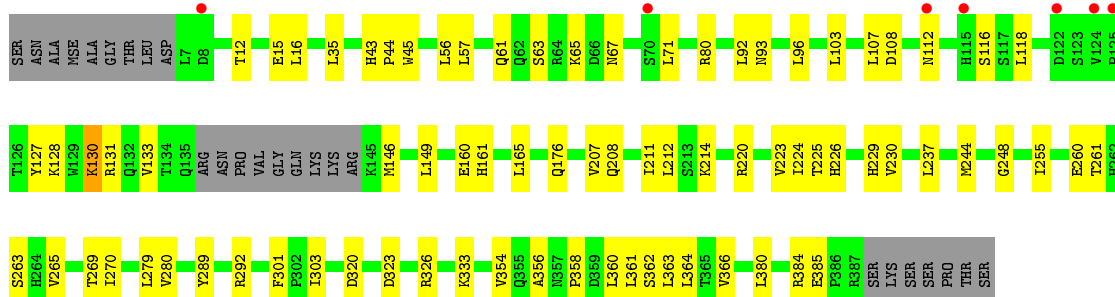




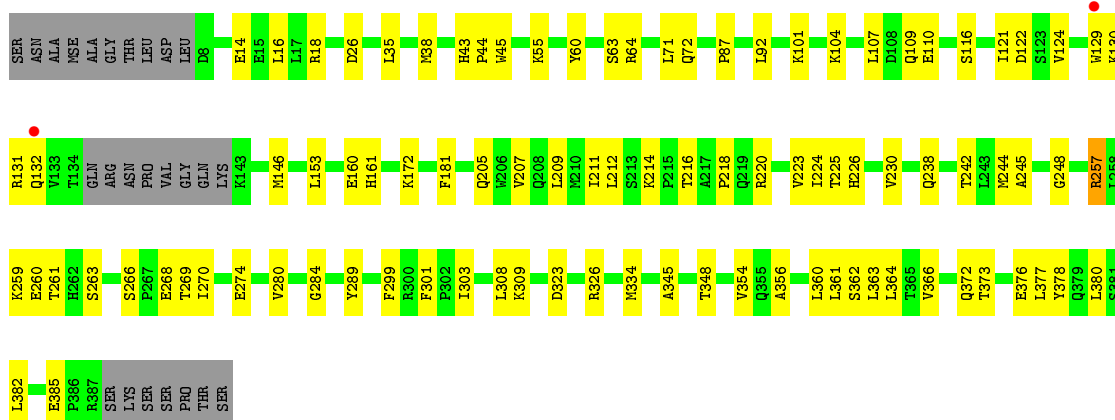
• Molecule 1: RAS guanyl-releasing protein 2



• Molecule 1: RAS guanyl-releasing protein 2



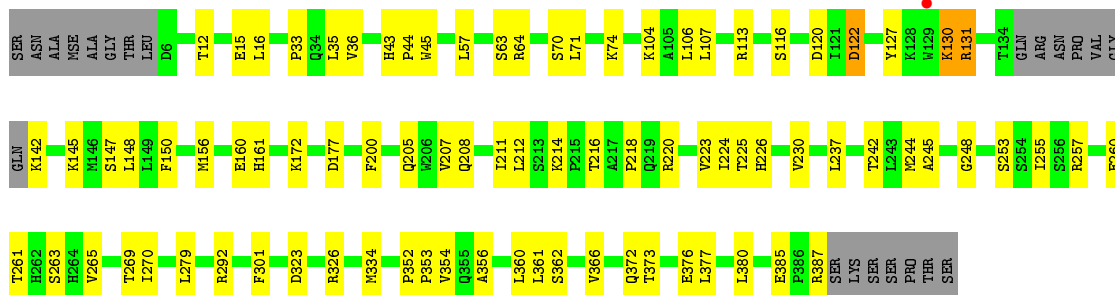
• Molecule 1: RAS guanyl-releasing protein 2





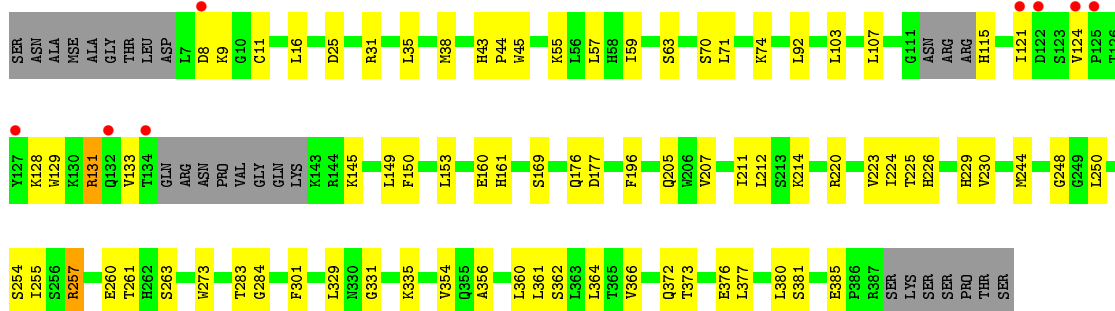
- Molecule 1: RAS guanyl-releasing protein 2

Chain M:  73% 21% 6%




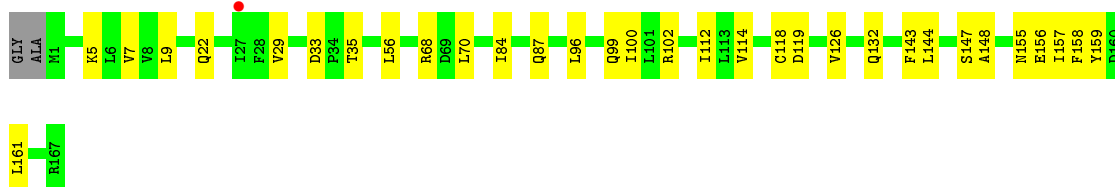
- Molecule 1: RAS guanyl-releasing protein 2

Chain O:  73% 20% 7%




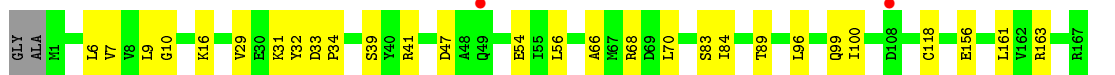
- Molecule 2: Ras-related protein Rap-1b

Chain B:  80% 19% 1%




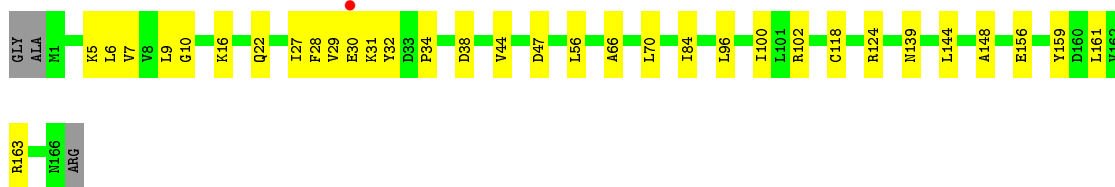
- Molecule 2: Ras-related protein Rap-1b

Chain D:  82% 17% 1%

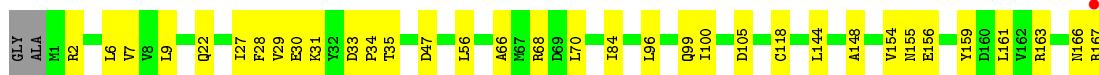
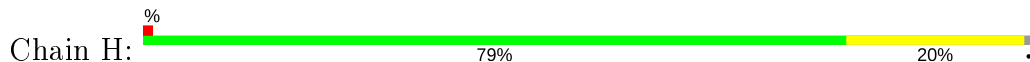


- Molecule 2: Ras-related protein Rap-1b

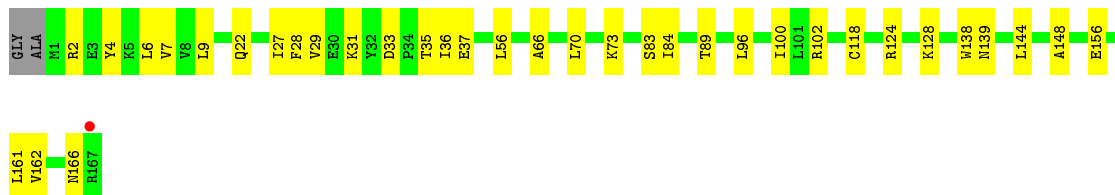
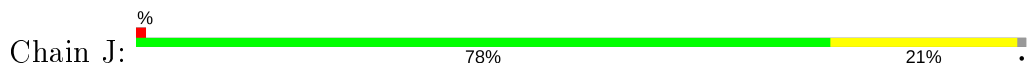
Chain F:  79% 20% 1%



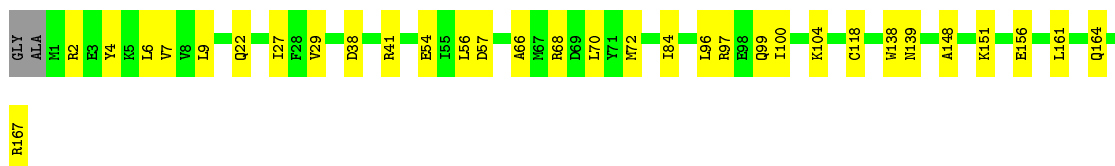
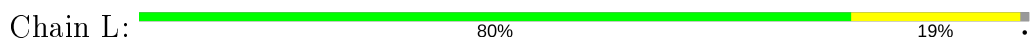
• Molecule 2: Ras-related protein Rap-1b



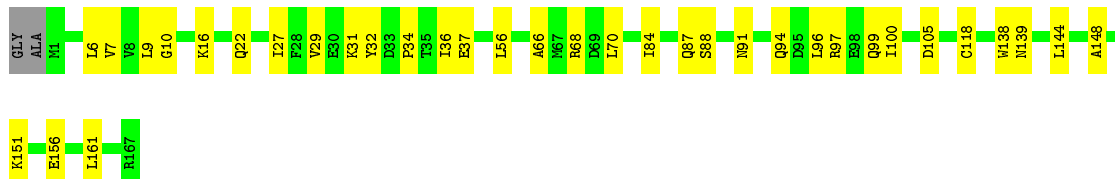
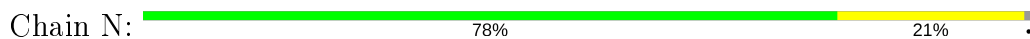
• Molecule 2: Ras-related protein Rap-1b



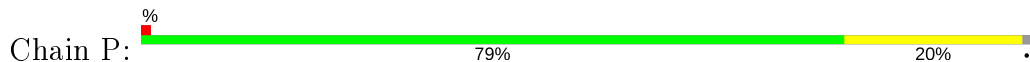
• Molecule 2: Ras-related protein Rap-1b



• Molecule 2: Ras-related protein Rap-1b



• Molecule 2: Ras-related protein Rap-1b





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.00Å 209.26Å 336.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.46 – 3.10 49.46 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.46-3.10) 90.1 (49.46-3.10)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.203 , 0.258 0.208 , 0.261	Depositor DCC
$R_{free}$ test set	4359 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtrriage
Anisotropy	0.694	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	34903	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4966e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/3124	0.40	0/4225
1	C	0.24	0/3142	0.41	0/4247
1	E	0.24	0/3128	0.41	0/4232
1	G	0.25	0/3130	0.41	0/4233
1	I	0.24	0/3046	0.41	0/4119
1	K	0.24	0/3058	0.40	0/4135
1	M	0.24	0/3089	0.40	0/4175
1	O	0.24	0/3030	0.41	0/4095
2	B	0.25	0/1340	0.43	0/1805
2	D	0.25	0/1347	0.44	0/1814
2	F	0.25	0/1336	0.43	0/1800
2	H	0.26	0/1347	0.44	0/1814
2	J	0.26	0/1347	0.45	0/1814
2	L	0.26	0/1347	0.43	0/1814
2	N	0.25	0/1347	0.43	0/1814
2	P	0.25	0/1347	0.44	0/1814
All	All	0.25	0/35505	0.42	0/47950

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	E	0	1
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1
2	L	0	1
2	N	0	1
2	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	29	VAL	Peptide
2	D	29	VAL	Peptide
1	E	140	GLY	Peptide
2	F	29	VAL	Peptide
2	H	29	VAL	Peptide
2	J	29	VAL	Peptide
2	L	29	VAL	Peptide
2	N	29	VAL	Peptide
2	P	29	VAL	Peptide

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3063	0	3079	45	0
1	C	3081	0	3112	59	0
1	E	3067	0	3079	55	0
1	G	3069	0	3090	62	0
1	I	2989	0	3001	58	0
1	K	2999	0	3011	60	0
1	M	3030	0	3050	55	0
1	O	2974	0	2992	51	0
2	B	1325	0	1315	20	0
2	D	1331	0	1322	19	0
2	F	1320	0	1309	20	0
2	H	1331	0	1322	23	0
2	J	1331	0	1322	21	0
2	L	1331	0	1322	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1331	0	1322	23	0
2	P	1331	0	1322	21	0
All	All	34903	0	34970	576	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 8.

All (576) 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:I:161:HIS:CG	1:I:360:LEU:HD12	2.11	0.85
1:I:225:THR:HG22	1:I:269:THR:HG21	1.66	0.78
1:I:356:ALA:HB1	1:I:361:LEU:HD21	1.66	0.76
1:A:80:ARG:HE	1:A:118:LEU:HG	1.50	0.76
1:M:244:MSE:HE1	2:N:70:LEU:HD22	1.68	0.76
1:M:208:GLN:HA	1:M:255:ILE:HD11	1.69	0.74
1:K:356:ALA:HB1	1:K:361:LEU:HD11	1.70	0.74
1:C:225:THR:HG22	1:C:269:THR:HG21	1.71	0.71
1:C:356:ALA:HB1	1:C:361:LEU:HD11	1.74	0.70
1:M:211:ILE:HD12	1:M:255:ILE:HD13	1.73	0.70
1:M:225:THR:HG22	1:M:269:THR:HG21	1.73	0.70
1:O:257:ARG:NH1	1:O:385:GLU:O	2.24	0.69
1:K:212:LEU:HD23	1:K:380:LEU:HB3	1.74	0.69
1:E:238:GLN:NE2	1:E:299:PHE:O	2.24	0.69
1:M:16:LEU:HD11	1:M:35:LEU:HD11	1.75	0.68
2:F:7:VAL:HG22	2:F:56:LEU:HD12	1.74	0.68
2:J:7:VAL:HG22	2:J:56:LEU:HD12	1.76	0.68
2:H:9:LEU:HD23	2:H:96:LEU:HG	1.76	0.68
1:M:356:ALA:HB1	1:M:361:LEU:HD11	1.77	0.67
1:I:130:LYS:HA	1:I:133:VAL:HB	1.76	0.67
1:I:211:ILE:HD13	1:I:224:ILE:HG12	1.77	0.67
1:M:211:ILE:HD13	1:M:224:ILE:HG12	1.76	0.67
1:C:280:VAL:O	1:C:280:VAL:HG12	1.95	0.66
1:K:16:LEU:HD11	1:K:35:LEU:HD11	1.77	0.66
2:P:7:VAL:HG22	2:P:56:LEU:HD12	1.78	0.66
2:H:30:GLU:OE1	2:H:31:LYS:HG2	1.97	0.66
1:O:145:LYS:O	1:O:149:LEU:HB2	1.97	0.65
1:K:225:THR:HG22	1:K:269:THR:HG21	1.78	0.65
1:K:280:VAL:HG12	1:K:280:VAL:O	1.97	0.65
1:I:211:ILE:HD12	1:I:255:ILE:HD13	1.79	0.65
2:H:22:GLN:HG2	2:H:154:VAL:HG11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:107:LEU:HD23	1:I:116:SER:HA	1.79	0.65
1:O:16:LEU:HD11	1:O:35:LEU:HD11	1.77	0.65
1:I:280:VAL:O	1:I:280:VAL:HG12	1.95	0.64
1:C:248:GLY:HA3	2:D:66:ALA:HB1	1.80	0.64
1:E:225:THR:HG22	1:E:269:THR:HG21	1.79	0.64
1:G:142:LYS:HD2	1:G:142:LYS:O	1.97	0.64
1:G:212:LEU:HD23	1:G:380:LEU:HB3	1.79	0.64
2:N:7:VAL:HG22	2:N:56:LEU:HD12	1.80	0.64
2:P:68:ARG:NH1	2:P:99:GLN:OE1	2.30	0.64
2:N:9:LEU:HD23	2:N:96:LEU:HG	1.80	0.64
1:A:220:ARG:HE	1:A:261:THR:HG21	1.62	0.63
1:E:211:ILE:HD12	1:E:255:ILE:HD13	1.78	0.63
1:G:130:LYS:O	1:G:134:THR:OG1	2.14	0.63
1:I:244:MSE:HE1	2:J:70:LEU:HD22	1.81	0.63
1:M:104:LYS:NZ	1:M:116:SER:O	2.32	0.63
1:C:16:LEU:HD11	1:C:35:LEU:HD11	1.81	0.63
1:A:356:ALA:HB1	1:A:361:LEU:HD11	1.81	0.63
1:G:356:ALA:HB1	1:G:361:LEU:HD11	1.81	0.63
1:C:156:MSE:HE2	1:C:233:LYS:HD2	1.81	0.62
1:E:244:MSE:HE1	2:F:70:LEU:HD22	1.81	0.62
1:G:141:GLN:O	1:G:142:LYS:HG3	1.99	0.62
1:G:16:LEU:HD11	1:G:35:LEU:HD11	1.80	0.62
1:O:212:LEU:HD23	1:O:380:LEU:HB3	1.82	0.62
1:C:160:GLU:HG2	1:C:354:VAL:HG22	1.80	0.62
2:L:68:ARG:NH1	2:L:99:GLN:OE1	2.32	0.62
2:L:7:VAL:HG22	2:L:56:LEU:HD12	1.80	0.62
1:A:257:ARG:NH1	1:A:385:GLU:O	2.23	0.62
2:L:9:LEU:HD23	2:L:96:LEU:HG	1.80	0.61
1:C:244:MSE:HE1	2:D:70:LEU:HD22	1.80	0.61
1:A:244:MSE:HE1	2:B:70:LEU:HD22	1.80	0.61
1:C:127:TYR:O	1:C:130:LYS:N	2.28	0.61
1:K:211:ILE:HA	1:K:223:VAL:HG21	1.83	0.61
1:O:356:ALA:HB1	1:O:361:LEU:HD11	1.82	0.61
2:D:9:LEU:HD23	2:D:96:LEU:HG	1.82	0.61
1:K:244:MSE:HE1	2:L:70:LEU:HD22	1.81	0.61
1:C:220:ARG:HE	1:C:261:THR:HG21	1.66	0.61
1:E:280:VAL:HG12	1:E:280:VAL:O	2.01	0.61
2:J:9:LEU:HB3	2:J:96:LEU:HD23	1.83	0.61
1:K:238:GLN:NE2	1:K:299:PHE:O	2.34	0.61
2:B:7:VAL:HG22	2:B:56:LEU:HD12	1.82	0.60
2:D:7:VAL:HG22	2:D:56:LEU:HD12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:14:GLU:OE1	1:K:55:LYS:NZ	2.33	0.60
1:A:211:ILE:HA	1:A:223:VAL:HG21	1.81	0.60
2:H:27:ILE:HG22	2:H:28:PHE:H	1.67	0.60
1:O:160:GLU:HG2	1:O:354:VAL:HG22	1.84	0.60
1:I:161:HIS:CG	1:I:360:LEU:CD1	2.84	0.60
1:E:220:ARG:HE	1:E:261:THR:HG21	1.67	0.60
1:C:211:ILE:HA	1:C:223:VAL:HG21	1.84	0.59
1:A:260:GLU:O	1:A:263:SER:OG	2.20	0.59
1:A:290:ARG:NH1	2:B:35:THR:OG1	2.35	0.59
1:C:211:ILE:HD13	1:C:224:ILE:HG12	1.84	0.59
1:K:284:GLY:HA2	2:L:41:ARG:HH22	1.67	0.59
1:G:144:ARG:HH12	1:G:148:LEU:HB2	1.67	0.59
2:H:30:GLU:OE1	2:H:31:LYS:CG	2.51	0.59
1:M:131:ARG:NH1	1:M:177:ASP:OD2	2.36	0.59
1:I:160:GLU:HG2	1:I:354:VAL:HG22	1.83	0.59
1:A:211:ILE:HD13	1:A:224:ILE:HG12	1.83	0.59
1:O:248:GLY:HA3	2:P:66:ALA:HB1	1.85	0.59
1:O:244:MSE:HE1	2:P:70:LEU:HD22	1.84	0.59
2:J:2:ARG:NH2	2:J:166:ASN:OD1	2.36	0.58
2:D:68:ARG:NH1	2:D:99:GLN:OE1	2.36	0.58
1:G:220:ARG:HE	1:G:261:THR:HG21	1.67	0.58
2:J:36:ILE:HD12	2:J:37:GLU:H	1.68	0.58
1:E:356:ALA:HB1	1:E:361:LEU:HD11	1.85	0.58
1:C:257:ARG:NH1	1:C:385:GLU:O	2.31	0.58
1:K:220:ARG:HE	1:K:261:THR:HG21	1.68	0.58
1:O:211:ILE:HD13	1:O:224:ILE:HG12	1.84	0.58
1:C:214:LYS:HB2	1:C:220:ARG:HG2	1.85	0.58
1:I:248:GLY:HA3	2:J:66:ALA:HB1	1.86	0.58
1:I:161:HIS:CD2	1:I:360:LEU:HD12	2.38	0.58
1:M:211:ILE:HA	1:M:223:VAL:HG21	1.85	0.58
1:O:211:ILE:HA	1:O:223:VAL:HG21	1.86	0.58
1:C:266:SER:OG	1:C:268:GLU:OE1	2.22	0.57
1:M:220:ARG:HE	1:M:261:THR:HG21	1.69	0.57
1:A:63:SER:HB3	1:A:71:LEU:HD23	1.86	0.57
1:E:112:ASN:HB2	1:E:114:ARG:HG2	1.87	0.57
1:M:212:LEU:HD23	1:M:380:LEU:HB3	1.86	0.57
1:M:145:LYS:HA	1:M:148:LEU:HD13	1.85	0.57
1:A:16:LEU:HD11	1:A:35:LEU:HD11	1.86	0.57
2:B:114:VAL:HG21	2:B:157:ILE:HD11	1.87	0.57
1:E:208:GLN:HA	1:E:255:ILE:HD11	1.86	0.57
1:E:211:ILE:HD13	1:E:224:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:260:GLU:O	1:G:263:SER:OG	2.23	0.57
1:G:285:ASN:ND2	2:H:34:PRO:O	2.33	0.57
1:I:211:ILE:HA	1:I:223:VAL:HG21	1.87	0.57
1:K:121:ILE:HD12	1:K:122:ASP:N	2.20	0.57
1:C:254:SER:O	1:C:381:SER:OG	2.12	0.56
1:K:146:MSE:HB2	1:K:363:LEU:HG	1.86	0.56
1:G:244:MSE:HE1	2:H:70:LEU:HD22	1.88	0.56
1:I:212:LEU:HD23	1:I:380:LEU:HB3	1.87	0.56
1:G:211:ILE:HA	1:G:223:VAL:HG21	1.86	0.55
2:H:6:LEU:HD22	2:H:161:LEU:HD13	1.87	0.55
2:N:27:ILE:HG12	2:N:151:LYS:HE3	1.87	0.55
1:O:220:ARG:HE	1:O:261:THR:HG21	1.70	0.55
2:L:6:LEU:HD22	2:L:161:LEU:HD13	1.87	0.55
1:A:373:THR:HG23	1:A:376:GLU:H	1.71	0.55
1:A:270:ILE:O	1:A:274:GLU:HG3	2.07	0.55
1:C:260:GLU:O	1:C:263:SER:OG	2.23	0.55
2:J:6:LEU:HD22	2:J:161:LEU:HD13	1.88	0.55
1:G:323:ASP:OD1	1:G:326:ARG:N	2.39	0.55
1:A:31:ARG:HH22	1:A:74:LYS:NZ	2.05	0.55
1:K:101:LYS:HE2	2:N:88:SER:HB2	1.89	0.55
1:K:104:LYS:NZ	1:K:116:SER:O	2.40	0.55
1:M:323:ASP:OD1	1:M:326:ARG:N	2.40	0.55
2:N:87:GLN:HE21	2:N:91:ASN:HD21	1.53	0.55
2:P:9:LEU:HB3	2:P:96:LEU:HD23	1.89	0.55
1:G:91:ASP:HB2	1:G:126:THR:HG22	1.88	0.55
1:A:212:LEU:HD23	1:A:380:LEU:HB3	1.89	0.54
1:A:214:LYS:HB2	1:A:220:ARG:HG2	1.90	0.54
1:E:260:GLU:O	1:E:263:SER:OG	2.24	0.54
1:O:260:GLU:O	1:O:263:SER:OG	2.24	0.54
1:O:11:CYS:O	1:O:329:LEU:N	2.38	0.54
1:C:153:LEU:HD21	1:C:360:LEU:HD11	1.89	0.54
1:M:260:GLU:O	1:M:263:SER:OG	2.25	0.54
1:C:37:ARG:NH2	1:C:342:GLU:OE1	2.39	0.54
2:N:6:LEU:HD22	2:N:161:LEU:HD13	1.89	0.54
2:B:9:LEU:HB3	2:B:96:LEU:HD23	1.90	0.54
1:G:266:SER:OG	1:G:268:GLU:OE1	2.26	0.54
2:P:156:GLU:OE1	2:P:156:GLU:N	2.40	0.54
1:O:254:SER:O	1:O:381:SER:OG	2.14	0.54
1:G:373:THR:HG23	1:G:376:GLU:H	1.72	0.54
2:H:7:VAL:HG22	2:H:56:LEU:HD12	1.89	0.54
1:O:55:LYS:O	1:O:59:ILE:HD13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:ILE:HD13	1:G:224:ILE:HG12	1.90	0.54
2:D:6:LEU:HD22	2:D:161:LEU:HD13	1.89	0.53
1:G:64:ARG:HE	1:G:110:GLU:HG3	1.73	0.53
1:G:270:ILE:O	1:G:274:GLU:HG3	2.07	0.53
2:J:156:GLU:OE1	2:J:156:GLU:N	2.41	0.53
1:M:205:GLN:HG3	1:M:377:LEU:HD11	1.89	0.53
2:F:6:LEU:HD22	2:F:161:LEU:HD13	1.89	0.53
1:E:248:GLY:HA3	2:F:66:ALA:HB1	1.90	0.53
1:K:260:GLU:O	1:K:263:SER:OG	2.26	0.53
1:K:270:ILE:O	1:K:274:GLU:HG3	2.09	0.53
1:E:211:ILE:HA	1:E:223:VAL:HG21	1.90	0.53
1:C:226:HIS:O	1:C:230:VAL:HG13	2.08	0.53
1:E:226:HIS:O	1:E:230:VAL:HG13	2.09	0.53
1:O:63:SER:HB2	1:O:71:LEU:HB3	1.91	0.53
1:K:323:ASP:OD1	1:K:326:ARG:N	2.42	0.53
1:E:253:SER:HB2	2:F:102:ARG:HB3	1.91	0.53
1:I:323:ASP:OD1	1:I:326:ARG:N	2.41	0.53
1:O:214:LYS:HB2	1:O:220:ARG:HG2	1.91	0.53
1:O:260:GLU:HB3	1:O:385:GLU:OE2	2.09	0.53
1:A:323:ASP:OD1	1:A:326:ARG:N	2.41	0.52
1:E:323:ASP:OD1	1:E:326:ARG:N	2.42	0.52
2:F:96:LEU:O	2:F:100:ILE:HG13	2.09	0.52
1:G:143:LYS:HZ1	1:G:146:MSE:HB2	1.73	0.52
1:K:260:GLU:HB3	1:K:385:GLU:OE2	2.09	0.52
1:E:91:ASP:OD2	1:E:128:LYS:N	2.42	0.52
1:M:70:SER:O	1:M:74:LYS:HG3	2.10	0.52
2:P:6:LEU:HD22	2:P:161:LEU:HD13	1.92	0.52
2:D:84:ILE:HD13	2:D:118:CYS:HA	1.92	0.52
1:E:260:GLU:HB3	1:E:385:GLU:OE2	2.10	0.52
1:E:283:THR:HG23	2:F:5:LYS:HE2	1.90	0.52
1:I:57:LEU:HD12	1:I:103:LEU:HD23	1.92	0.52
1:G:57:LEU:HD12	1:G:103:LEU:HD23	1.92	0.52
1:K:205:GLN:HG3	1:K:377:LEU:HD11	1.92	0.52
1:C:270:ILE:O	1:C:274:GLU:HG3	2.10	0.52
2:F:156:GLU:OE1	2:F:156:GLU:N	2.42	0.52
1:K:244:MSE:SE	1:K:280:VAL:HG11	2.60	0.52
2:N:156:GLU:N	2:N:156:GLU:OE1	2.41	0.52
1:O:250:LEU:O	1:O:255:ILE:HD11	2.10	0.52
2:B:156:GLU:OE1	2:B:156:GLU:N	2.42	0.52
1:C:104:LYS:NZ	1:C:116:SER:O	2.43	0.52
1:O:207:VAL:O	1:O:211:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:220:ARG:HE	1:I:261:THR:HG21	1.74	0.51
1:I:16:LEU:HD11	1:I:35:LEU:HD11	1.92	0.51
1:A:226:HIS:O	1:A:230:VAL:HG13	2.09	0.51
1:A:225:THR:HG22	1:A:269:THR:HG21	1.91	0.51
2:L:139:ASN:ND2	2:L:139:ASN:O	2.42	0.51
1:C:244:MSE:SE	1:C:280:VAL:HG11	2.60	0.51
1:K:226:HIS:O	1:K:230:VAL:HG13	2.10	0.51
2:D:156:GLU:N	2:D:156:GLU:OE1	2.42	0.51
2:H:156:GLU:N	2:H:156:GLU:OE1	2.40	0.51
1:O:63:SER:HB3	1:O:71:LEU:HD23	1.91	0.51
1:A:211:ILE:HG12	1:A:223:VAL:HG23	1.92	0.51
2:P:96:LEU:O	2:P:100:ILE:HG13	2.10	0.51
1:A:31:ARG:HH22	1:A:74:LYS:HZ3	1.59	0.51
2:F:84:ILE:HD13	2:F:118:CYS:HA	1.93	0.51
1:G:150:PHE:HA	1:G:153:LEU:HB2	1.93	0.51
2:B:22:GLN:NE2	2:B:148:ALA:O	2.44	0.51
1:C:143:LYS:O	1:C:147:SER:OG	2.21	0.51
1:G:226:HIS:O	1:G:230:VAL:HG13	2.10	0.51
1:I:165:LEU:CD1	1:I:361:LEU:HD12	2.40	0.51
1:K:60:TYR:OH	1:K:110:GLU:OE2	2.27	0.51
1:A:57:LEU:HD12	1:A:103:LEU:HD23	1.93	0.51
1:E:16:LEU:HD11	1:E:35:LEU:HD11	1.93	0.51
2:J:138:TRP:O	2:J:139:ASN:ND2	2.44	0.51
1:K:373:THR:HG23	1:K:376:GLU:H	1.76	0.51
2:L:41:ARG:HG3	2:L:54:GLU:HG3	1.94	0.50
1:M:160:GLU:HB3	1:M:354:VAL:HG13	1.93	0.50
2:J:96:LEU:O	2:J:100:ILE:HG13	2.10	0.50
2:N:139:ASN:ND2	2:N:139:ASN:O	2.44	0.50
1:G:12:THR:HG23	1:G:15:GLU:H	1.77	0.50
1:K:63:SER:HB2	1:K:71:LEU:HD23	1.92	0.50
1:M:226:HIS:O	1:M:230:VAL:HG13	2.11	0.50
1:A:12:THR:HG23	1:A:15:GLU:H	1.77	0.50
2:B:96:LEU:O	2:B:100:ILE:HG13	2.12	0.50
2:L:27:ILE:HG12	2:L:151:LYS:HE3	1.94	0.50
2:D:41:ARG:HG3	2:D:54:GLU:HG3	1.94	0.50
1:K:248:GLY:HA3	2:L:66:ALA:HB1	1.93	0.50
1:O:121:ILE:O	1:O:124:VAL:HG22	2.12	0.50
1:O:25:ASP:OD1	1:O:31:ARG:NH1	2.45	0.50
1:E:12:THR:HG23	1:E:15:GLU:H	1.77	0.50
1:K:129:TRP:O	1:K:132:GLN:NE2	2.43	0.50
1:M:127:TYR:HA	1:M:130:LYS:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:211:ILE:HG12	1:M:223:VAL:HG23	1.94	0.50
1:M:64:ARG:NH2	1:M:106:LEU:HG	2.26	0.50
1:I:208:GLN:HA	1:I:255:ILE:HD11	1.93	0.49
1:K:257:ARG:NH1	1:K:385:GLU:O	2.26	0.49
1:G:205:GLN:HG3	1:G:377:LEU:HD11	1.93	0.49
2:B:33:ASP:OD1	2:B:35:THR:HG22	2.12	0.49
1:C:212:LEU:HD23	1:C:380:LEU:HB3	1.94	0.49
1:C:250:LEU:O	1:C:255:ILE:HD11	2.12	0.49
2:L:2:ARG:HD2	2:L:4:TYR:CZ	2.46	0.49
1:G:248:GLY:HA3	2:H:66:ALA:HB1	1.93	0.49
1:K:309:LYS:NZ	2:L:57:ASP:O	2.36	0.49
2:D:47:ASP:OD1	2:D:163:ARG:NH1	2.46	0.49
1:G:248:GLY:HA2	2:H:70:LEU:HD13	1.95	0.49
2:P:22:GLN:NE2	2:P:148:ALA:O	2.44	0.49
1:E:205:GLN:OE1	1:E:372:GLN:N	2.32	0.49
1:I:226:HIS:O	1:I:230:VAL:HG13	2.12	0.49
1:I:320:ASP:OD1	1:I:333:LYS:NZ	2.41	0.49
1:O:226:HIS:O	1:O:230:VAL:HG13	2.11	0.49
1:M:373:THR:HG23	1:M:376:GLU:H	1.77	0.49
2:H:22:GLN:NE2	2:H:148:ALA:O	2.46	0.48
2:J:84:ILE:HD13	2:J:118:CYS:HA	1.94	0.48
1:M:63:SER:HB2	1:M:71:LEU:HD23	1.94	0.48
2:L:156:GLU:OE1	2:L:156:GLU:N	2.40	0.48
1:A:279:LEU:HD11	1:A:292:ARG:HG3	1.95	0.48
1:A:205:GLN:HG3	1:A:377:LEU:HD11	1.96	0.48
1:E:160:GLU:HG2	1:E:354:VAL:HG22	1.95	0.48
1:I:207:VAL:O	1:I:211:ILE:HG13	2.13	0.48
1:C:13:VAL:HG23	1:C:39:PHE:HZ	1.78	0.48
2:L:22:GLN:NE2	2:L:148:ALA:O	2.46	0.48
1:E:279:LEU:HD11	1:E:292:ARG:HG3	1.95	0.48
2:N:84:ILE:HD13	2:N:118:CYS:HA	1.95	0.48
1:E:257:ARG:NH1	1:E:385:GLU:O	2.32	0.48
1:I:260:GLU:HB3	1:I:385:GLU:OE2	2.14	0.48
1:K:214:LYS:HB2	1:K:220:ARG:HG2	1.96	0.48
2:D:96:LEU:O	2:D:100:ILE:HG13	2.14	0.48
1:I:248:GLY:HA2	2:J:70:LEU:HD13	1.96	0.48
1:G:207:VAL:O	1:G:211:ILE:HG13	2.14	0.48
2:H:96:LEU:O	2:H:100:ILE:HG13	2.14	0.48
1:I:260:GLU:O	1:I:263:SER:OG	2.31	0.48
1:I:93:ASN:HB3	1:I:96:LEU:HB3	1.96	0.48
1:K:211:ILE:HD13	1:K:224:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:207:VAL:O	1:K:211:ILE:HG13	2.14	0.48
1:M:205:GLN:OE1	1:M:372:GLN:N	2.36	0.48
1:O:225:THR:HG22	1:O:229:HIS:CE1	2.49	0.48
1:C:63:SER:OG	1:C:71:LEU:HB3	2.13	0.47
2:D:32:TYR:CE2	2:D:34:PRO:HG3	2.49	0.47
1:G:253:SER:O	1:G:257:ARG:HG2	2.13	0.47
1:I:214:LYS:HB2	1:I:220:ARG:HG2	1.96	0.47
2:N:96:LEU:O	2:N:100:ILE:HG13	2.14	0.47
1:O:115:HIS:ND1	1:O:115:HIS:O	2.44	0.47
1:I:63:SER:OG	1:I:71:LEU:HB3	2.14	0.47
2:L:96:LEU:O	2:L:100:ILE:HG13	2.13	0.47
1:M:248:GLY:HA2	2:N:70:LEU:HD13	1.96	0.47
1:E:160:GLU:HG2	1:E:354:VAL:HG13	1.95	0.47
1:I:43:HIS:CG	1:I:44:PRO:HD3	2.49	0.47
2:N:68:ARG:NH1	2:N:99:GLN:OE1	2.47	0.47
2:B:112:ILE:HG22	2:B:161:LEU:HD13	1.95	0.47
1:C:289:TYR:CZ	1:C:303:ILE:HG22	2.49	0.47
2:H:33:ASP:OD1	2:H:35:THR:HG22	2.13	0.47
1:K:160:GLU:HG2	1:K:354:VAL:HG22	1.96	0.47
1:M:160:GLU:HG2	1:M:354:VAL:HG22	1.96	0.47
2:N:22:GLN:NE2	2:N:148:ALA:O	2.46	0.47
1:O:150:PHE:HA	1:O:153:LEU:HD12	1.95	0.47
1:O:205:GLN:HG3	1:O:377:LEU:HD11	1.96	0.47
1:E:146:MSE:HE2	1:E:363:LEU:HB3	1.96	0.47
1:E:136:ARG:HB3	1:G:137:ASN:HB2	1.97	0.47
2:L:84:ILE:HD13	2:L:118:CYS:HA	1.95	0.47
1:O:248:GLY:HA2	2:P:70:LEU:HD13	1.96	0.47
1:C:107:LEU:O	1:C:110:GLU:HG2	2.14	0.47
1:I:127:TYR:O	1:I:127:TYR:CG	2.67	0.47
1:A:369:ASP:OD2	1:C:136:ARG:NH2	2.47	0.47
1:G:160:GLU:HG2	1:G:354:VAL:HG22	1.96	0.47
2:J:22:GLN:NE2	2:J:148:ALA:O	2.47	0.47
2:N:91:ASN:O	2:N:94:GLN:HG2	2.14	0.47
1:O:205:GLN:OE1	1:O:372:GLN:N	2.41	0.47
1:C:279:LEU:HD11	1:C:292:ARG:HG3	1.97	0.47
1:M:107:LEU:HD23	1:M:116:SER:HA	1.96	0.47
1:A:160:GLU:HG2	1:A:354:VAL:HG22	1.97	0.47
1:K:220:ARG:HE	1:K:261:THR:CG2	2.28	0.47
1:M:260:GLU:HB3	1:M:385:GLU:OE2	2.14	0.47
1:E:43:HIS:CG	1:E:44:PRO:HD3	2.50	0.46
1:K:248:GLY:HA2	2:L:70:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:43:HIS:CG	1:M:44:PRO:HD3	2.51	0.46
1:O:169:SER:HB3	1:O:196:PHE:HD1	1.81	0.46
2:F:10:GLY:HA3	2:F:16:LYS:HD3	1.96	0.46
1:G:64:ARG:HH11	1:G:110:GLU:HG2	1.80	0.46
1:I:265:VAL:HG21	1:I:270:ILE:HD11	1.97	0.46
1:I:358:PRO:HA	1:I:361:LEU:HD23	1.97	0.46
1:A:207:VAL:O	1:A:211:ILE:HG13	2.15	0.46
2:D:33:ASP:O	2:D:39:SER:OG	2.24	0.46
1:G:340:ILE:O	1:G:343:GLU:HB2	2.16	0.46
1:A:261:THR:HG23	1:A:385:GLU:OE2	2.16	0.46
1:C:43:HIS:CG	1:C:44:PRO:HD3	2.50	0.46
1:K:160:GLU:HB3	1:K:354:VAL:HG13	1.96	0.46
1:A:220:ARG:HE	1:A:261:THR:CG2	2.27	0.46
1:C:136:ARG:NH1	1:C:369:ASP:OD2	2.48	0.46
1:K:130:LYS:O	1:K:172:LYS:HD3	2.16	0.46
1:A:289:TYR:CZ	1:A:303:ILE:HG22	2.50	0.46
1:G:242:THR:O	1:G:245:ALA:HB3	2.16	0.46
1:I:244:MSE:SE	1:I:280:VAL:HG11	2.66	0.46
2:N:10:GLY:HA3	2:N:16:LYS:HD3	1.96	0.46
1:E:161:HIS:CD2	1:E:360:LEU:HD13	2.51	0.46
2:F:139:ASN:ND2	2:F:139:ASN:O	2.48	0.46
1:G:22:GLU:O	1:G:31:ARG:NH1	2.49	0.46
1:O:129:TRP:O	1:O:133:VAL:HG23	2.16	0.46
1:O:57:LEU:HD12	1:O:103:LEU:HD23	1.97	0.46
1:O:70:SER:O	1:O:74:LYS:HG3	2.16	0.46
1:K:64:ARG:NH1	1:K:109:GLN:OE1	2.36	0.46
2:P:95:ASP:C	2:P:99:GLN:HE21	2.18	0.46
2:F:161:LEU:HD23	2:F:161:LEU:HA	1.80	0.46
2:F:9:LEU:HB3	2:F:96:LEU:HD23	1.97	0.46
1:I:127:TYR:CD2	1:I:130:LYS:HG2	2.51	0.46
1:K:18:ARG:HH22	1:K:71:LEU:HD21	1.81	0.46
2:B:84:ILE:HD13	2:B:118:CYS:HA	1.97	0.45
1:G:211:ILE:HD12	1:G:255:ILE:HG12	1.98	0.45
2:H:155:ASN:HB3	2:H:159:TYR:CZ	2.52	0.45
1:C:284:GLY:HA2	2:D:41:ARG:HH22	1.82	0.45
1:G:70:SER:O	1:G:74:LYS:HG3	2.16	0.45
1:M:214:LYS:HB2	1:M:220:ARG:HG2	1.97	0.45
1:M:242:THR:O	1:M:245:ALA:HB3	2.15	0.45
1:C:207:VAL:O	1:C:211:ILE:HG13	2.16	0.45
1:E:107:LEU:O	1:E:110:GLU:HG2	2.16	0.45
1:E:357:ASN:O	1:E:361:LEU:HD13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:107:LEU:HD23	1:K:116:SER:HA	1.98	0.45
1:M:257:ARG:HE	1:M:387:ARG:HH12	1.65	0.45
2:P:161:LEU:HA	2:P:161:LEU:HD23	1.78	0.45
1:G:43:HIS:CG	1:G:44:PRO:HD3	2.51	0.45
2:N:32:TYR:CE2	2:N:34:PRO:HG3	2.51	0.45
1:O:161:HIS:CD2	1:O:360:LEU:HB3	2.51	0.45
1:C:242:THR:O	1:C:245:ALA:HB3	2.17	0.45
1:E:373:THR:HG23	1:E:376:GLU:H	1.82	0.45
1:C:121:ILE:HA	1:C:124:VAL:HG13	1.98	0.45
1:G:112:ASN:HB2	1:G:116:SER:H	1.81	0.45
2:H:84:ILE:HD13	2:H:118:CYS:HA	1.99	0.45
1:C:261:THR:HG23	1:C:385:GLU:OE2	2.16	0.45
1:E:93:ASN:HB3	1:E:96:LEU:HB3	1.99	0.45
1:I:80:ARG:HG3	1:I:118:LEU:O	2.17	0.45
1:I:108:ASP:HA	1:I:112:ASN:HB3	1.99	0.45
2:J:144:LEU:HA	2:J:144:LEU:HD12	1.89	0.45
1:M:248:GLY:HA3	2:N:66:ALA:HB1	1.99	0.45
1:E:161:HIS:CD2	1:E:360:LEU:HB3	2.52	0.45
1:G:260:GLU:HB3	1:G:385:GLU:OE2	2.17	0.45
2:J:27:ILE:HG22	2:J:28:PHE:H	1.82	0.45
1:A:331:GLY:O	1:A:335:LYS:HG3	2.18	0.44
1:O:131:ARG:NH2	1:O:177:ASP:OD1	2.50	0.44
1:I:161:HIS:ND1	1:I:360:LEU:HD12	2.32	0.44
1:O:43:HIS:CG	1:O:44:PRO:HD3	2.52	0.44
2:F:32:TYR:CE2	2:F:34:PRO:HG3	2.52	0.44
1:I:289:TYR:CZ	1:I:303:ILE:HG22	2.52	0.44
1:I:161:HIS:CE1	1:I:356:ALA:HA	2.52	0.44
2:J:36:ILE:HD13	1:K:26:ASP:HB2	1.99	0.44
2:L:161:LEU:HA	2:L:161:LEU:HD23	1.81	0.44
2:D:161:LEU:HA	2:D:161:LEU:HD23	1.78	0.44
2:P:84:ILE:HD13	2:P:118:CYS:HA	1.98	0.44
1:C:70:SER:O	1:C:74:LYS:HG3	2.18	0.44
1:G:261:THR:HG23	1:G:385:GLU:OE2	2.18	0.44
2:H:2:ARG:NH1	2:H:166:ASN:OD1	2.51	0.44
1:I:211:ILE:HG12	1:I:223:VAL:HG23	1.99	0.44
1:K:181:PHE:CE2	1:K:308:LEU:HD13	2.53	0.44
1:M:207:VAL:O	1:M:211:ILE:HG13	2.18	0.44
2:P:144:LEU:HD23	2:P:157:ILE:HG13	2.00	0.44
1:I:279:LEU:HD11	1:I:292:ARG:HG3	1.99	0.44
2:N:144:LEU:HD12	2:N:144:LEU:HA	1.81	0.44
1:G:148:LEU:HD13	1:G:148:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:146:MSE:HB2	1:I:363:LEU:HG	2.00	0.44
1:I:12:THR:HG23	1:I:15:GLU:H	1.83	0.44
1:I:63:SER:HB2	1:I:71:LEU:HD23	1.99	0.44
1:E:220:ARG:O	1:E:224:ILE:HG13	2.18	0.44
1:G:175:PHE:HE2	1:G:341:LEU:HD13	1.82	0.44
1:M:130:LYS:O	1:M:172:LYS:HD3	2.18	0.44
1:A:253:SER:HB2	2:B:102:ARG:HB3	2.00	0.44
1:C:352:PRO:HA	1:C:353:PRO:HD3	1.91	0.44
1:E:244:MSE:SE	1:E:280:VAL:HG11	2.67	0.44
1:G:137:ASN:N	1:G:137:ASN:OD1	2.51	0.44
1:E:289:TYR:CZ	1:E:303:ILE:HG22	2.53	0.43
2:F:144:LEU:HA	2:F:144:LEU:HD12	1.81	0.43
2:F:44:VAL:HG11	2:F:159:TYR:HE1	1.83	0.43
1:G:175:PHE:CE2	1:G:341:LEU:HD13	2.53	0.43
1:M:161:HIS:CD2	1:M:360:LEU:HB3	2.53	0.43
2:N:22:GLN:OE1	2:N:27:ILE:HG13	2.18	0.43
1:G:214:LYS:HB2	1:G:220:ARG:HG2	2.00	0.43
2:J:161:LEU:HD23	2:J:161:LEU:HA	1.79	0.43
1:K:362:SER:O	1:K:366:VAL:HG23	2.18	0.43
1:A:161:HIS:CE1	1:A:360:LEU:HB3	2.52	0.43
1:C:200:PHE:CE1	1:C:245:ALA:HB2	2.52	0.43
1:C:220:ARG:HE	1:C:261:THR:CG2	2.30	0.43
1:E:63:SER:O	1:E:67:ASN:N	2.52	0.43
1:I:161:HIS:CD2	1:I:360:LEU:CD1	3.02	0.43
1:O:103:LEU:HD13	1:O:107:LEU:HD23	1.99	0.43
1:O:283:THR:HG23	2:P:5:LYS:HE2	2.00	0.43
2:B:155:ASN:HB3	2:B:159:TYR:CZ	2.53	0.43
1:C:205:GLN:HG3	1:C:377:LEU:HD11	1.98	0.43
1:I:362:SER:O	1:I:366:VAL:HG23	2.18	0.43
1:M:64:ARG:HH22	1:M:106:LEU:HG	1.84	0.43
1:A:43:HIS:CG	1:A:44:PRO:HD3	2.53	0.43
2:D:96:LEU:HA	2:D:96:LEU:HD12	1.83	0.43
2:F:47:ASP:OD1	2:F:163:ARG:NH1	2.51	0.43
1:K:209:LEU:HD11	1:K:372:GLN:HG3	2.00	0.43
2:L:164:GLN:HA	2:L:167:ARG:HG2	2.01	0.43
1:O:220:ARG:HE	1:O:261:THR:CG2	2.32	0.43
1:A:153:LEU:HD21	1:A:360:LEU:HD11	2.00	0.43
1:A:362:SER:O	1:A:366:VAL:HG23	2.18	0.43
1:K:43:HIS:CG	1:K:44:PRO:HD3	2.54	0.43
1:K:64:ARG:HA	1:K:72:GLN:OE1	2.19	0.43
1:M:362:SER:O	1:M:366:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ILE:HG12	1:C:223:VAL:HG23	1.99	0.43
2:N:97:ARG:HD2	2:N:138:TRP:CE2	2.54	0.43
1:O:92:LEU:HD21	1:O:128:LYS:HB3	2.01	0.43
1:C:323:ASP:OD1	1:C:326:ARG:N	2.51	0.43
1:E:33:PRO:HA	1:E:36:VAL:HG12	2.01	0.43
1:M:279:LEU:HD11	1:M:292:ARG:HG3	2.00	0.43
1:O:373:THR:HG23	1:O:376:GLU:H	1.84	0.43
1:C:129:TRP:O	1:C:132:GLN:HB2	2.19	0.43
1:C:360:LEU:O	1:C:364:LEU:HB2	2.18	0.43
1:G:320:ASP:OD1	1:G:333:LYS:NZ	2.43	0.43
1:I:220:ARG:HE	1:I:261:THR:CG2	2.32	0.43
2:J:4:TYR:CE2	2:J:162:VAL:HG13	2.53	0.43
1:G:279:LEU:HD11	1:G:292:ARG:HG3	2.01	0.43
1:I:237:LEU:HA	1:I:237:LEU:HD12	1.91	0.43
1:I:56:LEU:HD23	1:I:56:LEU:HA	1.90	0.43
1:M:200:PHE:CE1	1:M:245:ALA:HB2	2.54	0.43
2:B:87:GLN:OE1	2:B:126:VAL:HG12	2.19	0.42
2:D:83:SER:HB3	2:D:89:THR:HG21	2.00	0.42
1:I:112:ASN:OD1	1:I:112:ASN:N	2.51	0.42
1:M:147:SER:HA	1:M:150:PHE:HD2	1.83	0.42
1:M:33:PRO:HA	1:M:36:VAL:HG12	2.01	0.42
1:O:38:MSE:SE	1:O:335:LYS:HG2	2.69	0.42
1:E:55:LYS:O	1:E:59:ILE:HG12	2.19	0.42
1:K:266:SER:OG	1:K:268:GLU:OE1	2.37	0.42
1:O:8:ASP:O	1:O:331:GLY:HA3	2.19	0.42
1:O:9:LYS:HA	1:O:9:LYS:HD3	1.89	0.42
2:F:38:ASP:OD1	2:F:38:ASP:N	2.41	0.42
1:G:137:ASN:N	1:G:138:PRO:HD3	2.33	0.42
1:I:176:GLN:HG3	1:I:176:GLN:H	1.58	0.42
1:K:261:THR:HG23	1:K:385:GLU:OE2	2.19	0.42
1:M:216:THR:OG1	1:M:218:PRO:HD2	2.18	0.42
1:O:131:ARG:HH22	1:O:177:ASP:CG	2.22	0.42
2:P:32:TYR:CE2	2:P:34:PRO:HG3	2.55	0.42
2:H:144:LEU:HA	2:H:144:LEU:HD12	1.89	0.42
1:I:280:VAL:CG1	1:I:280:VAL:O	2.65	0.42
1:O:160:GLU:HB3	1:O:354:VAL:HG13	2.01	0.42
1:A:218:PRO:HG3	1:A:264:HIS:CD2	2.55	0.42
1:E:340:ILE:O	1:E:343:GLU:HB2	2.20	0.42
1:G:289:TYR:CZ	1:G:303:ILE:HG22	2.54	0.42
2:B:144:LEU:HA	2:B:144:LEU:HD12	1.88	0.42
1:E:136:ARG:NH2	1:G:137:ASN:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:83:SER:HB3	2:J:89:THR:HG21	2.01	0.42
1:A:283:THR:HG23	2:B:5:LYS:HE2	2.02	0.42
2:F:22:GLN:NE2	2:F:148:ALA:O	2.52	0.42
1:E:352:PRO:HA	1:E:353:PRO:HD3	1.91	0.42
1:A:259:LYS:HB2	1:A:259:LYS:HE2	1.90	0.42
1:I:65:LYS:C	1:I:67:ASN:H	2.23	0.42
1:A:270:ILE:HA	1:A:270:ILE:HD13	1.83	0.42
2:B:132:GLN:HG3	2:B:143:PHE:CD2	2.55	0.42
2:B:119:ASP:N	2:B:147:SER:OG	2.52	0.42
2:L:72:MET:O	2:L:104:LYS:HE2	2.20	0.42
2:L:38:ASP:OD1	2:L:38:ASP:N	2.49	0.42
1:M:12:THR:HG23	1:M:15:GLU:H	1.84	0.42
1:M:212:LEU:HB3	1:M:380:LEU:HD22	2.02	0.42
1:E:216:THR:OG1	1:E:218:PRO:HD2	2.19	0.41
2:F:27:ILE:HG22	2:F:28:PHE:H	1.85	0.41
1:G:225:THR:HG22	1:G:229:HIS:CE1	2.55	0.41
1:G:331:GLY:O	1:G:335:LYS:HG3	2.19	0.41
1:G:63:SER:OG	1:G:68:SER:O	2.38	0.41
2:J:33:ASP:OD1	2:J:35:THR:HG22	2.19	0.41
2:L:96:LEU:HD12	2:L:96:LEU:HA	1.89	0.41
1:M:265:VAL:HG21	1:M:270:ILE:HD11	2.02	0.41
1:C:362:SER:O	1:C:366:VAL:HG23	2.21	0.41
1:E:121:ILE:H	1:E:121:ILE:HG13	1.66	0.41
1:G:290:ARG:NH1	2:H:35:THR:OG1	2.52	0.41
1:K:242:THR:O	1:K:245:ALA:HB3	2.19	0.41
2:N:96:LEU:HA	2:N:96:LEU:HD12	1.91	0.41
2:H:161:LEU:HD23	2:H:161:LEU:HA	1.79	0.41
2:H:47:ASP:OD1	2:H:163:ARG:NH1	2.53	0.41
1:E:345:ALA:O	1:E:348:THR:OG1	2.34	0.41
1:G:176:GLN:HG3	1:G:176:GLN:H	1.61	0.41
1:K:161:HIS:CE1	1:K:360:LEU:HD13	2.55	0.41
1:M:63:SER:OG	1:M:71:LEU:HB3	2.20	0.41
2:P:4:TYR:CE2	2:P:162:VAL:HG13	2.55	0.41
1:C:176:GLN:HG3	1:C:176:GLN:H	1.63	0.41
1:C:33:PRO:HA	1:C:36:VAL:HG12	2.02	0.41
1:E:289:TYR:CE1	1:E:303:ILE:HG22	2.54	0.41
1:M:120:ASP:OD1	1:M:122:ASP:N	2.50	0.41
1:A:113:ARG:HA	1:A:116:SER:HB3	2.01	0.41
1:A:140:GLY:N	1:C:369:ASP:OD1	2.42	0.41
1:G:161:HIS:CD2	1:G:360:LEU:HB3	2.55	0.41
1:K:38:MSE:HE3	1:K:334:MSE:SE	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:87:PRO:HB2	1:K:124:VAL:HG13	2.02	0.41
1:M:142:LYS:HB3	1:M:142:LYS:HE2	1.84	0.41
1:M:156:MSE:HE1	1:M:237:LEU:HD13	2.02	0.41
2:P:27:ILE:HG22	2:P:28:PHE:H	1.84	0.41
2:B:157:ILE:CG2	2:B:158:PHE:N	2.84	0.41
1:G:143:LYS:NZ	1:G:363:LEU:HG	2.35	0.41
1:I:92:LEU:HD11	1:I:131:ARG:HD3	2.02	0.41
1:K:216:THR:OG1	1:K:218:PRO:HD2	2.20	0.41
1:M:57:LEU:HD11	1:M:106:LEU:HD22	2.02	0.41
1:A:260:GLU:HB3	1:A:385:GLU:OE2	2.21	0.41
2:B:68:ARG:NH1	2:B:99:GLN:OE1	2.54	0.41
1:E:214:LYS:HB2	1:E:220:ARG:HG2	2.03	0.41
1:G:362:SER:O	1:G:366:VAL:HG23	2.21	0.41
2:H:68:ARG:NH1	2:H:99:GLN:OE1	2.53	0.41
1:C:113:ARG:HA	1:C:116:SER:HB3	2.03	0.41
1:E:121:ILE:O	1:E:124:VAL:HG12	2.20	0.41
1:E:207:VAL:O	1:E:211:ILE:HG13	2.21	0.41
1:G:93:ASN:HB3	1:G:96:LEU:HB3	2.03	0.41
1:K:280:VAL:CG1	1:K:280:VAL:O	2.68	0.41
1:K:289:TYR:CZ	1:K:303:ILE:HG22	2.56	0.41
1:K:378:TYR:O	1:K:382:LEU:HG	2.21	0.41
1:C:260:GLU:HB3	1:C:385:GLU:OE2	2.20	0.41
1:C:63:SER:HB2	1:C:71:LEU:HD23	2.03	0.41
2:N:36:ILE:HG13	2:N:37:GLU:H	1.86	0.41
1:O:250:LEU:HB3	1:O:273:TRP:CZ2	2.56	0.41
2:P:4:TYR:CE1	2:P:51:CYS:HB3	2.56	0.41
1:E:227:PHE:O	1:E:230:VAL:HG22	2.20	0.41
1:E:56:LEU:HA	1:E:56:LEU:HD23	1.90	0.41
1:G:345:ALA:O	1:G:348:THR:OG1	2.32	0.41
2:L:97:ARG:HD2	2:L:138:TRP:CE2	2.56	0.41
1:M:253:SER:O	1:M:257:ARG:HG2	2.21	0.41
1:K:153:LEU:HD21	1:K:360:LEU:HD11	2.03	0.40
1:K:92:LEU:CD1	1:K:131:ARG:HD2	2.51	0.40
1:O:284:GLY:O	2:P:37:GLU:HG3	2.21	0.40
1:I:356:ALA:CB	1:I:361:LEU:HD21	2.46	0.40
1:O:362:SER:O	1:O:366:VAL:HG23	2.21	0.40
1:A:129:TRP:O	1:A:133:VAL:N	2.45	0.40
1:E:220:ARG:HE	1:E:261:THR:CG2	2.33	0.40
1:K:345:ALA:O	1:K:348:THR:OG1	2.37	0.40
2:P:36:ILE:HD12	2:P:36:ILE:HA	1.89	0.40
1:C:248:GLY:HA2	2:D:70:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:HIS:CD2	1:C:360:LEU:HB3	2.56	0.40
2:D:10:GLY:HA3	2:D:16:LYS:HD3	2.03	0.40
1:E:212:LEU:HD13	1:E:212:LEU:HA	1.96	0.40
1:G:270:ILE:HA	1:G:270:ILE:HD13	1.84	0.40
1:M:161:HIS:CD2	1:M:360:LEU:HD13	2.56	0.40
1:C:229:HIS:O	1:C:232:GLU:HG2	2.21	0.40
1:C:55:LYS:O	1:C:59:ILE:HG12	2.22	0.40
1:I:220:ARG:O	1:I:224:ILE:HG13	2.22	0.40
2:J:128:LYS:HE3	2:J:128:LYS:HB2	1.88	0.40
1:K:63:SER:OG	1:K:71:LEU:HB3	2.21	0.40
1:M:352:PRO:HA	1:M:353:PRO:HD3	1.94	0.40
1:O:176:GLN:H	1:O:176:GLN:HG3	1.59	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 X-ray entries followed by that with respect to entries of similar resolution.

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	378/397 (95%)	373 (99%)	5 (1%)	0	100	100
1	C	379/397 (96%)	366 (97%)	12 (3%)	1 (0%)	41	73
1	E	379/397 (96%)	375 (99%)	4 (1%)	0	100	100
1	G	379/397 (96%)	368 (97%)	11 (3%)	0	100	100
1	I	368/397 (93%)	360 (98%)	8 (2%)	0	100	100
1	K	368/397 (93%)	365 (99%)	3 (1%)	0	100	100
1	M	371/397 (94%)	367 (99%)	4 (1%)	0	100	100
1	O	364/397 (92%)	358 (98%)	6 (2%)	0	100	100
2	B	165/169 (98%)	161 (98%)	4 (2%)	0	100	100
2	D	165/169 (98%)	157 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	164/169 (97%)	157 (96%)	7 (4%)	0	100	100
2	H	165/169 (98%)	160 (97%)	5 (3%)	0	100	100
2	J	165/169 (98%)	158 (96%)	7 (4%)	0	100	100
2	L	165/169 (98%)	161 (98%)	4 (2%)	0	100	100
2	N	165/169 (98%)	162 (98%)	3 (2%)	0	100	100
2	P	165/169 (98%)	160 (97%)	5 (3%)	0	100	100
All	All	4305/4528 (95%)	4208 (98%)	96 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	128	LYS

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	342/349 (98%)	335 (98%)	7 (2%)	55	80
1	C	345/349 (99%)	339 (98%)	6 (2%)	60	83
1	E	342/349 (98%)	336 (98%)	6 (2%)	59	82
1	G	343/349 (98%)	335 (98%)	8 (2%)	50	77
1	I	334/349 (96%)	325 (97%)	9 (3%)	44	74
1	K	335/349 (96%)	330 (98%)	5 (2%)	65	85
1	M	339/349 (97%)	332 (98%)	7 (2%)	53	79
1	O	333/349 (95%)	328 (98%)	5 (2%)	65	85
2	B	146/147 (99%)	146 (100%)	0	100	100
2	D	147/147 (100%)	146 (99%)	1 (1%)	84	93
2	F	146/147 (99%)	143 (98%)	3 (2%)	53	79
2	H	147/147 (100%)	145 (99%)	2 (1%)	67	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	147/147 (100%)	143 (97%)	4 (3%)	44	74
2	L	147/147 (100%)	147 (100%)	0	100	100
2	N	147/147 (100%)	145 (99%)	2 (1%)	67	86
2	P	147/147 (100%)	144 (98%)	3 (2%)	55	80
All	All	3887/3968 (98%)	3819 (98%)	68 (2%)	60	83

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	TRP
1	A	80	ARG
1	A	144	ARG
1	A	150	PHE
1	A	189	ASP
1	A	257	ARG
1	A	301	PHE
1	C	8	ASP
1	C	45	TRP
1	C	189	ASP
1	C	257	ARG
1	C	301	PHE
1	C	364	LEU
2	D	31	LYS
1	E	45	TRP
1	E	120	ASP
1	E	131	ARG
1	E	161	HIS
1	E	257	ARG
1	E	301	PHE
2	F	30	GLU
2	F	31	LYS
2	F	124	ARG
1	G	45	TRP
1	G	132	GLN
1	G	141	GLN
1	G	142	LYS
1	G	143	LYS
1	G	144	ARG
1	G	189	ASP
1	G	301	PHE
2	H	105	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	167	ARG
1	I	45	TRP
1	I	61	GLN
1	I	128	LYS
1	I	130	LYS
1	I	149	LEU
1	I	229	HIS
1	I	301	PHE
1	I	364	LEU
1	I	384	ARG
2	J	31	LYS
2	J	73	LYS
2	J	102	ARG
2	J	124	ARG
1	K	45	TRP
1	K	257	ARG
1	K	259	LYS
1	K	301	PHE
1	K	364	LEU
1	M	45	TRP
1	M	113	ARG
1	M	122	ASP
1	M	130	LYS
1	M	131	ARG
1	M	301	PHE
1	M	334	MSE
2	N	31	LYS
2	N	105	ASP
1	O	45	TRP
1	O	131	ARG
1	O	257	ARG
1	O	301	PHE
1	O	364	LEU
2	P	31	LYS
2	P	124	ARG
2	P	167	ARG

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	379	GLN
1	E	115	HIS

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Mol	Chain	Res	Type
1	E	161	HIS
1	G	379	GLN
1	G	383	GLN
2	J	139	ASN
2	N	91	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 carbohydrates 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 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	371/397 (93%)	-0.23	2 (0%) 91 81	36, 66, 140, 191	0
1	C	372/397 (93%)	-0.27	2 (0%) 91 81	37, 66, 126, 192	0
1	E	372/397 (93%)	0.06	7 (1%) 66 46	55, 103, 163, 201	0
1	G	372/397 (93%)	-0.26	2 (0%) 91 81	35, 64, 155, 208	0
1	I	363/397 (91%)	-0.09	7 (1%) 66 46	38, 78, 151, 223	0
1	K	363/397 (91%)	-0.19	2 (0%) 89 78	36, 70, 125, 203	0
1	M	366/397 (92%)	-0.32	1 (0%) 94 88	28, 58, 132, 218	0
1	O	361/397 (90%)	-0.13	8 (2%) 62 41	34, 66, 137, 210	0
2	B	167/169 (98%)	-0.18	1 (0%) 89 78	42, 85, 123, 154	1 (0%)
2	D	167/169 (98%)	-0.12	2 (1%) 79 61	44, 82, 122, 176	0
2	F	166/169 (98%)	0.12	1 (0%) 89 78	63, 96, 148, 189	0
2	H	167/169 (98%)	-0.24	1 (0%) 89 78	38, 66, 100, 159	0
2	J	167/169 (98%)	-0.18	1 (0%) 89 78	50, 72, 116, 175	0
2	L	167/169 (98%)	-0.23	0 100 100	45, 72, 107, 148	0
2	N	167/169 (98%)	-0.33	0 100 100	33, 59, 94, 149	0
2	P	167/169 (98%)	-0.31	1 (0%) 89 78	37, 59, 98, 150	0
All	All	4275/4528 (94%)	-0.18	38 (0%) 84 69	28, 72, 138, 223	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	122	ASP	6.1
1	C	122	ASP	5.4
1	K	129	TRP	4.4
1	O	124	VAL	4.4
1	O	121	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	122	ASP	3.9
2	F	30	GLU	3.7
1	I	122	ASP	3.6
1	G	69	ASN	3.6
2	B	27	ILE	3.6
2	J	167	ARG	3.4
1	E	141	GLN	3.3
1	O	127	TYR	3.1
1	O	125	PRO	2.8
1	A	69	ASN	2.6
1	I	115	HIS	2.5
1	I	112	ASN	2.5
1	O	8	ASP	2.4
1	I	125	PRO	2.4
1	E	7	LEU	2.3
1	E	129	TRP	2.3
1	I	8	ASP	2.2
2	D	108	ASP	2.2
1	M	129	TRP	2.2
1	E	136	ARG	2.2
1	I	124	VAL	2.2
1	G	122	ASP	2.2
1	O	132	GLN	2.2
2	P	167	ARG	2.2
1	C	129	TRP	2.1
1	O	134	THR	2.1
1	K	132	GLN	2.1
1	E	11	CYS	2.1
1	I	70	SER	2.1
1	A	75	THR	2.1
2	H	167	ARG	2.1
2	D	49	GLN	2.0
1	E	211	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.