



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 3, 2018 – 08:47 PM EST

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

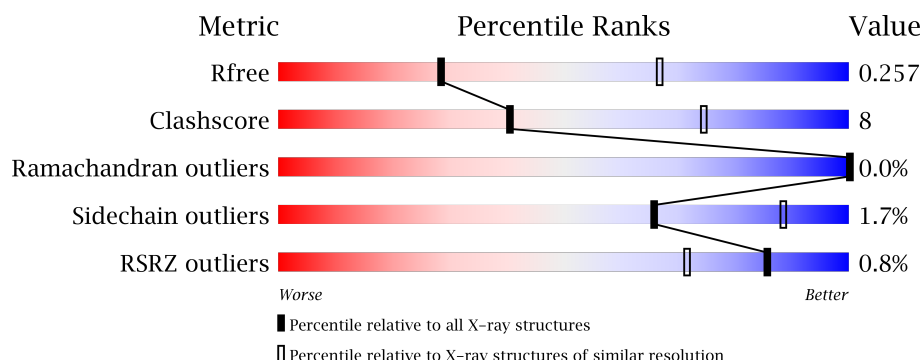
1 Overall quality at a glance

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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

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Mol	Chain	Length	Quality of chain
1	K	397	
1	M	397	
1	O	397	
2	B	169	
2	D	169	
2	F	169	
2	H	169	
2	J	169	
2	L	169	
2	N	169	
2	P	169	

2 Entry composition

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

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
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:

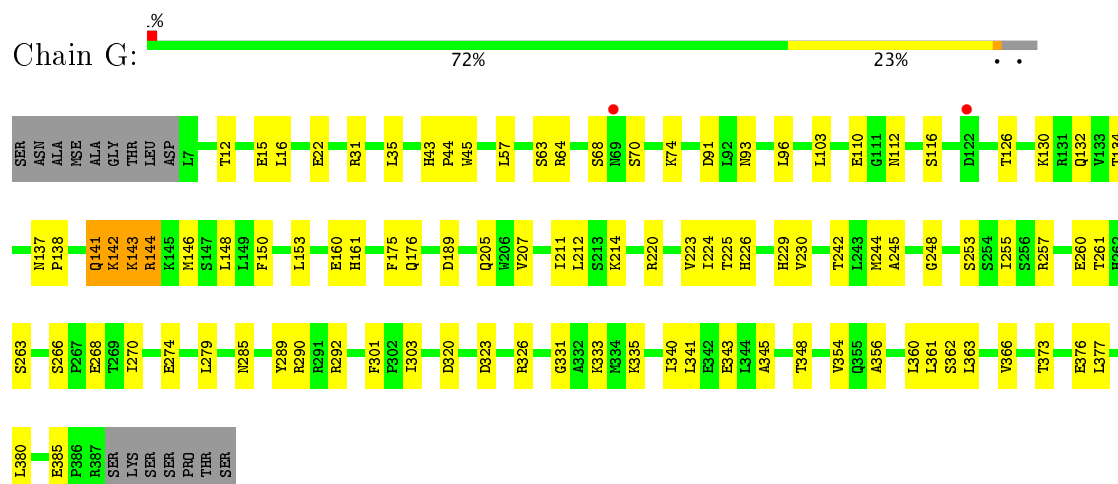
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P61224
B	0	ALA	-	expression tag	UNP P61224
D	-1	GLY	-	expression tag	UNP P61224
D	0	ALA	-	expression tag	UNP P61224
F	-1	GLY	-	expression tag	UNP P61224
F	0	ALA	-	expression tag	UNP P61224
H	-1	GLY	-	expression tag	UNP P61224

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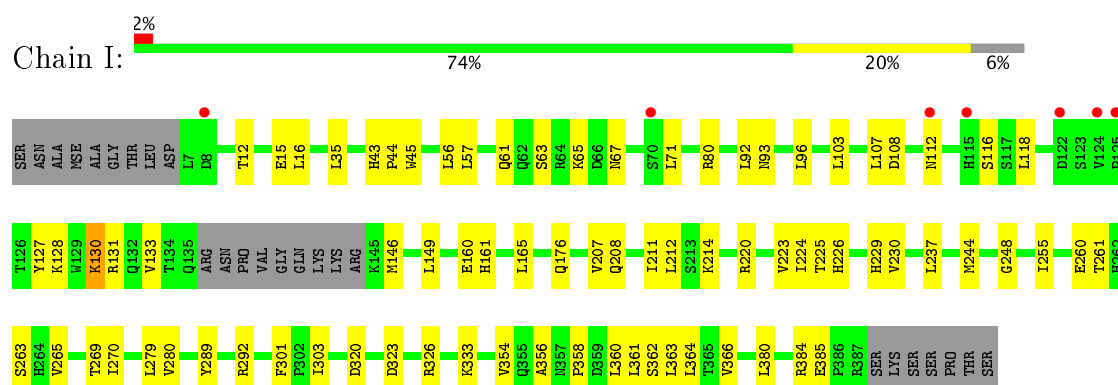
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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	ALA	-	expression tag	UNP P61224
J	-1	GLY	-	expression tag	UNP P61224
J	0	ALA	-	expression tag	UNP P61224
L	-1	GLY	-	expression tag	UNP P61224
L	0	ALA	-	expression tag	UNP P61224
N	-1	GLY	-	expression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

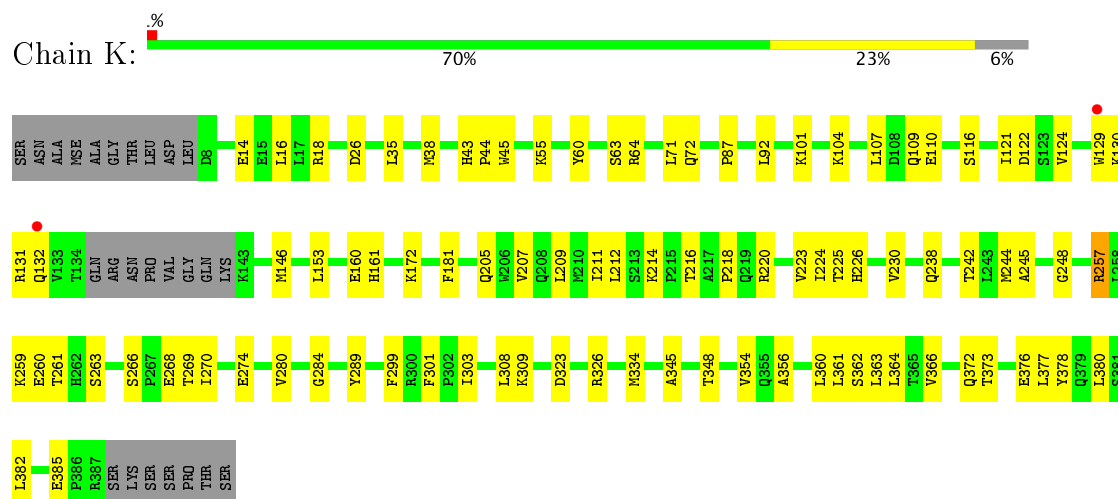
- Molecule 1: RAS guanyl-releasing protein 2



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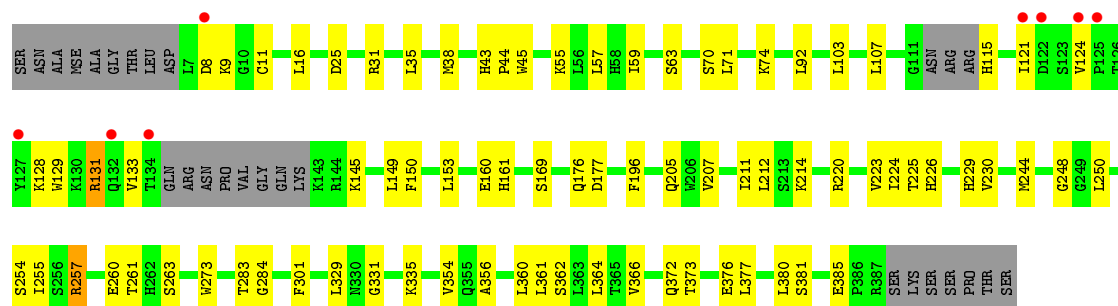
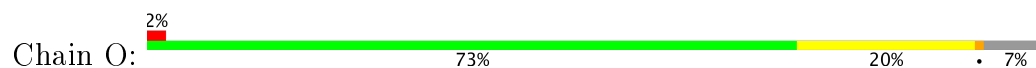


- Molecule 1: RAS guanyl-releasing protein 2

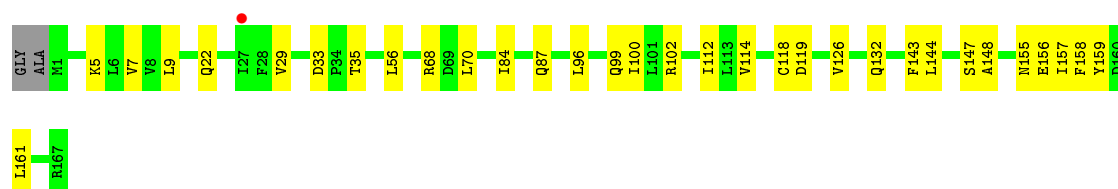
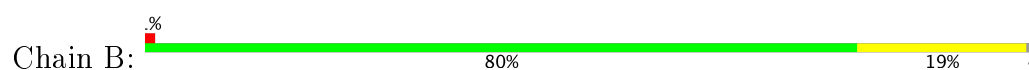




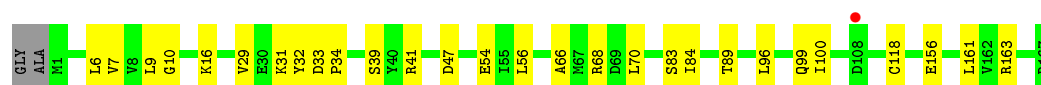
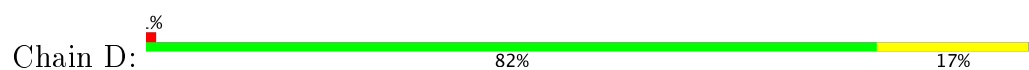
• Molecule 1: RAS guanyl-releasing protein 2



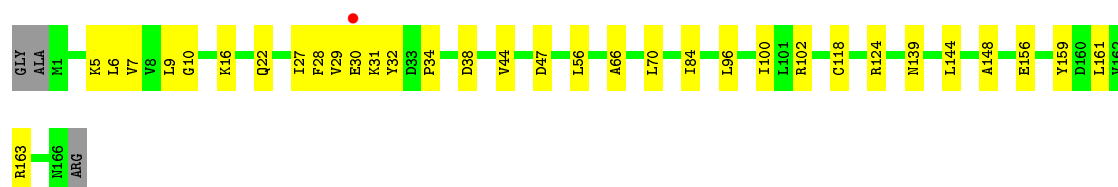
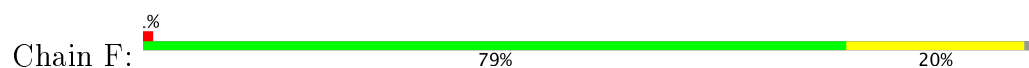
• Molecule 2: Ras-related protein Rap-1b




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




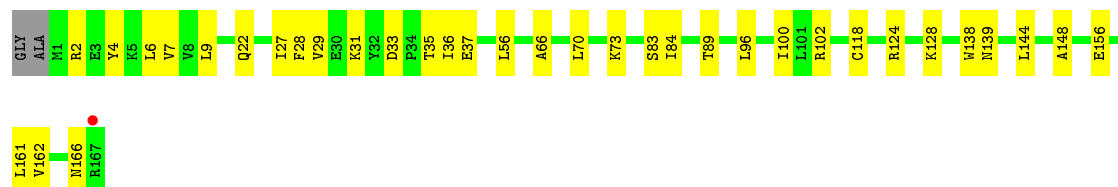
- Molecule 2: Ras-related protein Rap-1b

Chain H:  79% 20%




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

Chain J:  78% 21%




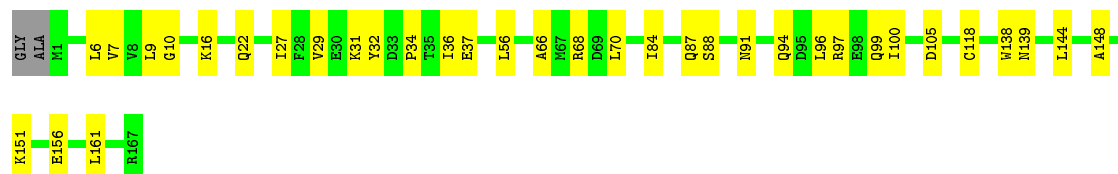
- Molecule 2: Ras-related protein Rap-1b

Chain L:  80% 19%




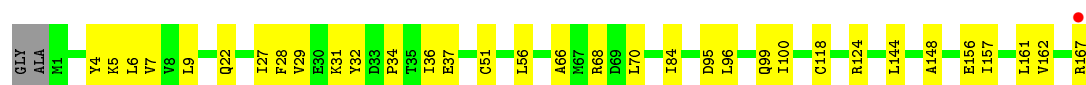
- Molecule 2: Ras-related protein Rap-1b

Chain N:  78% 21%



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

Chain P:  79% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.00 Å 209.26 Å 336.76 Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.12 Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.203 , 0.258 0.201 , 0.257	Depositor DCC
R_{free} test set	3998 reflections (4.87%)	DCC
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34903	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.84 % 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 4.6999e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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.

5 of 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

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
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.

The worst 5 of 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

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%)	44	79
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
2	F	164/169 (97%)	157 (96%)	7 (4%)	0	100	100
2	H	165/169 (98%)	160 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	60	86
1	C	345/349 (99%)	339 (98%)	6 (2%)	66	88
1	E	342/349 (98%)	336 (98%)	6 (2%)	64	87
1	G	343/349 (98%)	335 (98%)	8 (2%)	56	83
1	I	334/349 (96%)	325 (97%)	9 (3%)	50	81
1	K	335/349 (96%)	330 (98%)	5 (2%)	70	89
1	M	339/349 (97%)	332 (98%)	7 (2%)	59	85
1	O	333/349 (95%)	328 (98%)	5 (2%)	70	89
2	B	146/147 (99%)	146 (100%)	0	100	100
2	D	147/147 (100%)	146 (99%)	1 (1%)	87	95
2	F	146/147 (99%)	143 (98%)	3 (2%)	59	85
2	H	147/147 (100%)	145 (99%)	2 (1%)	71	90
2	J	147/147 (100%)	143 (97%)	4 (3%)	50	81
2	L	147/147 (100%)	147 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	147/147 (100%)	145 (99%)	2 (1%)	71	90
2	P	147/147 (100%)	144 (98%)	3 (2%)	60	86
All	All	3887/3968 (98%)	3819 (98%)	68 (2%)	66	88

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	301	PHE
1	I	229	HIS
1	O	257	ARG
2	H	105	ASP
1	I	61	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	379	GLN
2	N	91	ASN
1	G	383	GLN
1	E	115	HIS
2	J	139	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, 95th 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 ²)	Q<0.9
1	A	371/397 (93%)	-0.25	1 (0%) 93 86	36, 66, 140, 191	0
1	C	372/397 (93%)	-0.28	2 (0%) 90 80	37, 66, 126, 192	0
1	E	372/397 (93%)	0.04	6 (1%) 72 51	55, 103, 163, 201	0
1	G	372/397 (93%)	-0.28	2 (0%) 90 80	35, 64, 155, 208	0
1	I	363/397 (91%)	-0.10	7 (1%) 67 46	38, 78, 151, 223	0
1	K	363/397 (91%)	-0.21	2 (0%) 89 77	36, 70, 125, 203	0
1	M	366/397 (92%)	-0.34	1 (0%) 93 86	28, 58, 132, 218	0
1	O	361/397 (90%)	-0.14	8 (2%) 62 41	34, 66, 137, 210	0
2	B	167/169 (98%)	-0.19	1 (0%) 89 77	42, 85, 123, 154	1 (0%)
2	D	167/169 (98%)	-0.13	1 (0%) 89 77	44, 82, 122, 176	0
2	F	166/169 (98%)	0.11	1 (0%) 89 77	63, 96, 148, 189	0
2	H	167/169 (98%)	-0.25	0 100 100	38, 66, 100, 159	0
2	J	167/169 (98%)	-0.19	1 (0%) 89 77	50, 72, 116, 175	0
2	L	167/169 (98%)	-0.24	0 100 100	45, 72, 107, 148	0
2	N	167/169 (98%)	-0.34	0 100 100	33, 59, 94, 149	0
2	P	167/169 (98%)	-0.31	1 (0%) 89 77	37, 59, 98, 150	0
All	All	4275/4528 (94%)	-0.19	34 (0%) 86 71	28, 72, 138, 223	1 (0%)

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	122	ASP	6.1
1	C	122	ASP	5.2
1	K	129	TRP	4.4
1	O	124	VAL	4.3
1	O	121	ILE	4.1

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.