



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:09 PM UTC

PDB ID : 6AXF / pdb_00006axf
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

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

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

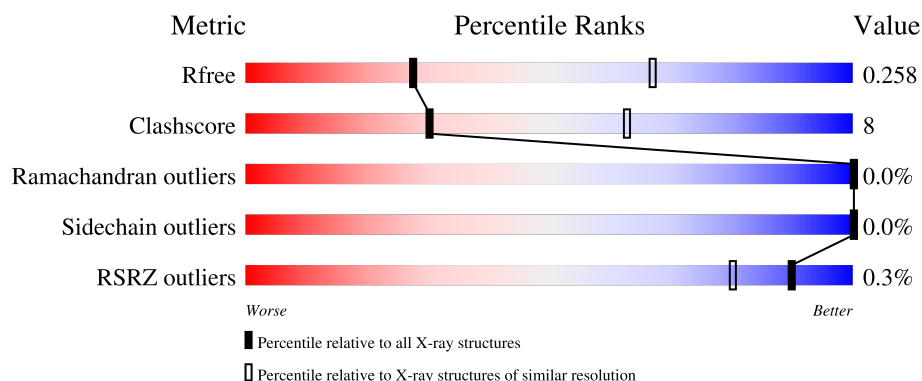
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 of the lower 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 $\leq 5\%$. 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	 71% 23% 6%
1	M	397	 74% 20% 6%
1	O	397	 74% 19% 7%
2	B	169	 80% 19% .
2	D	169	 % 83% 16% .
2	F	169	 80% 18% .
2	H	169	 79% 20% .
2	J	169	 80% 19% .
2	L	169	 79% 20% .
2	N	169	 79% 20% .
2	P	169	 79% 20% .

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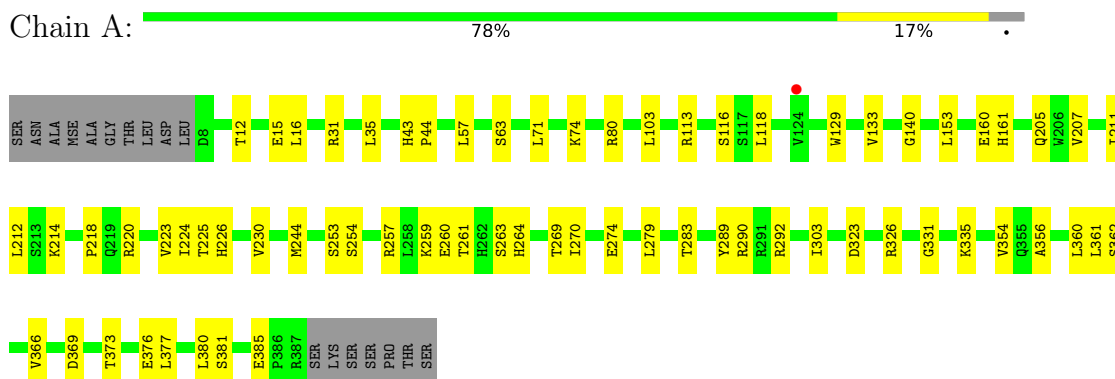
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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	ALA	-	expression tag	UNP P61224
J	-1	GLY	-	expression tag	UNP P61224
J	0	ALA	-	expression tag	UNP P61224
L	-1	GLY	-	expression tag	UNP P61224
L	0	ALA	-	expression tag	UNP P61224
N	-1	GLY	-	expression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

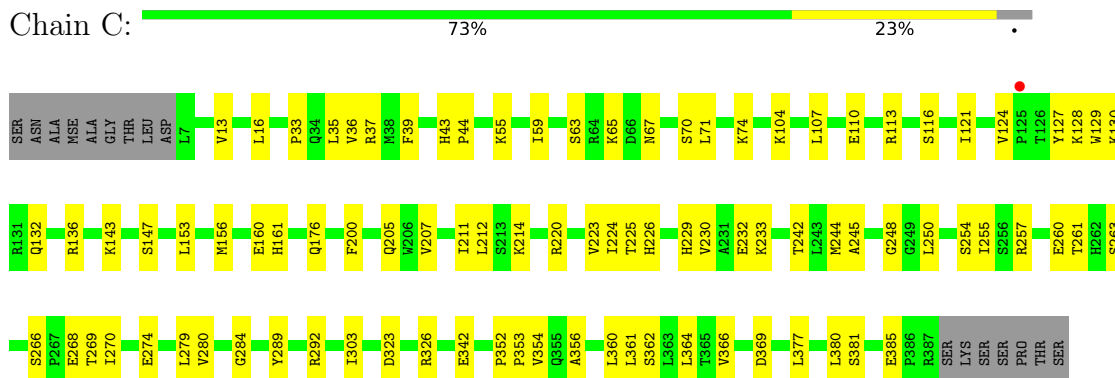
3 Residue-property plots

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 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.

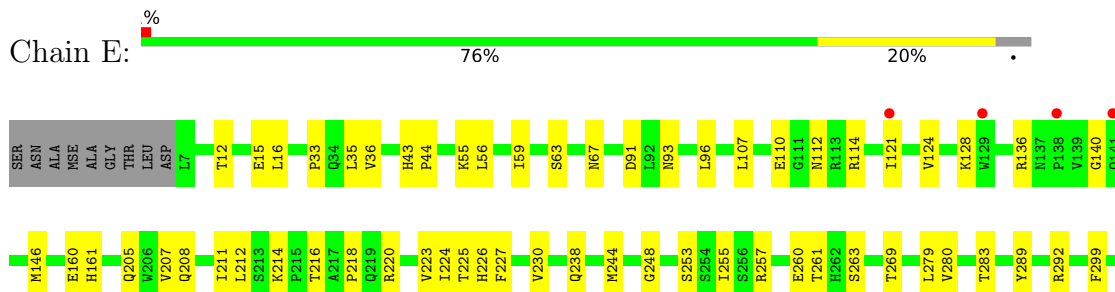
• Molecule 1: RAS guanyl-releasing protein 2



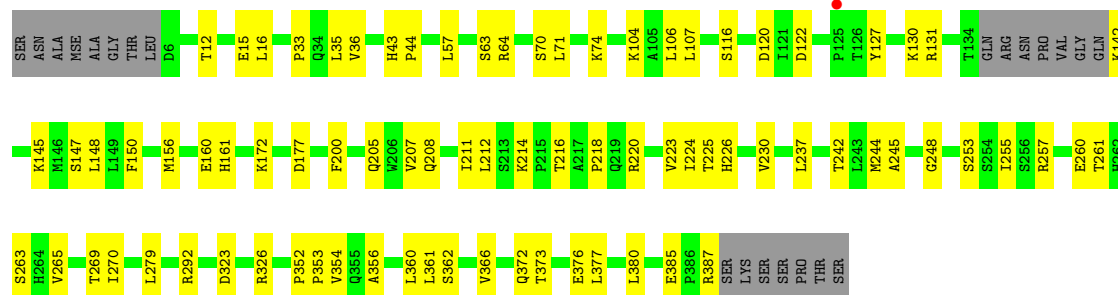
• Molecule 1: RAS guanyl-releasing protein 2



• Molecule 1: RAS guanyl-releasing protein 2

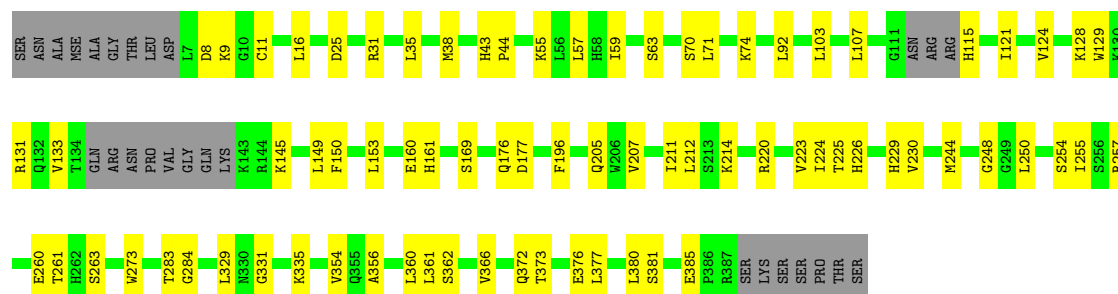


Chain M:  74% 20% 6%



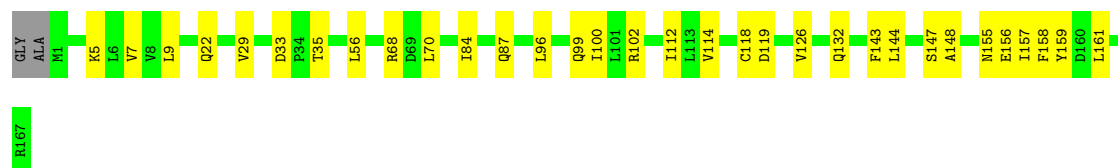
- Molecule 1: RAS guanyl-releasing protein 2

Chain O:  74% 19% 7%



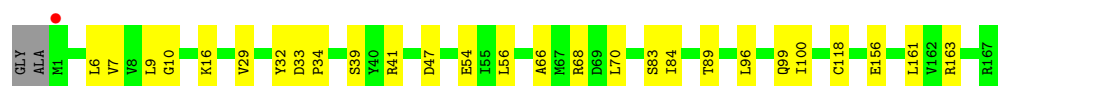
- Molecule 2: Ras-related protein Rap-1b

Chain B:  80% 19% .



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

Chain D:  83% 16% .



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

Chain F:  80% 18% .



ARG

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

Chain H:  79% 20%

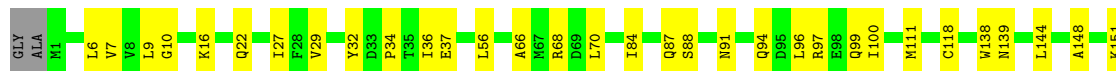
- Molecule 2: Ras-related protein Rap-1b

Chain J:  80% 19%

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

Chain L:  79% 20%

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

Chain N:  79% 20%

- 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	139.00Å 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) 90.0 (49.46-3.10)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.203 , 0.258 0.209 , 0.258	Depositor DCC
R_{free} test set	4365 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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 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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.13	0/3124	0.32	0/4225
1	C	0.14	0/3142	0.35	0/4247
1	E	0.14	0/3128	0.33	0/4232
1	G	0.14	0/3130	0.35	0/4233
1	I	0.14	0/3046	0.35	0/4119
1	K	0.13	0/3058	0.32	0/4135
1	M	0.13	0/3089	0.32	0/4175
1	O	0.14	0/3030	0.33	0/4095
2	B	0.12	0/1340	0.34	0/1805
2	D	0.13	0/1347	0.34	0/1814
2	F	0.12	0/1336	0.34	0/1800
2	H	0.12	0/1347	0.35	0/1814
2	J	0.13	0/1347	0.37	0/1814
2	L	0.13	0/1347	0.33	0/1814
2	N	0.13	0/1347	0.35	0/1814
2	P	0.12	0/1347	0.34	0/1814
All	All	0.13	0/35505	0.34	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	46	0
1	C	3081	0	3112	60	0
1	E	3067	0	3079	56	0
1	G	3069	0	3090	62	0
1	I	2989	0	3001	59	0
1	K	2999	0	3011	61	0
1	M	3030	0	3050	56	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	22	0
2	L	1331	0	1322	24	0
2	N	1331	0	1322	24	0
2	P	1331	0	1322	23	0
All	All	34903	0	34970	587	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 587 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%)	36	67
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%)	342 (100%)	0	100	100
1	C	345/349 (99%)	345 (100%)	0	100	100
1	E	342/349 (98%)	342 (100%)	0	100	100
1	G	343/349 (98%)	343 (100%)	0	100	100
1	I	334/349 (96%)	334 (100%)	0	100	100
1	K	335/349 (96%)	335 (100%)	0	100	100
1	M	339/349 (97%)	339 (100%)	0	100	100
1	O	333/349 (95%)	333 (100%)	0	100	100
2	B	146/147 (99%)	146 (100%)	0	100	100
2	D	147/147 (100%)	147 (100%)	0	100	100
2	F	146/147 (99%)	146 (100%)	0	100	100
2	H	147/147 (100%)	146 (99%)	1 (1%)	76	82
2	J	147/147 (100%)	147 (100%)	0	100	100
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%)	147 (100%)	0	100	100
2	P	147/147 (100%)	147 (100%)	0	100	100
All	All	3887/3968 (98%)	3886 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	44	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	93	ASN
1	K	370	GLN
1	O	383	GLN
1	I	372	GLN
2	J	49	GLN

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 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 ⓘ

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%)	-0.23	1 (0%) 90 80	36, 66, 140, 191	0
1	C	372/397 (93%)	-0.31	1 (0%) 90 80	37, 66, 126, 192	0
1	E	372/397 (93%)	0.07	4 (1%) 78 59	55, 103, 163, 201	0
1	G	372/397 (93%)	-0.29	5 (1%) 75 56	35, 64, 155, 208	0
1	I	363/397 (91%)	-0.17	0 100 100	38, 78, 151, 223	0
1	K	363/397 (91%)	-0.24	0 100 100	36, 70, 125, 203	0
1	M	366/397 (92%)	-0.34	1 (0%) 90 80	28, 58, 132, 218	0
1	O	361/397 (90%)	-0.23	0 100 100	34, 66, 137, 210	0
2	B	167/169 (98%)	-0.14	0 100 100	42, 85, 123, 154	0
2	D	167/169 (98%)	-0.15	1 (0%) 85 70	44, 82, 122, 176	0
2	F	166/169 (98%)	0.03	0 100 100	63, 95, 148, 189	0
2	H	167/169 (98%)	-0.36	0 100 100	38, 66, 100, 159	0
2	J	167/169 (98%)	-0.24	0 100 100	50, 72, 116, 175	0
2	L	167/169 (98%)	-0.25	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%)	-0.29	0 100 100	37, 59, 98, 150	0
All	All	4275/4528 (94%)	-0.22	13 (0%) 90 80	28, 72, 138, 223	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	138	PRO	3.5
1	E	121	ILE	3.2
1	G	124	VAL	2.5
2	D	1	MET	2.4
1	G	126	THR	2.4

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 oligosaccharides 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.