



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:30 am BST

PDB ID : 3QNI  
Title : Crystal structure of human PACSIN 1 F-BAR domain  
Authors : Meng, G.; Bai, X.; Zheng, X.  
Deposited on : 2011-02-08  
Resolution : 2.80 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
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

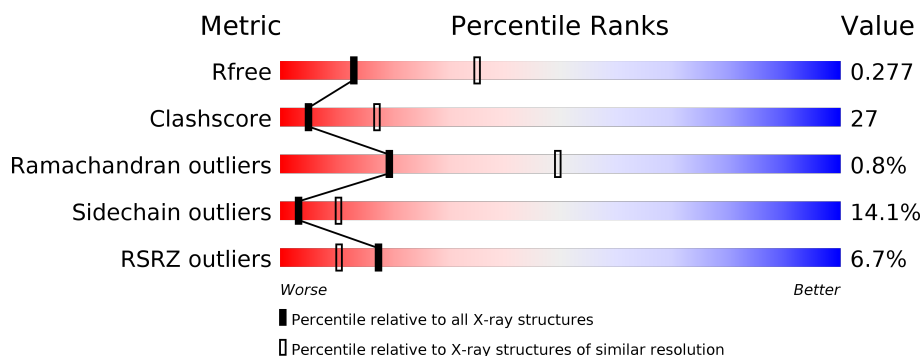
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	307	
1	B	307	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4662 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 Protein kinase C and casein kinase substrate in neurons protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2246	1412	399	421	14			
1	B	266	Total	C	N	O	S	0	0	0
			2215	1395	392	414	14			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	97	Total	O	0	0
			97	97		
3	B	102	Total	O	0	0
			102	102		

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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A:
- 
- Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows positions 1 to 300. A color scale at the top indicates conservation levels: 7% (red), 50% (green), 30% (yellow), 7% (orange), and 11% (grey).
- Key residues (high information content) include:
- Position 1: MET (0.14 bits)
  - Position 2: SER (0.13 bits)
  - Position 3: SER (0.13 bits)
  - Position 4: SER (0.13 bits)
  - Position 5: TTR (0.13 bits)
  - Position 6: ASP (0.13 bits)
  - Position 7: GLU (0.13 bits)
  - Position 8: ALA (0.13 bits)
  - Position 9: SER (0.13 bits)
  - Position 10: LEU (0.13 bits)
  - Position 11: ALA (0.13 bits)
  - Position 12: PRO (0.13 bits)
  - Position 13: GLU (0.13 bits)
  - Position 14: GLU (0.13 bits)
  - Position 15: T15 (0.13 bits)
  - Position 16: F19 (0.13 bits)
  - Position 17: G23 (0.13 bits)
  - Position 18: R26 (0.13 bits)
  - Position 19: R27 (0.13 bits)
  - Position 20: T28 (0.13 bits)
  - Position 21: V29 (0.13 bits)
  - Position 22: R30 (0.13 bits)
  - Position 23: I32 (0.13 bits)
  - Position 24: D33 (0.13 bits)
  - Position 25: D34 (0.13 bits)
  - Position 26: R37 (0.13 bits)
  - Position 27: L42 (0.13 bits)
  - Position 28: N43 (0.13 bits)
  - Position 29: N44 (0.13 bits)
  - Position 30: Q45 (0.13 bits)
  - Position 31: R51 (0.13 bits)
  - Position 32: A55 (0.13 bits)
  - Position 33: Q58 (0.13 bits)
  - Position 34: Q59 (0.13 bits)
  - Position 35: L60 (0.13 bits)
  - Position 36: N63 (0.13 bits)
  - Position 37: A64 (0.13 bits)
  - Position 38: R65 (0.13 bits)
  - Position 39: R66 (0.13 bits)
  - Position 40: E72 (0.13 bits)
  - Position 41: K73 (0.13 bits)
  - Position 42: Q76 (0.13 bits)
  - Position 43: Y77 (0.13 bits)
  - Position 44: E78 (0.13 bits)
  - Position 45: S79 (0.13 bits)
  - Position 46: L80 (0.13 bits)
  - Position 47: R81 (0.13 bits)
  - Position 48: R82 (0.13 bits)

- Chain B:
- 
- | Amino Acid | Frequency (%) |
|------------|---------------|
| Met        | 5%            |
| Ser        | 51%           |
| Ser        | 29%           |
| Ser        | 6%            |
| Tyr        | 13%           |
| Asp        |               |
| Ala        |               |
| Ser        |               |
| Leu        |               |
| Ala        |               |
| Pro        |               |
| Glu        |               |
| Glu        |               |
| Thr        |               |
| T16        |               |
| D17        |               |
| R27        |               |
| R30        |               |
| R31        |               |
| R36        |               |
| R37        |               |
| L38        |               |
| C39        |               |
| N40        |               |
| D41        |               |
| L42        |               |
| N43        |               |
| R49        |               |
| R57        |               |
| T61        |               |
| A64        |               |
| E72        |               |
| K73        |               |
| G74        |               |
| P75        |               |
| Q76        |               |
| L80        |               |
| N84        |               |
| G85        |               |
| A86        |               |
| L87        |               |
| N88        |               |
| T89        |               |
| E90        |               |
| Q99        |               |
| E100       |               |
| L101       |               |

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.90Å 83.74Å 86.51Å 90.00° 114.40° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (30.00-2.80) 93.8 (29.83-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.33 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.204 , 0.284 0.205 , 0.277	Depositor DCC
$R_{free}$ test set	1117 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.1	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4662	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.81	2/2289 (0.1%)	0.88	8/3068 (0.3%)
1	B	0.77	0/2260	0.85	4/3029 (0.1%)
All	All	0.79	2/4549 (0.0%)	0.87	12/6097 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	GLU	CG-CD	5.44	1.60	1.51
1	A	45	CYS	CB-SG	-5.18	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	VAL	CB-CA-C	-13.58	85.59	111.40
1	B	169	LEU	N-CA-CB	-10.01	90.37	110.40
1	A	80	LEU	CA-CB-CG	-7.14	98.88	115.30
1	B	260	GLU	N-CA-C	-6.81	92.62	111.00
1	A	31	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	196	ASP	N-CA-CB	-5.90	99.98	110.60
1	A	307	PRO	N-CA-CB	5.82	110.28	103.30
1	A	194	LYS	N-CA-C	5.56	126.02	111.00
1	B	168	LYS	CB-CA-C	5.52	121.45	110.40
1	A	31	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	168	LYS	N-CA-C	5.23	125.12	111.00
1	B	144	LYS	N-CA-C	5.04	124.62	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	2246	0	2192	151	0
1	B	2215	0	2171	124	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	97	0	0	16	0
3	B	102	0	0	22	0
All	All	4662	0	4363	239	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 27.

All (239) 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:A:167:GLU:HA	1:A:198:CYS:SG	1.39	1.62
1:A:264:TYR:CD1	1:B:259:ALA:HB2	1.54	1.41
1:A:264:TYR:CE1	1:B:259:ALA:HB2	1.53	1.40
1:B:126:MET:CB	1:B:127:GLY:HA3	1.48	1.33
1:B:126:MET:HB3	1:B:127:GLY:CA	1.53	1.30
1:A:195:VAL:O	1:A:195:VAL:CG1	1.70	1.29
1:A:264:TYR:CD1	1:B:259:ALA:CB	2.13	1.29
1:A:167:GLU:CA	1:A:198:CYS:SG	2.23	1.26
1:A:264:TYR:CE1	1:B:259:ALA:CB	2.20	1.22
1:B:145:PRO:HG2	3:B:335:HOH:O	1.41	1.21
1:A:169:LEU:O	1:A:169:LEU:HD23	1.37	1.19
1:B:261:ASN:HD22	1:B:262:SER:N	1.37	1.18
1:B:125:ILE:HG22	3:B:312:HOH:O	1.43	1.18
1:B:167:GLU:O	1:B:171:MET:HB2	1.44	1.17
1:B:261:ASN:ND2	1:B:263:SER:H	1.43	1.16
1:B:169:LEU:CD1	3:B:309:HOH:O	1.96	1.13
1:A:196:ASP:HB3	1:A:197:LYS:CE	1.81	1.10
1:B:169:LEU:HD13	3:B:309:HOH:O	1.53	1.07
1:A:196:ASP:HB3	1:A:197:LYS:HE3	1.36	1.04
1:B:261:ASN:C	1:B:261:ASN:HD22	1.61	1.03
1:A:31:ARG:HH22	1:A:235:GLN:NE2	1.57	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:HE3	1:B:303:GLU:OE2	1.59	1.01
1:A:266:HIS:HB3	3:A:392:HOH:O	1.62	0.99
1:B:167:GLU:HG2	1:B:171:MET:HG3	1.46	0.96
1:A:258:LEU:O	1:A:261:ASN:HB2	1.65	0.96
1:A:31:ARG:NH2	1:A:235:GLN:HE22	1.64	0.95
1:B:261:ASN:ND2	1:B:263:SER:N	2.16	0.94
1:A:125:ILE:HG22	1:A:126:MET:HG2	1.47	0.93
1:A:200:GLN:NE2	1:A:201:ASP:OD1	2.02	0.93
1:A:264:TYR:HD1	1:B:259:ALA:CB	1.63	0.92
1:B:126:MET:HB3	1:B:127:GLY:HA3	0.93	0.91
1:B:126:MET:HB2	1:B:127:GLY:HA3	1.49	0.91
1:A:257:ASN:HB3	1:A:260:GLU:HG2	1.52	0.90
1:A:23:GLY:O	1:A:26:LYS:HG3	1.70	0.89
1:A:264:TYR:HE1	1:B:259:ALA:CB	1.79	0.89
1:A:118:LYS:O	3:A:333:HOH:O	1.92	0.87
1:B:261:ASN:HD21	1:B:263:SER:H	0.89	0.86
1:B:36:HIS:HD2	3:B:351:HOH:O	1.58	0.86
1:B:261:ASN:ND2	1:B:262:SER:N	2.23	0.85
1:B:297:MET:HE3	1:B:297:MET:HA	1.58	0.84
1:A:196:ASP:HB3	1:A:197:LYS:HE2	1.57	0.84
1:A:146:TRP:CZ3	1:A:220:THR:HG22	2.13	0.83
1:B:125:ILE:HG23	1:B:126:MET:N	1.93	0.82
1:A:146:TRP:HZ3	1:A:220:THR:HG22	1.44	0.82
1:B:261:ASN:C	1:B:261:ASN:ND2	2.29	0.82
1:B:260:GLU:CB	3:B:380:HOH:O	2.25	0.82
1:B:123:LYS:O	1:B:124:GLN:HB2	1.80	0.82
1:B:279:ASP:HB3	1:B:282:GLU:HB2	1.61	0.81
1:B:126:MET:CB	1:B:127:GLY:CA	2.29	0.81
1:B:261:ASN:HD21	1:B:263:SER:N	1.74	0.80
1:A:90:GLU:OE2	1:B:49:ARG:NH2	2.15	0.80
1:A:264:TYR:CD1	1:B:259:ALA:HB3	2.15	0.79
1:A:264:TYR:HE1	1:B:259:ALA:HB2	1.32	0.79
1:A:196:ASP:CB	1:A:197:LYS:HE2	2.13	0.79
1:A:264:TYR:CE1	1:B:259:ALA:HB3	2.17	0.79
1:A:167:GLU:HA	1:A:198:CYS:HG	1.48	0.78
1:A:37:ARG:NH2	1:B:75:PRO:HD3	1.99	0.77
1:A:31:ARG:HH22	1:A:235:GLN:HE22	1.21	0.76
1:B:31:ARG:HH22	1:B:235:GLN:NE2	1.84	0.76
1:B:167:GLU:O	1:B:171:MET:CB	2.31	0.75
1:A:282:GLU:HG2	1:A:285:ARG:HH22	1.51	0.75
1:B:167:GLU:CG	1:B:171:MET:HG3	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:MET:HB3	1:B:127:GLY:HA2	1.66	0.74
1:B:31:ARG:HH22	1:B:235:GLN:HE22	1.35	0.73
1:A:170:ALA:CB	3:A:387:HOH:O	2.35	0.73
1:B:88:MET:HE2	1:B:88:MET:H	1.53	0.72
1:A:196:ASP:CG	1:A:197:LYS:HE2	2.10	0.72
1:A:195:VAL:O	1:A:195:VAL:HG12	0.90	0.72
1:B:126:MET:HB2	3:B:312:HOH:O	1.90	0.71
1:A:257:ASN:HB3	1:A:260:GLU:CG	2.20	0.71
1:A:88:MET:CE	1:A:88:MET:H	2.03	0.70
1:B:158:LYS:HA	1:B:161:HIS:HB2	1.72	0.68
1:A:200:GLN:C	1:A:200:GLN:CD	2.52	0.68
1:A:31:ARG:NH2	1:A:235:GLN:NE2	2.27	0.68
1:A:241:ARG:NH1	1:B:76:GLN:OE1	2.27	0.67
1:A:205:THR:O	1:A:208:LYS:N	2.28	0.67
1:A:170:ALA:HB2	3:A:387:HOH:O	1.94	0.66
1:B:126:MET:SD	3:B:359:HOH:O	2.53	0.66
1:A:258:LEU:HB2	1:B:264:TYR:OH	1.95	0.66
1:A:31:ARG:HH11	1:A:31:ARG:HG2	1.59	0.66
1:A:200:GLN:O	1:A:203:GLN:HB3	1.95	0.66
1:A:167:GLU:N	1:A:198:CYS:SG	2.68	0.66
1:B:85:GLY:HA2	1:B:88:MET:CE	2.25	0.66
1:A:286:TRP:O	1:A:290:THR:HB	1.97	0.65
1:A:196:ASP:CB	1:A:197:LYS:CE	2.65	0.65
1:A:201:ASP:O	1:A:204:LYS:N	2.30	0.65
1:A:37:ARG:HH21	1:B:75:PRO:CD	2.10	0.64
1:B:269:ARG:HG3	1:B:269:ARG:HH11	1.62	0.64
1:A:257:ASN:CB	1:A:260:GLU:HG2	2.24	0.64
1:A:169:LEU:O	1:A:169:LEU:CD2	2.30	0.64
1:B:169:LEU:HD12	3:B:309:HOH:O	1.77	0.64
1:A:169:LEU:C	1:A:169:LEU:HD23	2.16	0.63
1:A:264:TYR:HE1	1:B:259:ALA:N	1.97	0.63
1:A:290:THR:HG22	1:A:291:SER:HB2	1.80	0.63
1:B:86:ALA:HA	3:B:396:HOH:O	1.98	0.63
1:A:272:GLU:HB2	1:B:253:LYS:HE3	1.80	0.62
1:A:197:LYS:CD	1:A:197:LYS:H	2.12	0.62
1:A:205:THR:O	1:A:206:GLN:C	2.34	0.62
1:B:292:GLY:O	1:B:295:MET:HG3	2.00	0.62
1:A:296:PRO:HA	3:A:320:HOH:O	2.00	0.61
1:A:29:VAL:HA	1:A:32:ILE:HD12	1.82	0.61
1:A:281:GLN:H	1:A:281:GLN:CD	2.04	0.61
1:A:143:GLN:HG3	1:A:223:TYR:HE1	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:HIS:HD2	1:B:131:GLU:OE2	1.85	0.60
1:B:146:TRP:CZ3	1:B:220:THR:OG1	2.54	0.60
1:B:261:ASN:HA	3:B:318:HOH:O	2.01	0.59
1:B:36:HIS:CD2	3:B:351:HOH:O	2.43	0.59
1:A:37:ARG:NH2	1:B:75:PRO:CD	2.64	0.59
1:B:85:GLY:HA2	1:B:88:MET:HE3	1.85	0.59
1:B:158:LYS:O	1:B:162:LEU:HB2	2.03	0.58
1:B:167:GLU:HB3	1:B:168:LYS:NZ	2.18	0.58
1:A:88:MET:HE2	1:A:88:MET:H	1.69	0.58
1:B:101:VAL:HG22	1:B:255:HIS:O	2.03	0.58
1:A:202:VAL:HG12	1:A:203:GLN:N	2.19	0.57
1:A:264:TYR:HE1	1:B:259:ALA:H	1.52	0.57
1:B:267:VAL:HG22	1:B:268:TYR:CD2	2.40	0.57
1:A:104:ASN:HB3	1:A:255:HIS:CG	2.40	0.57
1:A:200:GLN:O	1:A:203:GLN:N	2.38	0.56
1:B:152:GLU:OE1	3:B:349:HOH:O	2.17	0.56
1:A:55:ALA:O	1:A:59:GLN:HG3	2.06	0.56
1:A:130:LYS:HD2	3:A:348:HOH:O	2.05	0.56
1:B:87:ILE:O	1:B:90:GLU:HG3	2.06	0.56
1:A:254:ARG:HD2	3:A:364:HOH:O	2.03	0.56
1:A:264:TYR:O	1:A:267:VAL:HG13	2.06	0.55
1:A:261:ASN:HB3	1:A:264:TYR:H	1.70	0.55
1:A:259:ALA:C	1:A:261:ASN:H	2.10	0.55
1:A:197:LYS:H	1:A:197:LYS:CE	2.20	0.55
1:A:27:ARG:NH1	1:B:295:MET:HE1	2.21	0.55
1:A:205:THR:OG1	1:A:206:GLN:N	2.39	0.55
1:A:264:TYR:OH	1:B:258:LEU:HB2	2.07	0.55
1:B:143:GLN:HG3	1:B:223:TYR:HE1	1.73	0.54
1:A:264:TYR:HD1	1:B:259:ALA:HB1	1.63	0.54
1:A:37:ARG:NH1	3:A:359:HOH:O	2.04	0.54
1:B:168:LYS:O	3:B:398:HOH:O	2.19	0.53
1:A:43:MET:HG2	1:A:113:VAL:CG2	2.38	0.53
1:A:33:ASP:O	1:A:34:ASP:C	2.45	0.53
1:A:124:GLN:OE1	1:A:130:LYS:HB2	2.09	0.53
1:A:31:ARG:NH1	1:A:31:ARG:HG2	2.23	0.53
1:A:167:GLU:CB	1:A:198:CYS:SG	2.97	0.52
1:A:88:MET:HE1	1:A:88:MET:H	1.73	0.52
1:A:241:ARG:NH2	3:A:334:HOH:O	2.43	0.52
1:A:233:GLN:HG2	3:A:399:HOH:O	2.09	0.52
1:A:146:TRP:O	1:A:150:MET:HB2	2.10	0.52
1:A:200:GLN:CG	1:A:201:ASP:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:HD11	1:B:239:GLU:HB2	1.93	0.51
1:A:79:SER:HB3	1:A:278:ALA:HA	1.90	0.51
1:B:139:PHE:CE2	1:B:230:VAL:HB	2.46	0.50
1:A:37:ARG:HH21	1:B:75:PRO:HD2	1.75	0.50
1:B:64:ALA:HA	1:B:88:MET:HG3	1.93	0.50
1:A:200:GLN:OE1	1:A:200:GLN:O	2.30	0.50
1:B:39:CYS:O	1:B:43:MET:HG3	2.12	0.50
1:A:42:LEU:HD23	1:A:113:VAL:HG11	1.94	0.50
1:A:200:GLN:HG3	1:A:201:ASP:N	2.27	0.49
1:B:146:TRP:HZ2	3:B:371:HOH:O	1.95	0.49
1:A:72:GLU:HG3	1:A:73:LYS:N	2.26	0.49
1:A:27:ARG:HH12	1:B:295:MET:HE1	1.78	0.49
1:A:305:TRP:O	1:A:306:ASN:C	2.49	0.49
1:A:257:ASN:OD1	1:A:260:GLU:HG2	2.12	0.49
1:A:31:ARG:HH22	1:A:235:GLN:HE21	1.52	0.49
1:A:87:ILE:O	1:A:90:GLU:HG3	2.13	0.49
1:B:143:GLN:OE1	3:B:326:HOH:O	2.20	0.49
1:A:43:MET:CG	1:A:113:VAL:CG2	2.91	0.49
1:A:238:GLU:OE2	1:A:241:ARG:NH2	2.46	0.48
1:A:66:ARG:NH2	1:B:48:GLU:OE2	2.47	0.48
1:A:88:MET:N	1:A:88:MET:CE	2.76	0.48
1:B:200:GLN:HA	1:B:203:GLN:HG3	1.96	0.48
1:A:31:ARG:HH11	1:A:31:ARG:CG	2.27	0.48
1:A:51:LYS:NZ	3:A:366:HOH:O	2.47	0.48
1:A:253:LYS:HD2	1:B:272:GLU:HG3	1.96	0.47
1:A:170:ALA:HB3	3:A:387:HOH:O	2.07	0.47
1:B:126:MET:HG2	3:B:359:HOH:O	2.15	0.47
1:B:151:LYS:HG2	1:B:152:GLU:N	2.27	0.47
1:B:161:HIS:C	3:B:319:HOH:O	2.52	0.47
1:B:199:LYS:HA	1:B:199:LYS:HD2	1.78	0.47
1:A:292:GLY:O	1:A:295:MET:HB2	2.15	0.47
1:B:123:LYS:HB3	1:B:123:LYS:HE3	1.40	0.47
1:B:57:GLY:O	1:B:61:THR:HG23	2.15	0.47
1:A:159:ALA:O	1:A:162:LEU:HB3	2.13	0.47
1:A:296:PRO:CA	3:A:320:HOH:O	2.62	0.47
1:B:279:ASP:HB3	1:B:282:GLU:CB	2.40	0.47
1:A:200:GLN:OE1	1:A:200:GLN:C	2.53	0.47
1:B:157:LYS:HG3	1:B:209:TYR:CZ	2.50	0.46
1:A:104:ASN:HB3	1:A:255:HIS:ND1	2.31	0.46
1:B:72:GLU:HG3	1:B:73:LYS:N	2.28	0.46
1:B:123:LYS:HG2	1:B:129:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:PRO:HD3	3:B:346:HOH:O	2.16	0.46
1:B:297:MET:HE3	1:B:297:MET:CA	2.40	0.45
1:A:64:ALA:HA	1:A:88:MET:HG3	1.98	0.45
1:A:27:ARG:HH12	1:B:295:MET:CE	2.29	0.45
1:A:245:LEU:HD23	1:B:80:LEU:HD23	1.99	0.45
1:A:19:PHE:HB2	1:B:295:MET:HE2	1.99	0.45
1:A:58:GLN:CA	1:A:58:GLN:HE21	2.30	0.45
1:B:72:GLU:OE2	3:B:385:HOH:O	2.21	0.45
1:A:205:THR:O	1:A:207:GLU:N	2.50	0.45
1:A:258:LEU:HA	1:A:258:LEU:HD23	1.47	0.44
1:A:80:LEU:HD22	1:B:245:LEU:HD13	1.98	0.44
1:B:215:ASP:HA	1:B:218:LYS:HD2	2.00	0.44
1:B:37:ARG:NH1	1:B:41:ASP:OD2	2.51	0.44
1:A:143:GLN:HG3	1:A:223:TYR:CE1	2.50	0.44
1:A:139:PHE:CE1	1:A:230:VAL:HB	2.53	0.44
1:B:104:ASN:O	1:B:105:LEU:C	2.56	0.44
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.86	0.44
1:A:201:ASP:O	1:A:202:VAL:C	2.53	0.43
1:A:90:GLU:HG2	1:A:271:LEU:HD22	2.00	0.43
1:B:167:GLU:HB3	1:B:168:LYS:HZ1	1.82	0.43
1:B:167:GLU:HB3	1:B:168:LYS:HZ2	1.82	0.43
1:A:19:PHE:N	1:B:295:MET:HE3	2.33	0.43
1:A:276:ARG:NH2	3:A:384:HOH:O	2.50	0.43
1:B:156:ALA:O	1:B:157:LYS:C	2.57	0.43
1:A:76:GLN:HE21	1:A:77:TYR:N	2.16	0.43
1:A:43:MET:SD	1:A:113:VAL:HG23	2.58	0.43
1:B:304:GLU:O	1:B:305:TRP:CB	2.66	0.43
1:A:197:LYS:H	1:A:197:LYS:HD2	1.83	0.43
1:A:291:SER:O	1:B:27:ARG:NH1	2.51	0.43
1:B:148:LYS:O	1:B:151:LYS:HD2	2.19	0.43
1:B:216:VAL:O	1:B:217:GLY:C	2.58	0.43
1:A:124:GLN:NE2	1:A:124:GLN:HA	2.34	0.42
1:A:264:TYR:HE1	1:B:259:ALA:CA	2.29	0.42
1:B:120:ALA:HB2	3:B:382:HOH:O	2.19	0.42
1:A:63:TRP:CZ2	1:B:49:ARG:HB2	2.53	0.42
1:A:257:ASN:CG	1:A:260:GLU:HG2	2.39	0.42
1:A:60:LEU:CD1	1:A:94:VAL:HG12	2.49	0.42
1:B:84:TRP:O	1:B:88:MET:HE1	2.19	0.42
1:A:146:TRP:CH2	1:A:220:THR:HG22	2.53	0.42
1:A:82:ARG:HD2	3:A:388:HOH:O	2.19	0.42
1:B:200:GLN:HA	1:B:203:GLN:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:GLN:O	1:A:201:ASP:C	2.53	0.41
1:A:291:SER:OG	1:B:27:ARG:HD2	2.19	0.41
1:A:88:MET:HE1	1:A:88:MET:N	2.35	0.41
1:B:140:ARG:HD3	3:B:366:HOH:O	2.20	0.41
1:B:17:ASP:O	1:B:27:ARG:NH2	2.53	0.41
1:A:225:GLU:CD	3:A:351:HOH:O	2.59	0.41
1:B:198:CYS:O	1:B:202:VAL:HG23	2.20	0.41
1:A:205:THR:C	1:A:207:GLU:N	2.70	0.41
1:A:160:TYR:HD1	1:A:205:THR:OG1	2.04	0.40
1:B:252:ILE:O	1:B:256:LEU:HG	2.21	0.40
1:A:112:LYS:HD3	1:A:248:VAL:HG22	2.03	0.40
1:A:200:GLN:CD	1:A:201:ASP:N	2.73	0.40
1:A:208:LYS:HE2	1:A:212:VAL:HG23	2.03	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	269/307 (88%)	250 (93%)	15 (6%)	4 (2%)	10	33
1	B	262/307 (85%)	246 (94%)	16 (6%)	0	100	100
All	All	531/614 (86%)	496 (93%)	31 (6%)	4 (1%)	19	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	A	195	VAL
1	A	260	GLU
1	A	216	VAL

### 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	234/273 (86%)	200 (86%)	34 (14%)	3	9
1	B	233/273 (85%)	201 (86%)	32 (14%)	3	11
All	All	467/546 (86%)	401 (86%)	66 (14%)	3	10

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	31	ARG
1	A	37	ARG
1	A	58	GLN
1	A	72	GLU
1	A	80	LEU
1	A	88	MET
1	A	90	GLU
1	A	103	ASN
1	A	118	LYS
1	A	123	LYS
1	A	125	ILE
1	A	130	LYS
1	A	140	ARG
1	A	150	MET
1	A	165	LYS
1	A	171	MET
1	A	197	LYS
1	A	198	CYS
1	A	200	GLN
1	A	202	VAL
1	A	204	LYS
1	A	208	LYS
1	A	215	ASP
1	A	222	GLN
1	A	227	MET
1	A	233	GLN

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Mol	Chain	Res	Type
1	A	250	LEU
1	A	263	SER
1	A	267	VAL
1	A	281	GLN
1	A	288	ARG
1	A	290	THR
1	A	291	SER
1	B	16	THR
1	B	17	ASP
1	B	30	LYS
1	B	31	ARG
1	B	37	ARG
1	B	42	LEU
1	B	49	ARG
1	B	88	MET
1	B	99	GLN
1	B	123	LYS
1	B	141	LYS
1	B	148	LYS
1	B	151	LYS
1	B	165	LYS
1	B	168	LYS
1	B	171	MET
1	B	196	ASP
1	B	197	LYS
1	B	199	LYS
1	B	200	GLN
1	B	203	GLN
1	B	204	LYS
1	B	220	THR
1	B	233	GLN
1	B	245	LEU
1	B	250	LEU
1	B	261	ASN
1	B	267	VAL
1	B	271	LEU
1	B	273	GLN
1	B	289	SER
1	B	297	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	58	GLN
1	A	99	GLN
1	A	161	HIS
1	A	206	GLN
1	A	226	ASN
1	A	235	GLN
1	B	99	GLN
1	B	103	ASN
1	B	104	ASN
1	B	122	HIS
1	B	200	GLN
1	B	226	ASN
1	B	229	GLN
1	B	235	GLN
1	B	236	GLN
1	B	261	ASN
1	B	281	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



No monomer is involved in short contacts.

## 5.7 Other polymers

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	273/307 (88%)	0.07	20 (7%) 15 8	41, 63, 143, 195	1 (0%)
1	B	266/307 (86%)	0.09	16 (6%) 21 14	43, 63, 145, 216	0
All	All	539/614 (87%)	0.08	36 (6%) 17 10	41, 63, 145, 216	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	CYS	8.2
1	A	193	ASP	6.9
1	A	196	ASP	5.8
1	A	194	LYS	5.5
1	B	170	ALA	5.4
1	B	197	LYS	5.3
1	A	192	GLN	5.1
1	B	200	GLN	4.9
1	B	171	MET	4.6
1	A	198	CYS	4.6
1	B	196	ASP	4.6
1	A	171	MET	3.6
1	B	305	TRP	3.5
1	B	203	GLN	3.4
1	A	169	LEU	3.4
1	A	306	ASN	3.3
1	B	201	ASP	3.3
1	B	169	LEU	3.3
1	A	195	VAL	3.2
1	B	163	ALA	3.1
1	A	201	ASP	3.1
1	A	307	PRO	3.0
1	A	301	GLN	2.9
1	B	168	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	168	LYS	2.8
1	A	197	LYS	2.6
1	A	200	GLN	2.5
1	B	160	TYR	2.3
1	A	203	GLN	2.3
1	B	199	LYS	2.3
1	A	167	GLU	2.2
1	B	204	LYS	2.1
1	A	126	MET	2.1
1	A	162	LEU	2.1
1	A	302	PHE	2.0
1	B	162	LEU	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	B	400	1/1	0.97	0.04	52,52,52,52	0
2	CA	A	400	1/1	0.99	0.09	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.