



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2017 – 04:52 AM EDT

PDB ID : 3SUZ  
Title : Crystal structure of Rat Mint2 PPC  
Authors : Shen, Y.; Long, J.; Yan, X.; Xie, X.  
Deposited on : unknown  
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692  
EDS : rb-20030345  
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-20030345

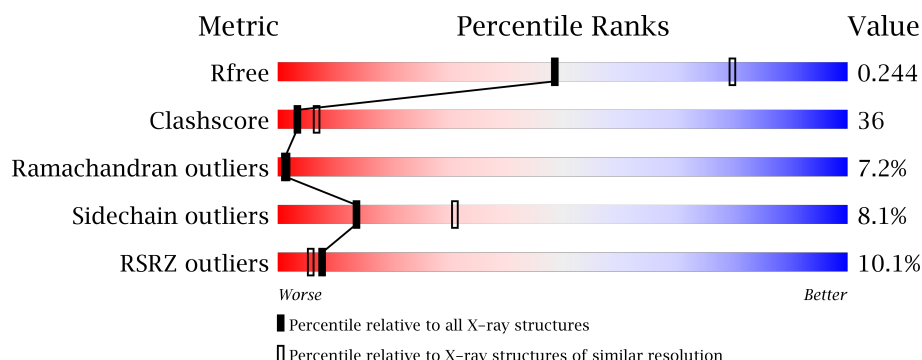
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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. 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	388	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2185 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 Amyloid beta A4 precursor protein-binding family A member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2134	1337	375	407	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	363	GLY	-	EXPRESSION TAG	UNP O35431
A	364	SER	-	EXPRESSION TAG	UNP O35431

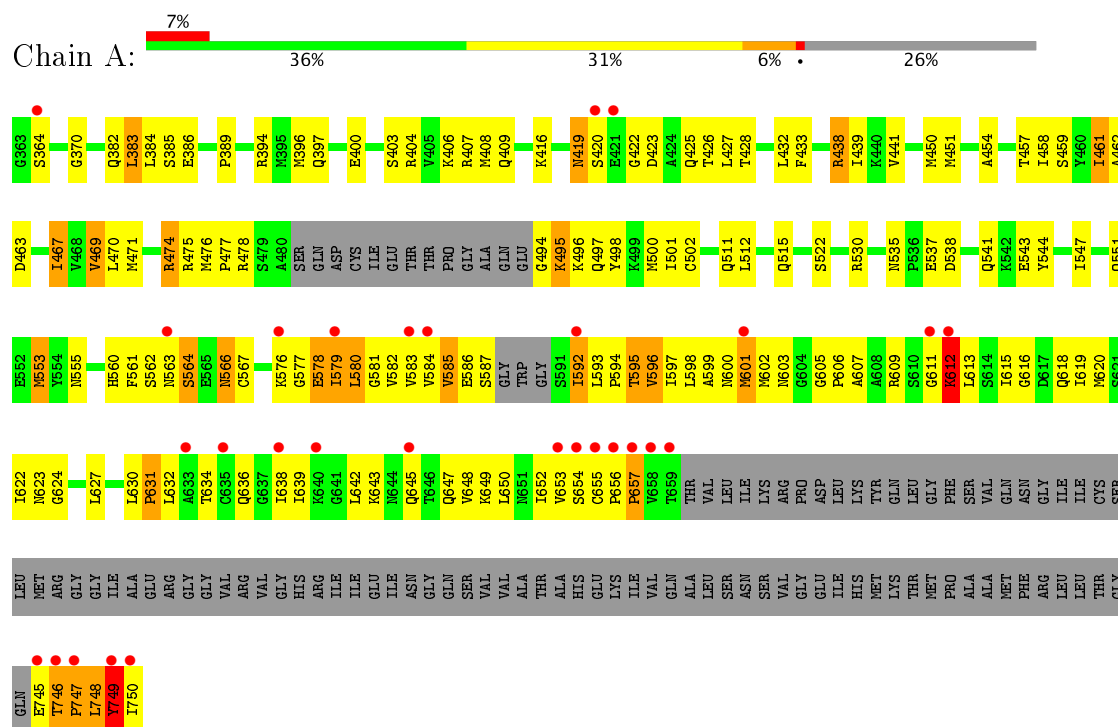
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	51	Total	O	0	0
			51	51		

### 3 Residue-property plots

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: Amyloid beta A4 precursor protein-binding family A member 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.66 Å   111.66 Å   84.59 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	31.83 – 2.70 31.83 – 2.69	Depositor EDS
% Data completeness (in resolution range)	91.4 (31.83-2.70) 94.6 (31.83-2.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 2.68 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.265 , 0.289 0.268 , 0.244	Depositor DCC
$R_{free}$ test set	811 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.5	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 68.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2185	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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 [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	0.38	0/2156	0.63	0/2908

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2134	0	2117	151	0
2	A	51	0	0	4	0
All	All	2185	0	2117	151	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 36.

All (151) 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:593:LEU:HB3	1:A:594:PRO:HD2	1.41	0.99
1:A:585:VAL:HG21	1:A:632:LEU:HD21	1.47	0.96
1:A:384:LEU:HB3	1:A:496:LYS:HB2	1.49	0.95
1:A:745:GLU:HG3	1:A:746:THR:HG22	1.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:ILE:HD11	1:A:643:LYS:HE2	1.50	0.93
1:A:535:ASN:HB3	1:A:537:GLU:OE2	1.71	0.89
1:A:394:ARG:HH11	1:A:397:GLN:HE22	1.15	0.88
1:A:583:VAL:HG12	1:A:600:ASN:H	1.44	0.82
1:A:461:ILE:HD13	1:A:462:ALA:N	1.95	0.82
1:A:580:LEU:HD12	1:A:580:LEU:H	1.47	0.79
1:A:602:MET:HA	1:A:602:MET:HE2	1.68	0.76
1:A:655:CYS:N	1:A:656:PRO:HD3	2.00	0.76
1:A:584:VAL:HG22	1:A:585:VAL:H	1.53	0.73
1:A:579:ILE:CD1	1:A:643:LYS:HE2	2.18	0.72
1:A:566:ASN:O	1:A:653:VAL:HA	1.90	0.71
1:A:593:LEU:HB3	1:A:594:PRO:CD	2.19	0.69
1:A:576:LYS:O	1:A:578:GLU:N	2.21	0.69
1:A:416:LYS:HE3	1:A:425:GLN:HA	1.75	0.68
1:A:599:ALA:HB3	1:A:616:GLY:H	1.57	0.68
1:A:582:VAL:HB	1:A:748:LEU:O	1.95	0.66
1:A:553:MET:HE3	1:A:553:MET:HA	1.78	0.66
1:A:584:VAL:HG22	1:A:585:VAL:N	2.11	0.65
1:A:594:PRO:HB3	2:A:34:HOH:O	1.97	0.64
1:A:561:PHE:C	1:A:563:ASN:H	2.00	0.64
1:A:622:ILE:HG12	1:A:650:LEU:CD2	2.27	0.64
1:A:580:LEU:N	1:A:580:LEU:HD12	2.12	0.63
1:A:605:GLY:O	1:A:609:ARG:HB2	1.97	0.63
1:A:578:GLU:HG2	1:A:579:ILE:N	2.14	0.61
1:A:403:SER:O	1:A:407:ARG:HG3	2.01	0.61
1:A:543:GLU:O	1:A:547:ILE:HG13	2.01	0.61
1:A:585:VAL:HG11	1:A:632:LEU:HD11	1.82	0.60
1:A:583:VAL:CG1	1:A:600:ASN:H	2.13	0.60
1:A:522:SER:HA	1:A:541:GLN:NE2	2.17	0.60
1:A:404:ARG:O	1:A:408:MET:HG3	2.02	0.60
1:A:522:SER:HA	1:A:541:GLN:HE21	1.66	0.59
1:A:612:LYS:HA	1:A:612:LYS:NZ	2.18	0.59
1:A:632:LEU:HD12	1:A:636:GLN:CD	2.23	0.59
1:A:579:ILE:HG21	1:A:750:ILE:HA	1.85	0.58
1:A:383:LEU:HG	1:A:500:MET:HB2	1.86	0.58
1:A:409:GLN:HE22	1:A:426:THR:CB	2.17	0.58
1:A:634:THR:O	1:A:638:ILE:HG13	2.04	0.58
1:A:432:LEU:HD12	1:A:441:VAL:HG22	1.87	0.57
1:A:459:SER:HB3	2:A:50:HOH:O	2.04	0.57
1:A:476:MET:CE	1:A:624:GLY:HA2	2.34	0.57
1:A:636:GLN:O	1:A:639:ILE:HG12	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:PRO:O	1:A:632:LEU:HD22	2.05	0.56
1:A:475:ARG:HG3	1:A:475:ARG:HH11	1.71	0.56
1:A:579:ILE:HG22	1:A:750:ILE:O	2.06	0.56
1:A:553:MET:CE	1:A:553:MET:HA	2.36	0.56
1:A:613:LEU:HB2	2:A:29:HOH:O	2.06	0.55
1:A:454:ALA:HB3	1:A:457:THR:HG23	1.88	0.55
1:A:579:ILE:CG2	1:A:750:ILE:O	2.54	0.55
1:A:600:ASN:HA	1:A:615:ILE:HG23	1.89	0.55
1:A:385:SER:N	1:A:496:LYS:HB3	2.23	0.54
1:A:585:VAL:CG1	1:A:632:LEU:HD11	2.37	0.54
1:A:578:GLU:HG2	1:A:579:ILE:H	1.73	0.54
1:A:469:VAL:HG12	1:A:502:CYS:SG	2.48	0.53
1:A:582:VAL:H	1:A:602:MET:HG3	1.73	0.53
1:A:578:GLU:O	1:A:579:ILE:HG12	2.08	0.53
1:A:585:VAL:HG21	1:A:632:LEU:CD2	2.32	0.53
1:A:582:VAL:N	1:A:602:MET:HG3	2.24	0.53
1:A:583:VAL:HB	1:A:598:LEU:O	2.08	0.53
1:A:394:ARG:HD3	1:A:397:GLN:NE2	2.25	0.52
1:A:416:LYS:CE	1:A:425:GLN:HA	2.38	0.52
1:A:537:GLU:H	1:A:537:GLU:CD	2.13	0.52
1:A:475:ARG:NH1	1:A:475:ARG:HG3	2.25	0.52
1:A:579:ILE:CD1	1:A:643:LYS:HG2	2.39	0.52
1:A:562:SER:C	1:A:564:SER:H	2.13	0.52
1:A:406:LYS:HE3	1:A:467:ILE:CD1	2.41	0.51
1:A:594:PRO:O	1:A:596:VAL:N	2.44	0.51
1:A:427:LEU:C	1:A:427:LEU:HD12	2.30	0.51
1:A:578:GLU:C	1:A:579:ILE:HG12	2.30	0.51
1:A:631:PRO:C	1:A:632:LEU:HD22	2.31	0.51
1:A:585:VAL:HG11	1:A:632:LEU:CD1	2.41	0.50
1:A:654:SER:C	1:A:656:PRO:HD3	2.32	0.50
1:A:450:MET:O	1:A:451:MET:HG3	2.11	0.50
1:A:476:MET:HE1	2:A:36:HOH:O	2.11	0.49
1:A:561:PHE:C	1:A:563:ASN:N	2.65	0.49
1:A:748:LEU:HD12	1:A:748:LEU:N	2.27	0.49
1:A:439:ILE:HD12	1:A:458:ILE:CD1	2.43	0.49
1:A:602:MET:HE1	1:A:747:PRO:HG2	1.94	0.49
1:A:601:MET:O	1:A:602:MET:HB2	2.13	0.49
1:A:579:ILE:HD11	1:A:643:LYS:CE	2.34	0.48
1:A:386:GLU:CG	1:A:389:PRO:HB3	2.44	0.48
1:A:593:LEU:O	1:A:595:THR:N	2.45	0.48
1:A:579:ILE:HD12	1:A:750:ILE:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:HE3	1:A:467:ILE:HD12	1.96	0.48
1:A:587:SER:HA	1:A:598:LEU:HD21	1.96	0.47
1:A:581:GLY:HA2	1:A:749:TYR:HD1	1.80	0.46
1:A:642:LEU:HA	1:A:645:GLN:HG2	1.96	0.46
1:A:649:LYS:O	1:A:650:LEU:HD23	2.16	0.46
1:A:494:GLY:O	1:A:495:LYS:CB	2.64	0.46
1:A:622:ILE:HG12	1:A:650:LEU:HD22	1.98	0.46
1:A:396:MET:O	1:A:400:GLU:HG3	2.17	0.45
1:A:409:GLN:HE22	1:A:426:THR:HB	1.79	0.45
1:A:476:MET:HE2	1:A:624:GLY:HA2	1.97	0.45
1:A:477:PRO:HB2	1:A:567:CYS:SG	2.56	0.45
1:A:511:GLN:O	1:A:515:GLN:HG3	2.17	0.45
1:A:463:ASP:HA	1:A:467:ILE:O	2.17	0.45
1:A:592:ILE:HG23	1:A:592:ILE:O	2.17	0.45
1:A:581:GLY:HA3	1:A:602:MET:CB	2.47	0.45
1:A:439:ILE:HD12	1:A:458:ILE:HD13	1.99	0.44
1:A:384:LEU:CB	1:A:496:LYS:HB2	2.34	0.44
1:A:585:VAL:HG21	1:A:632:LEU:HD11	1.99	0.44
1:A:623:ASN:ND2	1:A:648:VAL:HG13	2.32	0.44
1:A:382:GLN:HB2	1:A:474:ARG:HH12	1.82	0.44
1:A:553:MET:CE	1:A:553:MET:CA	2.96	0.43
1:A:592:ILE:O	1:A:593:LEU:HG	2.18	0.43
1:A:579:ILE:O	1:A:606:PRO:HD2	2.18	0.43
1:A:611:GLY:O	1:A:613:LEU:N	2.51	0.43
1:A:652:ILE:HG22	1:A:654:SER:H	1.82	0.43
1:A:461:ILE:HG12	1:A:470:LEU:HD23	2.00	0.43
1:A:655:CYS:N	1:A:656:PRO:CD	2.78	0.43
1:A:450:MET:C	1:A:451:MET:HG3	2.39	0.43
1:A:612:LYS:HZ3	1:A:612:LYS:HA	1.81	0.43
1:A:501:ILE:O	1:A:501:ILE:HG23	2.18	0.43
1:A:612:LYS:CE	1:A:612:LYS:HA	2.48	0.43
1:A:476:MET:HE1	1:A:624:GLY:HA2	1.98	0.43
1:A:584:VAL:CG2	1:A:585:VAL:N	2.81	0.43
1:A:551:GLN:O	1:A:555:ASN:ND2	2.52	0.42
1:A:598:LEU:HD22	1:A:598:LEU:N	2.34	0.42
1:A:580:LEU:CD1	1:A:580:LEU:H	2.23	0.42
1:A:584:VAL:CG2	1:A:585:VAL:H	2.27	0.42
1:A:583:VAL:HG11	1:A:599:ALA:HA	2.01	0.42
1:A:478:ARG:HB3	1:A:560:HIS:CE1	2.54	0.42
1:A:579:ILE:HD11	1:A:643:LYS:HG2	2.02	0.42
1:A:597:ILE:O	1:A:618:GLN:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:GLY:O	1:A:613:LEU:HD23	2.20	0.42
1:A:627:LEU:HA	1:A:630:LEU:HD12	2.02	0.42
1:A:541:GLN:O	1:A:544:TYR:HB3	2.20	0.41
1:A:603:ASN:O	1:A:605:GLY:N	2.52	0.41
1:A:370:GLY:HA3	1:A:433:PHE:CE1	2.55	0.41
1:A:620:MET:O	1:A:627:LEU:N	2.52	0.41
1:A:409:GLN:NE2	1:A:426:THR:OG1	2.53	0.41
1:A:438:ARG:HB3	1:A:438:ARG:NH2	2.34	0.41
1:A:622:ILE:HA	1:A:650:LEU:HD23	2.02	0.41
1:A:585:VAL:HG12	1:A:597:ILE:CB	2.50	0.41
1:A:585:VAL:CG2	1:A:632:LEU:HD11	2.51	0.41
1:A:619:ILE:HA	1:A:652:ILE:HD13	2.03	0.41
1:A:748:LEU:O	1:A:749:TYR:O	2.39	0.41
1:A:385:SER:O	1:A:498:TYR:HB2	2.20	0.41
1:A:382:GLN:HB2	1:A:474:ARG:NH1	2.36	0.41
1:A:419:ASN:ND2	1:A:422:GLY:O	2.53	0.41
1:A:581:GLY:HA3	1:A:602:MET:HB3	2.03	0.40
1:A:530:ARG:HG2	1:A:530:ARG:HH11	1.84	0.40
1:A:656:PRO:CB	1:A:657:PRO:HA	2.50	0.40
1:A:419:ASN:HD21	1:A:423:ASP:HB2	1.86	0.40
1:A:394:ARG:HH11	1:A:397:GLN:NE2	1.97	0.40
1:A:471:MET:HE3	1:A:471:MET:HB3	1.97	0.40
1:A:562:SER:C	1:A:564:SER:N	2.75	0.40
1:A:652:ILE:HG22	1:A:654:SER:N	2.37	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	279/388 (72%)	221 (79%)	38 (14%)	20 (7%)	<b>1</b> <b>1</b>

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	564	SER
1	A	566	ASN
1	A	595	THR
1	A	607	ALA
1	A	747	PRO
1	A	749	TYR
1	A	364	SER
1	A	420	SER
1	A	495	LYS
1	A	577	GLY
1	A	612	LYS
1	A	631	PRO
1	A	586	GLU
1	A	592	ILE
1	A	647	GLN
1	A	578	GLU
1	A	596	VAL
1	A	746	THR
1	A	601	MET
1	A	585	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	222/328 (68%)	204 (92%)	18 (8%)	14	31

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	383	LEU
1	A	419	ASN
1	A	428	THR
1	A	438	ARG
1	A	461	ILE

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Mol	Chain	Res	Type
1	A	467	ILE
1	A	469	VAL
1	A	474	ARG
1	A	497	GLN
1	A	512	LEU
1	A	538	ASP
1	A	553	MET
1	A	579	ILE
1	A	580	LEU
1	A	612	LYS
1	A	657	PRO
1	A	748	LEU
1	A	749	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	GLN
1	A	409	GLN
1	A	419	ASN
1	A	453	HIS
1	A	497	GLN
1	A	511	GLN
1	A	515	GLN
1	A	541	GLN
1	A	571	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

There are no ligands in this entry.

## 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	287/388 (73%)	0.48	29 (10%) 8 6	40, 70, 140, 148	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	750	ILE	7.7
1	A	655	CYS	4.8
1	A	612	LYS	4.5
1	A	745	GLU	4.3
1	A	421	GLU	4.2
1	A	658	VAL	3.9
1	A	657	PRO	3.7
1	A	633	ALA	3.6
1	A	746	THR	3.6
1	A	592	ILE	3.4
1	A	584	VAL	3.1
1	A	747	PRO	3.1
1	A	640	LYS	3.1
1	A	749	TYR	2.9
1	A	420	SER	2.8
1	A	611	GLY	2.7
1	A	653	VAL	2.6
1	A	656	PRO	2.5
1	A	654	SER	2.5
1	A	576	LYS	2.4
1	A	583	VAL	2.4
1	A	645	GLN	2.3
1	A	579	ILE	2.3
1	A	638	ILE	2.3
1	A	635	CYS	2.2
1	A	601	MET	2.2
1	A	364	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	659	THR	2.2
1	A	563	ASN	2.1

## 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.