



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:20 PM UTC

PDB ID : 3SUZ / pdb_00003suz
Title : Crystal structure of Rat Mint2 PPC
Authors : Shen, Y.; Long, J.; Yan, X.; Xie, X.
Deposited on : 2011-07-11
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

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
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

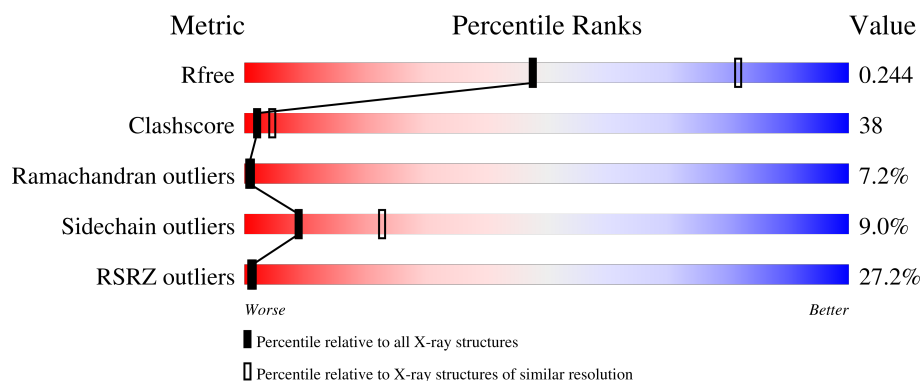
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	388	20% 35% 31% 7% 26%

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

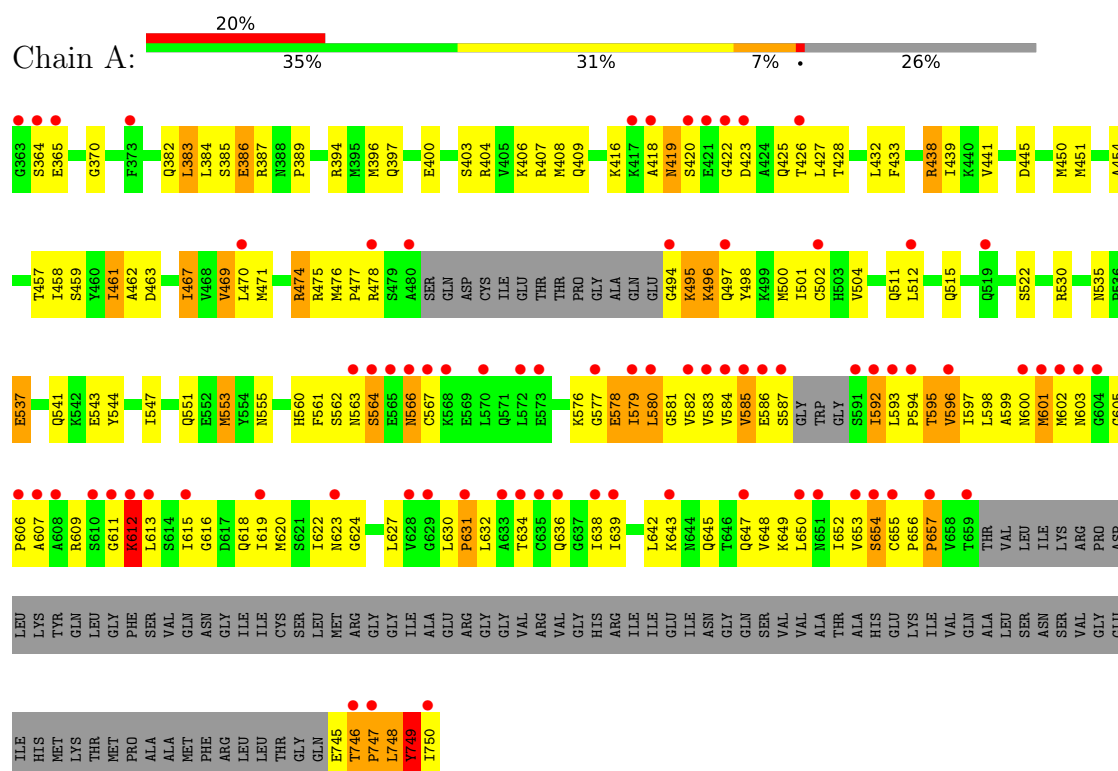
- Molecule 2 is water.

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

3 Residue-property plots [i](#)

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: 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, α , β , γ	111.66Å 111.66Å 84.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.83 – 2.70 31.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.4 (31.83-2.70) 94.8 (31.83-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.68Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.265 , 0.289 0.268 , 0.244	Depositor DCC
R_{free} test set	817 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	57.5	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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	0.47	0/2156	0.96	6/2908 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	ALA	N-CA-C	-8.15	97.81	109.96
1	A	387	ARG	N-CA-C	7.22	119.77	111.11
1	A	654	SER	CB-CA-C	-5.67	109.52	117.23
1	A	445	ASP	N-CA-C	5.50	118.11	111.40
1	A	504	VAL	N-CA-C	5.20	115.34	107.80
1	A	496	LYS	N-CA-C	-5.15	100.77	108.96

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	160	0
2	A	51	0	0	3	0
All	All	2185	0	2117	160	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 38.

All (160) 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:476:MET:HE1	1:A:624:GLY:HA2	1.48	0.95
1:A:745:GLU:HG3	1:A:746:THR:HG22	1.45	0.94
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:H	1:A:580:LEU:HD12	1.47	0.79
1:A:602:MET:HA	1:A:602:MET:HE2	1.67	0.77
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:561:PHE:C	1:A:563:ASN:H	2.00	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: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:632:LEU:HD12	1:A:636:GLN:CD	2.23	0.64
1:A:622:ILE:HG12	1:A:650:LEU:CD2	2.27	0.64
1:A:580:LEU:HD12	1:A:580:LEU:N	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:LEU:HD12	1:A:441:VAL:HG22	1.87	0.57
1:A:394:ARG:CZ	1:A:500:MET:HE2	2.34	0.57
1:A:459:SER:HB3	2:A:50:HOH:O	2.04	0.57
1:A:636:GLN:O	1:A:639:ILE:HG12	2.03	0.57
1:A:537:GLU:H	1:A:537:GLU:CD	2.13	0.56
1:A:427:LEU:HD12	1:A:427:LEU:C	2.30	0.56
1:A:562:SER:C	1:A:564:SER:H	2.13	0.56
1:A:631:PRO:O	1:A:632:LEU:HD22	2.05	0.56
1:A:475:ARG:HH11	1:A:475:ARG:HG3	1.71	0.56
1:A:579:ILE:HG22	1:A:750:ILE:O	2.06	0.56
1:A:553:MET:HA	1:A:553:MET:CE	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:631:PRO:C	1:A:632:LEU:HD22	2.31	0.55
1:A:578:GLU:C	1:A:579:ILE:HG12	2.30	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:654:SER:C	1:A:656:PRO:HD3	2.32	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:561:PHE:C	1:A:563:ASN:N	2.65	0.53
1:A:397:GLN:NE2	1:A:471:MET:HE1	2.24	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:475:ARG:HG3	1:A:475:ARG:NH1	2.25	0.52
1:A:579:ILE:CD1	1:A:643:LYS:HG2	2.39	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:585:VAL:HG11	1:A:632:LEU:CD1	2.41	0.50
1:A:450:MET:O	1:A:451:MET:HG3	2.11	0.50
1:A:748:LEU:N	1:A:748:LEU:HD12	2.27	0.49
1:A:439:ILE:HD12	1:A:458:ILE:CD1	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:450:MET:C	1:A:451:MET:HG3	2.39	0.48
1:A:406:LYS:HE3	1:A:467:ILE:HD12	1.96	0.48
1:A:602:MET:HE1	1:A:747:PRO:HG2	1.96	0.47
1:A:587:SER:HA	1:A:598:LEU:HD21	1.96	0.47
1:A:576:LYS:C	1:A:578:GLU:H	2.19	0.46
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:386:GLU:H	1:A:386:GLU:CD	2.16	0.45
1:A:553:MET:O	1:A:553:MET:HE2	2.16	0.45
1:A:477:PRO:HB2	1:A:567:CYS:SG	2.56	0.45
1:A:553:MET:HA	1:A:553:MET:HE3	1.99	0.45
1:A:511:GLN:O	1:A:515:GLN:HG3	2.17	0.45
1:A:562:SER:C	1:A:564:SER:N	2.75	0.45
1:A:463:ASP:HA	1:A:467:ILE:O	2.17	0.45
1:A:581:GLY:HA3	1:A:602:MET:CB	2.47	0.45
1:A:592:ILE:O	1:A:592:ILE:HG23	2.17	0.45
1:A:384:LEU:CB	1:A:496:LYS:HB2	2.34	0.44
1:A:439:ILE:HD12	1:A:458:ILE:HD13	1.99	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:476:MET:CE	1:A:624:GLY:HA2	2.34	0.44
1:A:611:GLY:C	1:A:613:LEU:H	2.26	0.43
1:A:553:MET:CE	1:A:553:MET:CA	2.96	0.43
1:A:579:ILE:O	1:A:606:PRO:HD2	2.18	0.43
1:A:592:ILE:O	1:A:593:LEU:HG	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:612:LYS:HA	1:A:612:LYS:HZ3	1.81	0.43
1:A:501:ILE:O	1:A:501:ILE:HG23	2.18	0.43
1:A:612:LYS:HA	1:A:612:LYS:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:580:LEU:CD1	2.23	0.42
1:A:583:VAL:HG11	1:A:599:ALA:HA	2.01	0.42
1:A:584:VAL:CG2	1:A:585:VAL:H	2.27	0.42
1:A:461:ILE:HD13	1:A:461:ILE:C	2.44	0.42
1:A:478:ARG:HB3	1:A:560:HIS:CE1	2.54	0.42
1:A:576:LYS:C	1:A:578:GLU:N	2.77	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
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:553:MET:HE2	1:A:553:MET:CA	2.51	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:612:LYS:C	1:A:613:LEU:HD22	2.45	0.41
1:A:385:SER:O	1:A:498:TYR:HB2	2.20	0.41
1:A:611:GLY:C	1:A:613:LEU:N	2.78	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: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:397:GLN:HE21	1:A:471:MET:HE1	1.84	0.40
1:A:530:ARG:HH11	1:A:530:ARG:HG2	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: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%)	1 1

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 [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	222/328 (68%)	202 (91%)	20 (9%)	9 23

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	365	GLU
1	A	383	LEU
1	A	386	GLU
1	A	419	ASN
1	A	428	THR
1	A	438	ARG
1	A	461	ILE
1	A	467	ILE
1	A	469	VAL
1	A	474	ARG
1	A	497	GLN
1	A	512	LEU
1	A	537	GLU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	397	GLN
1	A	399	GLN
1	A	409	GLN
1	A	419	ASN
1	A	447	GLN
1	A	453	HIS
1	A	497	GLN
1	A	511	GLN
1	A	515	GLN
1	A	541	GLN

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Mol	Chain	Res	Type
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 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 [i](#)

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, 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	287/388 (73%)	1.34	78 (27%) ⓘ ⓘ	40, 70, 140, 148	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	750	ILE	7.0
1	A	583	VAL	5.1
1	A	573	GLU	4.7
1	A	634	THR	4.3
1	A	635	CYS	4.2
1	A	363	GLY	3.9
1	A	567	CYS	3.9
1	A	364	SER	3.6
1	A	421	GLU	3.6
1	A	647	GLN	3.5
1	A	610	SER	3.5
1	A	426	THR	3.5
1	A	611	GLY	3.4
1	A	420	SER	3.4
1	A	612	LYS	3.4
1	A	633	ALA	3.4
1	A	603	ASN	3.4
1	A	572	LEU	3.3
1	A	747	PRO	3.3
1	A	579	ILE	3.3
1	A	619	ILE	3.3
1	A	657	PRO	3.2
1	A	601	MET	3.2
1	A	584	VAL	3.2
1	A	653	VAL	3.2
1	A	593	LEU	3.2
1	A	639	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	655	CYS	3.1
1	A	564	SER	3.1
1	A	651	ASN	3.1
1	A	568	LYS	3.1
1	A	563	ASN	3.0
1	A	659	THR	3.0
1	A	566	ASN	2.9
1	A	602	MET	2.9
1	A	623	ASN	2.9
1	A	592	ILE	2.9
1	A	423	ASP	2.8
1	A	494	GLY	2.8
1	A	580	LEU	2.8
1	A	628	VAL	2.8
1	A	636	GLN	2.7
1	A	570	LEU	2.7
1	A	587	SER	2.7
1	A	600	ASN	2.6
1	A	373	PHE	2.6
1	A	480	ALA	2.6
1	A	594	PRO	2.6
1	A	606	PRO	2.6
1	A	608	ALA	2.6
1	A	470	LEU	2.5
1	A	650	LEU	2.5
1	A	502	CYS	2.5
1	A	746	THR	2.5
1	A	591	SER	2.5
1	A	512	LEU	2.5
1	A	596	VAL	2.5
1	A	638	ILE	2.3
1	A	613	LEU	2.3
1	A	565	GLU	2.3
1	A	577	GLY	2.3
1	A	654	SER	2.2
1	A	365	GLU	2.2
1	A	418	ALA	2.2
1	A	604	GLY	2.2
1	A	629	GLY	2.2
1	A	497	GLN	2.2
1	A	417	LYS	2.2
1	A	582	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	422	GLY	2.1
1	A	643	LYS	2.1
1	A	615	ILE	2.1
1	A	478	ARG	2.1
1	A	631	PRO	2.1
1	A	607	ALA	2.1
1	A	519	GLN	2.1
1	A	585	VAL	2.0
1	A	586	GLU	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 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.