



# Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2026 – 08:07 PM EDT

PDB ID : 9YAT / pdb\_00009yat  
Title : Rana catesbeiana saxiphilin mutant - T563A  
Authors : Chen, Z.; Zakrzewska, S.; Minor, D.L.  
Deposited on : 2025-09-16  
Resolution : 2.50 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

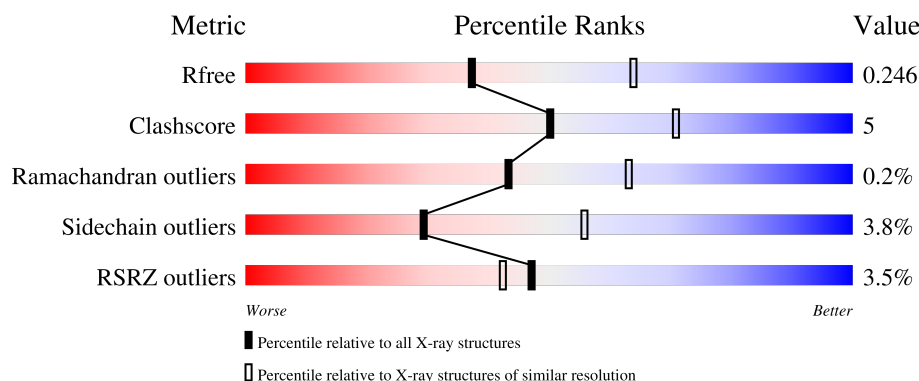
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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  $\geq 3$ , 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	853	 3% 84% 13% ..
1	B	853	 4% 80% 15% ..

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12922 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 Saxiphilin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	832	Total	C	N	O	S	0	0	0
			6413	4008	1110	1236	59			
1	B	822	Total	C	N	O	S	0	0	0
			6338	3959	1095	1225	59			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	563	ALA	THR	engineered mutation	UNP P31226
A	826	SER	-	expression tag	UNP P31226
A	827	ASN	-	expression tag	UNP P31226
A	828	SER	-	expression tag	UNP P31226
A	829	LEU	-	expression tag	UNP P31226
A	830	GLU	-	expression tag	UNP P31226
A	831	VAL	-	expression tag	UNP P31226
A	832	LEU	-	expression tag	UNP P31226
A	833	PHE	-	expression tag	UNP P31226
A	834	GLN	-	expression tag	UNP P31226
B	563	ALA	THR	engineered mutation	UNP P31226
B	826	SER	-	expression tag	UNP P31226
B	827	ASN	-	expression tag	UNP P31226
B	828	SER	-	expression tag	UNP P31226
B	829	LEU	-	expression tag	UNP P31226
B	830	GLU	-	expression tag	UNP P31226
B	831	VAL	-	expression tag	UNP P31226
B	832	LEU	-	expression tag	UNP P31226
B	833	PHE	-	expression tag	UNP P31226
B	834	GLN	-	expression tag	UNP P31226

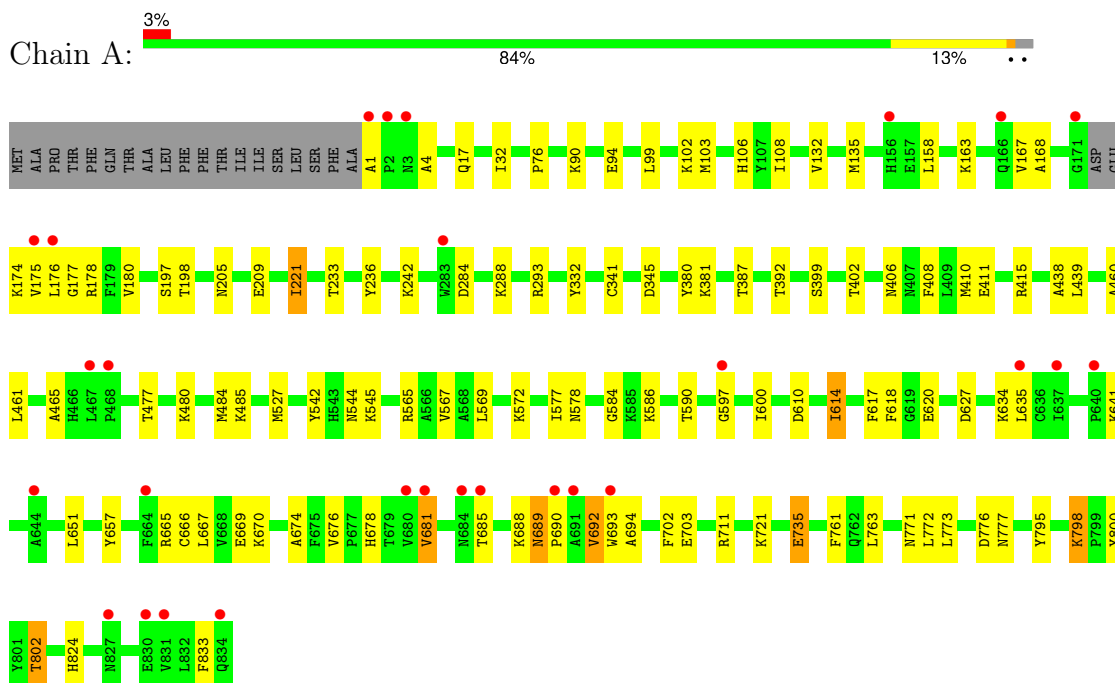
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	96	Total 96	O 96	0	0
2	B	75	Total 75	O 75	0	0

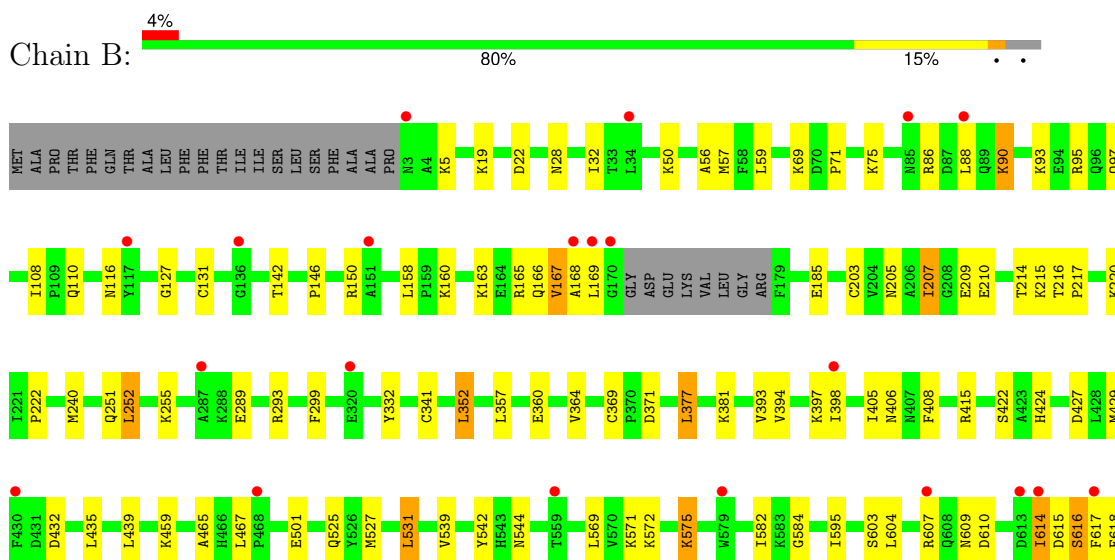
### 3 Residue-property plots [i](#)

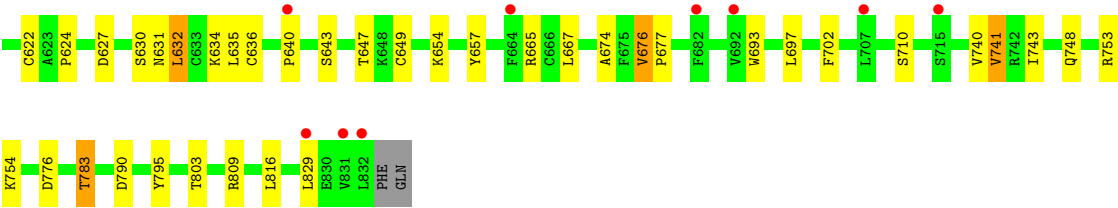
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Saxiphilin



- Molecule 1: Saxiphilin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.30Å 109.69Å 253.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.66 – 2.50 47.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.66-2.50) 99.0 (47.66-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.207 , 0.246 0.207 , 0.246	Depositor DCC
$R_{free}$ test set	4727 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.3	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 55.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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

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	0.12	0/6541	0.32	0/8827
1	B	0.13	0/6464	0.32	0/8724
All	All	0.12	0/13005	0.32	0/17551

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

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	6413	0	6288	61	0
1	B	6338	0	6204	73	0
2	A	96	0	0	2	0
2	B	75	0	0	1	0
All	All	12922	0	12492	134	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 5.

All (134) 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:B:647:THR:HB	1:B:654:LYS:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:GLN:HG3	1:B:595:ILE:HD11	1.68	0.75
1:B:205:ASN:HD21	1:B:207:ILE:HG22	1.52	0.73
1:A:1:ALA:HB3	1:A:4:ALA:HB2	1.70	0.73
1:B:216:THR:HG21	1:B:222:PRO:HA	1.75	0.69
1:A:411:GLU:OE1	1:A:415:ARG:NH1	2.26	0.68
1:A:410:MET:HE1	1:A:438:ALA:HA	1.74	0.67
1:A:590:THR:HG22	1:A:597:GLY:HA3	1.78	0.65
1:A:284:ASP:HB3	1:A:288:LYS:HD2	1.80	0.63
1:A:569:LEU:HD11	1:A:702:PHE:HB3	1.80	0.63
1:A:692:VAL:HG22	1:A:693:TRP:H	1.65	0.62
1:B:754:LYS:NZ	2:B:901:HOH:O	2.19	0.62
1:A:94:GLU:OE1	2:A:901:HOH:O	2.16	0.62
1:B:676:VAL:HG22	1:B:677:PRO:HD2	1.80	0.62
1:A:565:ARG:HB2	1:A:678:HIS:HD2	1.65	0.61
1:B:631:ASN:HA	1:B:634:LYS:HD2	1.83	0.60
1:B:108:ILE:O	1:B:110:GLN:NE2	2.35	0.60
1:B:127:GLY:HA3	1:B:146:PRO:HG3	1.83	0.59
1:A:798:LYS:O	1:A:802:THR:OG1	2.19	0.58
1:B:584:GLY:N	1:B:617:PHE:O	2.30	0.58
1:B:32:ILE:HG21	1:B:408:PHE:HB2	1.85	0.58
1:B:614:ILE:HA	1:B:632:LEU:HD11	1.86	0.58
1:A:635:LEU:HD22	1:A:670:LYS:HD3	1.86	0.57
1:A:569:LEU:HD22	1:A:681:VAL:HG22	1.86	0.56
1:B:240:MET:HE2	1:B:352:LEU:HD11	1.88	0.55
1:A:689:ASN:HB2	1:A:694:ALA:O	2.06	0.55
1:A:565:ARG:H	1:A:678:HIS:CD2	2.24	0.55
1:B:398:ILE:H	1:B:398:ILE:HD12	1.71	0.55
1:B:657:TYR:HE1	1:B:665:ARG:HG2	1.72	0.55
1:A:242:LYS:NZ	1:A:345:ASP:OD1	2.28	0.54
1:A:477:THR:HG22	1:A:773:LEU:HD21	1.88	0.54
1:B:160:LYS:HA	1:B:163:LYS:HD2	1.89	0.54
1:B:252:LEU:HD12	1:B:299:PHE:HE1	1.72	0.53
1:A:657:TYR:OH	1:A:669:GLU:OE1	2.25	0.53
1:A:667:LEU:HB2	1:A:674:ALA:HB2	1.90	0.53
1:B:582:ILE:HG22	1:B:618:PHE:HE1	1.73	0.53
1:B:28:ASN:O	1:B:415:ARG:NH1	2.42	0.52
1:A:735:GLU:H	1:A:735:GLU:CD	2.18	0.51
1:B:56:ALA:HB2	1:B:405:ILE:HD13	1.94	0.51
1:A:406:ASN:OD1	1:A:439:LEU:HB2	2.12	0.50
1:A:577:ILE:HG22	1:A:711:ARG:HH12	1.76	0.50
1:B:205:ASN:ND2	1:B:209:GLU:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PRO:HB3	1:A:392:THR:HG21	1.94	0.50
1:B:166:GLN:C	1:B:168:ALA:H	2.20	0.50
1:B:127:GLY:O	1:B:150:ARG:NH2	2.45	0.50
1:B:604:LEU:HD23	1:B:607:ARG:HH21	1.76	0.49
1:A:665:ARG:HB2	1:A:693:TRP:CZ2	2.47	0.49
1:A:168:ALA:O	1:A:178:ARG:NH2	2.45	0.49
1:B:357:LEU:HG	1:B:377:LEU:HG	1.94	0.49
1:A:32:ILE:HG21	1:A:408:PHE:HB2	1.94	0.49
1:A:163:LYS:O	1:A:167:VAL:HG13	2.13	0.49
1:B:667:LEU:HB2	1:B:674:ALA:HB2	1.94	0.49
1:A:135:MET:HG2	1:A:833:PHE:HE2	1.78	0.49
1:B:165:ARG:O	1:B:167:VAL:N	2.43	0.49
1:B:790:ASP:CG	1:B:809:ARG:HH12	2.21	0.49
1:B:90:LYS:HA	1:B:93:LYS:HE2	1.94	0.48
1:B:381:LYS:HD2	1:B:829:LEU:HD11	1.94	0.48
1:A:627:ASP:OD1	1:A:627:ASP:N	2.41	0.48
1:B:406:ASN:OD1	1:B:439:LEU:HB2	2.13	0.48
1:B:251:GLN:O	1:B:255:LYS:NZ	2.45	0.48
1:B:369:CYS:HB2	1:B:371:ASP:OD1	2.13	0.48
1:B:624:PRO:HA	1:B:649:CYS:HA	1.96	0.47
1:B:59:LEU:HD12	1:B:394:VAL:HG11	1.96	0.47
1:A:399:SER:HB2	1:A:402:THR:OG1	2.14	0.47
1:A:175:VAL:HG23	1:A:177:GLY:H	1.78	0.47
1:B:332:TYR:CG	1:B:341:CYS:HB2	2.50	0.47
1:B:627:ASP:HB3	1:B:630:SER:HB2	1.96	0.47
1:B:539:VAL:HG12	1:B:783:THR:HA	1.97	0.47
1:B:542:TYR:CZ	1:B:544:ASN:HB3	2.49	0.47
1:A:236:TYR:CE2	1:A:387:THR:HG22	2.50	0.46
1:B:69:LYS:HB3	1:B:69:LYS:HE2	1.80	0.46
1:A:614:ILE:H	1:A:614:ILE:HG13	1.60	0.46
1:B:289:GLU:HG3	1:B:293:ARG:HD3	1.98	0.46
1:A:567:VAL:HG12	1:A:721:LYS:HA	1.97	0.45
1:A:545:LYS:HE2	1:A:777:ASN:HB2	1.99	0.45
1:B:50:LYS:HE2	1:B:71:PRO:O	2.17	0.45
1:B:95:ARG:HG3	1:B:108:ILE:HG22	1.99	0.45
1:A:620:GLU:HB3	1:A:635:LEU:HG	1.99	0.45
1:B:693:TRP:CD1	1:B:693:TRP:H	2.35	0.45
1:B:210:GLU:OE1	1:B:215:LYS:HE3	2.17	0.44
1:B:569:LEU:HD11	1:B:702:PHE:HB3	1.98	0.44
1:B:753:ARG:NH2	1:B:776:ASP:O	2.50	0.44
1:B:676:VAL:HG13	1:B:677:PRO:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ASN:HD21	1:A:209:GLU:HB2	1.82	0.44
1:B:97:GLN:NE2	1:B:435:LEU:HD13	2.33	0.44
1:B:603:SER:OG	1:B:803:THR:O	2.33	0.44
1:A:617:PHE:HD2	1:A:618:PHE:CD1	2.35	0.44
1:B:429:MET:HE2	1:B:429:MET:HB3	1.92	0.43
1:A:380:TYR:CZ	1:A:381:LYS:HE2	2.53	0.43
1:A:485:LYS:HD3	1:A:772:LEU:HB2	2.00	0.43
1:A:221:ILE:H	1:A:221:ILE:HG13	1.52	0.43
1:B:203:CYS:HB2	1:B:214:THR:HG21	2.00	0.43
1:A:685:THR:HA	1:A:689:ASN:HB3	2.00	0.43
1:A:460:ALA:HA	1:A:465:ALA:HB2	2.01	0.43
1:A:586:LYS:HE3	1:A:635:LEU:HD11	2.01	0.43
1:B:75:LYS:HG2	1:B:397:LYS:HA	2.01	0.43
1:A:99:LEU:HD23	1:A:108:ILE:HD13	2.01	0.43
1:A:480:LYS:O	1:A:484:MET:HG3	2.19	0.43
1:A:332:TYR:CG	1:A:341:CYS:HB2	2.54	0.43
1:B:657:TYR:CE1	1:B:665:ARG:HG2	2.53	0.42
1:B:609:ASN:HB3	1:B:617:PHE:CZ	2.53	0.42
1:A:90:LYS:NZ	2:A:905:HOH:O	2.40	0.42
1:A:205:ASN:ND2	1:A:209:GLU:HB2	2.35	0.42
1:B:640:PRO:HA	1:B:643:SER:HB3	2.02	0.42
1:B:636:CYS:HA	1:B:657:TYR:HD2	1.85	0.42
1:A:175:VAL:HB	1:A:178:ARG:HD3	2.02	0.42
1:A:771:ASN:H	1:A:776:ASP:CG	2.27	0.42
1:B:697:LEU:HD23	1:B:697:LEU:HA	1.84	0.42
1:A:103:MET:HE3	1:A:106:HIS:CG	2.54	0.42
1:A:542:TYR:CZ	1:A:544:ASN:HB3	2.54	0.42
1:B:531:LEU:HD13	1:B:531:LEU:HA	1.91	0.42
1:A:572:LYS:HG2	1:A:703:GLU:CD	2.45	0.42
1:B:217:PRO:HD2	1:B:220:LYS:HD3	2.01	0.42
1:B:527:MET:HE3	1:B:531:LEU:HD21	2.01	0.42
1:B:467:LEU:HD12	1:B:467:LEU:H	1.85	0.42
1:B:527:MET:HG3	1:B:795:TYR:CZ	2.55	0.41
1:A:584:GLY:N	1:A:617:PHE:O	2.50	0.41
1:A:657:TYR:CG	1:A:666:CYS:HB2	2.55	0.41
1:B:22:ASP:OD2	1:B:424:HIS:NE2	2.52	0.41
1:B:575:LYS:HE2	1:B:575:LYS:HB3	1.86	0.41
1:A:197:SER:OG	1:A:198:THR:N	2.51	0.41
1:B:427:ASP:H	1:B:432:ASP:CG	2.28	0.41
1:B:622:CYS:HB2	1:B:635:LEU:HB2	2.03	0.41
1:A:527:MET:HG3	1:A:795:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:LYS:H	1:B:654:LYS:HD2	1.84	0.41
1:B:740:VAL:O	1:B:741:VAL:C	2.63	0.41
1:A:600:ILE:HD11	1:A:800:TYR:CE2	2.56	0.40
1:A:761:PHE:HE2	1:A:763:LEU:HD23	1.86	0.40
1:B:459:LYS:HE2	1:B:465:ALA:HA	2.03	0.40
1:B:57:MET:O	1:B:393:VAL:HA	2.20	0.40
1:A:651:LEU:HD23	1:A:651:LEU:HA	1.89	0.40
1:B:19:LYS:HE3	1:B:422:SER:HB2	2.02	0.40
1:A:690:PRO:HB2	1:A:692:VAL:HG12	2.03	0.40
1:B:131:CYS:H	1:B:142:THR:HB	1.87	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	828/853 (97%)	797 (96%)	30 (4%)	1 (0%)	48	68
1	B	818/853 (96%)	782 (96%)	33 (4%)	3 (0%)	30	49
All	All	1646/1706 (96%)	1579 (96%)	63 (4%)	4 (0%)	43	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	167	VAL
1	B	616	SER
1	A	692	VAL
1	B	741	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	712/730 (98%)	688 (97%)	24 (3%)	32	60
1	B	705/730 (97%)	675 (96%)	30 (4%)	26	51
All	All	1417/1460 (97%)	1363 (96%)	54 (4%)	29	56

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	102	LYS
1	A	132	VAL
1	A	158	LEU
1	A	174	LYS
1	A	176	LEU
1	A	180	VAL
1	A	221	ILE
1	A	233	THR
1	A	293	ARG
1	A	461	LEU
1	A	578	ASN
1	A	610	ASP
1	A	614	ILE
1	A	634	LYS
1	A	641	LYS
1	A	676	VAL
1	A	681	VAL
1	A	688	LYS
1	A	689	ASN
1	A	735	GLU
1	A	798	LYS
1	A	802	THR
1	A	824	HIS
1	B	5	LYS
1	B	86	ARG
1	B	88	LEU

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Mol	Chain	Res	Type
1	B	90	LYS
1	B	116	ASN
1	B	158	LEU
1	B	169	LEU
1	B	185	GLU
1	B	207	ILE
1	B	252	LEU
1	B	352	LEU
1	B	360	GLU
1	B	364	VAL
1	B	377	LEU
1	B	501	GLU
1	B	531	LEU
1	B	571	LYS
1	B	572	LYS
1	B	575	LYS
1	B	610	ASP
1	B	614	ILE
1	B	615	ASP
1	B	616	SER
1	B	632	LEU
1	B	676	VAL
1	B	710	SER
1	B	743	ILE
1	B	748	GLN
1	B	783	THR
1	B	816	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	118	GLN
1	A	148	GLN
1	A	166	GLN
1	A	248	GLN
1	A	315	GLN
1	A	466	HIS
1	A	580	ASN
1	A	660	ASN
1	A	678	HIS
1	A	689	ASN

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Mol	Chain	Res	Type
1	B	28	ASN
1	B	73	ASN
1	B	166	GLN
1	B	228	HIS
1	B	248	GLN
1	B	315	GLN
1	B	326	ASN
1	B	580	ASN
1	B	824	HIS

### 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, 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	832/853 (97%)	0.18	28 (3%)	48 43	49, 84, 173, 238	0
1	B	822/853 (96%)	0.32	30 (3%)	46 41	55, 95, 163, 223	0
All	All	1654/1706 (96%)	0.25	58 (3%)	47 42	49, 90, 170, 238	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	GLY	5.4
1	A	1	ALA	4.8
1	A	664	PHE	4.8
1	B	829	LEU	4.5
1	B	88	LEU	4.4
1	B	831	VAL	4.3
1	A	834	GLN	4.0
1	B	832	LEU	3.8
1	B	169	LEU	3.7
1	A	2	PRO	3.4
1	B	85	ASN	3.4
1	B	613	ASP	3.3
1	A	176	LEU	3.3
1	A	171	GLY	3.2
1	B	468	PRO	3.2
1	A	468	PRO	3.1
1	A	691	ALA	3.0
1	A	693	TRP	2.9
1	B	664	PHE	2.9
1	A	681	VAL	2.7
1	B	398	ILE	2.7
1	B	614	ILE	2.7
1	A	635	LEU	2.7
1	B	617	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	644	ALA	2.6
1	A	831	VAL	2.5
1	A	684	ASN	2.5
1	B	151	ALA	2.5
1	A	685	THR	2.5
1	A	597	GLY	2.4
1	A	467	LEU	2.4
1	A	3	ASN	2.4
1	B	168	ALA	2.4
1	B	136	GLY	2.4
1	A	690	PRO	2.3
1	B	715	SER	2.3
1	B	34	LEU	2.3
1	B	3	ASN	2.3
1	B	579	TRP	2.3
1	A	156	HIS	2.3
1	B	692	VAL	2.3
1	B	287	ALA	2.3
1	B	607	ARG	2.3
1	A	827	ASN	2.2
1	B	640	PRO	2.2
1	B	117	TYR	2.2
1	A	637	ILE	2.2
1	A	283	TRP	2.2
1	B	682	PHE	2.2
1	A	166	GLN	2.1
1	A	830	GLU	2.1
1	B	320	GLU	2.1
1	A	640	PRO	2.1
1	A	680	VAL	2.0
1	B	559	THR	2.0
1	A	175	VAL	2.0
1	B	430	PHE	2.0
1	B	707	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.