



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2022 – 10:31 AM EDT

PDB ID : 8D6Q  
Title : Rana catesbeiana saxiphilin mutant - Y558I  
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Deposited on : 2022-06-06  
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

<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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

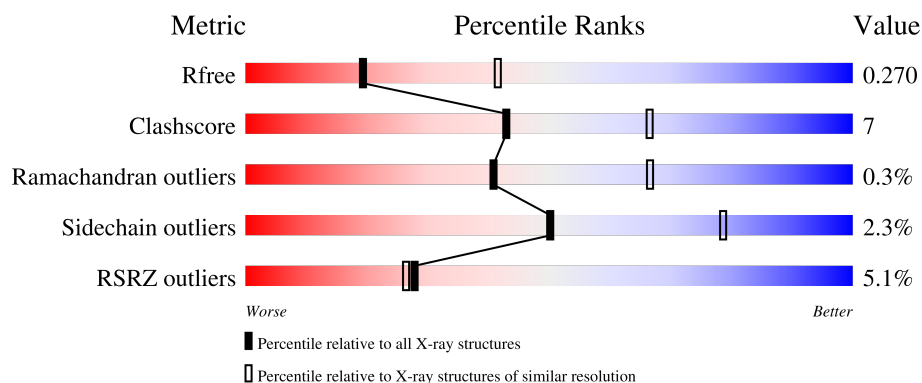
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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  $\geq 3$ , 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	851	 6% 82% 13% . .
1	B	851	 4% 76% 18% . .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12701 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	818	Total	C	N	O	S	0	0	0
			6311	3942	1090	1220	59			
1	B	818	Total	C	N	O	S	0	0	0
			6311	3942	1090	1220	59			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	558	ILE	TYR	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
B	558	ILE	TYR	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

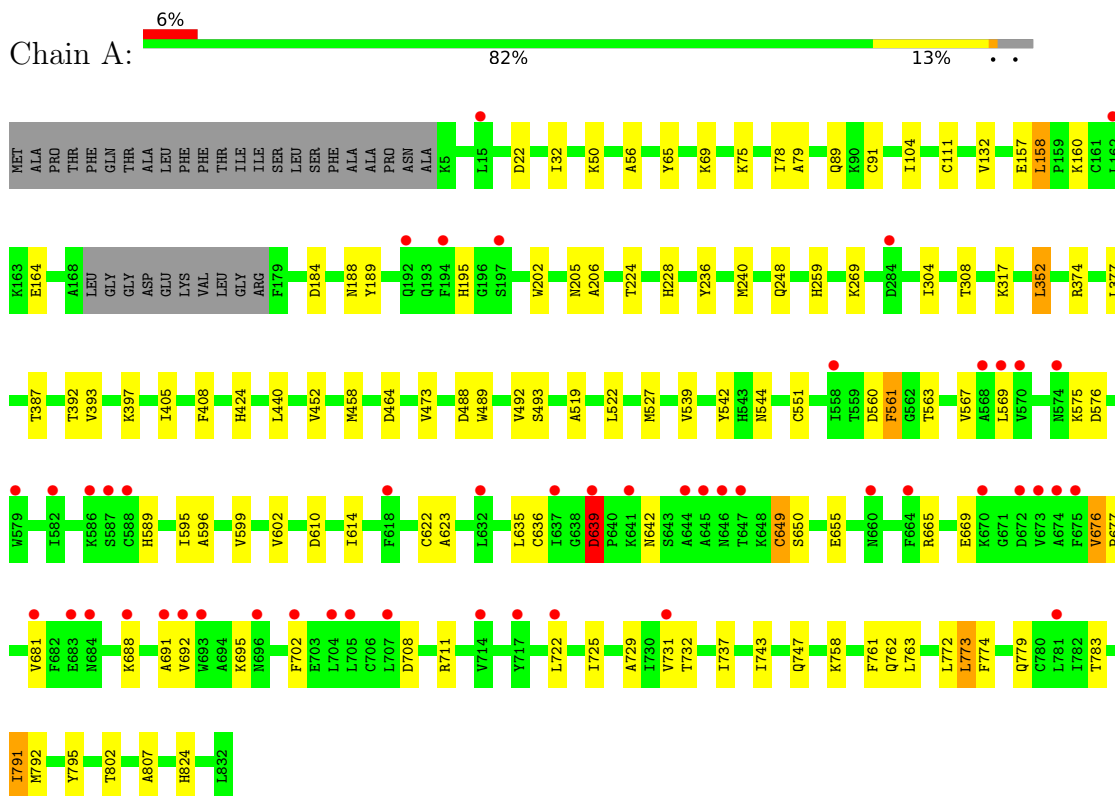
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		
2	B	39	Total	O	0	0
			39	39		

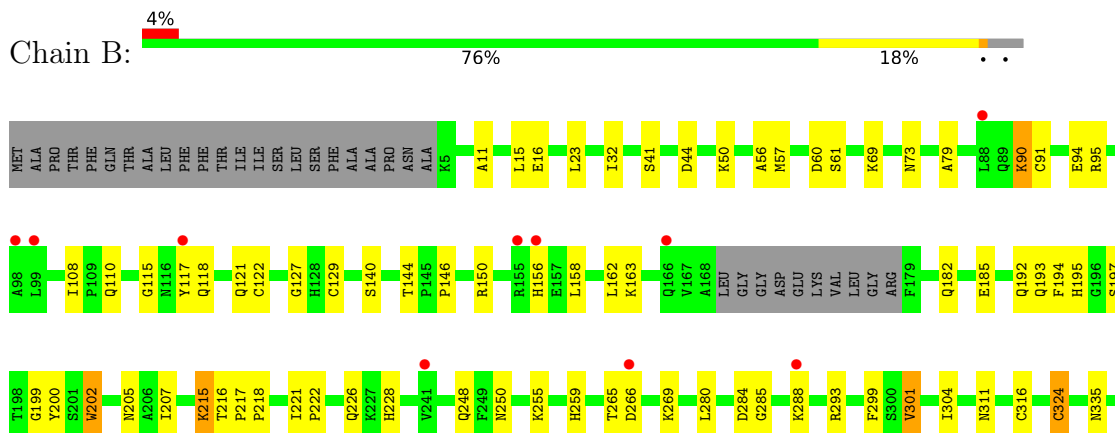
### 3 Residue-property plots [i](#)

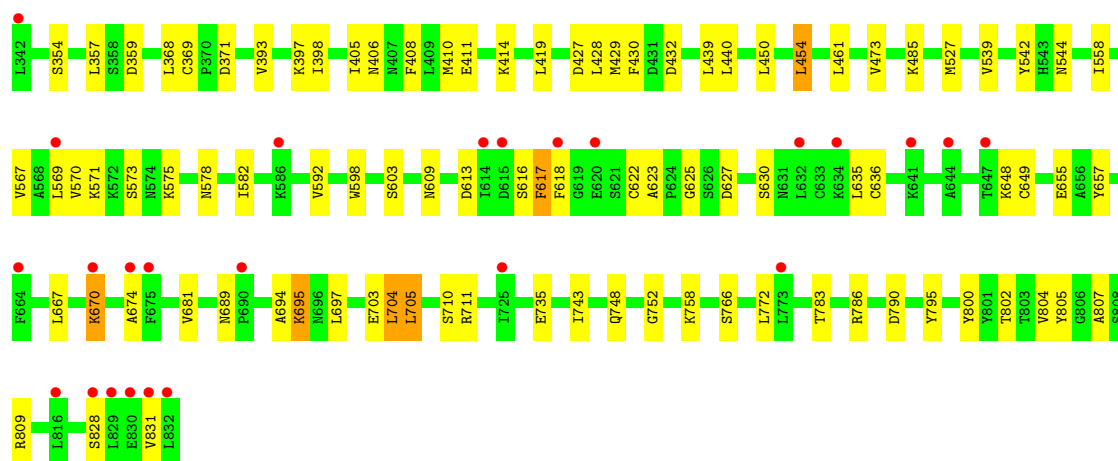
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, $\alpha$ , $\beta$ , $\gamma$	96.39Å 107.14Å 254.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.61 – 2.70 47.61 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.61-2.70) 99.7 (47.61-2.70)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.234 , 0.272 0.232 , 0.270	Depositor DCC
$R_{free}$ test set	3673 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	90.3	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 83.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12701	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	134.0	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	0.26	0/6436	0.47	0/8686
1	B	0.26	0/6436	0.46	0/8686
All	All	0.26	0/12872	0.47	0/17372

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	6311	0	6183	69	0
1	B	6311	0	6183	102	0
2	A	40	0	0	7	0
2	B	39	0	0	7	0
All	All	12701	0	12366	170	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 7.

All (170) 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:316:CYS:SG	2:B:913:HOH:O	2.26	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:GLN:O	1:B:121:GLN:NE2	2.18	0.77
1:A:551:CYS:SG	2:A:911:HOH:O	2.46	0.73
1:B:266:ASP:OD2	1:B:335:ASN:ND2	2.22	0.73
1:A:589:HIS:HD2	1:A:623:ALA:HB2	1.54	0.71
1:B:324:CYS:SG	2:B:913:HOH:O	2.48	0.71
1:A:636:CYS:SG	2:A:907:HOH:O	2.49	0.69
1:B:146:PRO:HA	1:B:150:ARG:HH12	1.58	0.69
1:A:610:ASP:OD1	2:A:901:HOH:O	2.11	0.68
1:A:308:THR:HB	1:B:293:ARG:HD3	1.76	0.68
1:A:602:VAL:HG23	1:A:614:ILE:HG21	1.74	0.67
1:A:649:CYS:SG	2:A:907:HOH:O	2.52	0.66
1:B:121:GLN:O	2:B:902:HOH:O	2.13	0.66
1:B:694:ALA:HA	1:B:697:LEU:HG	1.77	0.66
1:B:802:THR:HG22	1:B:807:ALA:HB2	1.77	0.66
1:B:265:THR:HA	1:B:269:LYS:HB2	1.76	0.66
1:A:489:TRP:O	1:A:493:SER:HB3	1.96	0.65
1:B:122:CYS:SG	2:B:902:HOH:O	2.54	0.65
1:B:689:ASN:O	1:B:695:LYS:NZ	2.29	0.65
1:B:284:ASP:HB3	1:B:288:LYS:HD2	1.79	0.65
1:B:285:GLY:O	2:B:901:HOH:O	2.13	0.64
1:B:625:GLY:H	1:B:649:CYS:HB3	1.61	0.64
1:B:216:THR:HG21	1:B:222:PRO:HA	1.81	0.63
1:B:657:TYR:OH	1:B:670:LYS:NZ	2.32	0.62
1:B:539:VAL:HG12	1:B:783:THR:HA	1.80	0.62
1:B:16:GLU:HG2	1:B:429:MET:HG3	1.80	0.61
1:A:32:ILE:HG21	1:A:408:PHE:HB2	1.82	0.61
1:A:224:THR:HG22	1:A:791:ILE:HD11	1.83	0.60
1:A:676:VAL:HG12	1:A:677:PRO:HD2	1.83	0.59
1:B:636:CYS:O	1:B:648:LYS:NZ	2.30	0.59
1:A:69:LYS:NZ	1:A:464:ASP:OD2	2.30	0.59
1:A:240:MET:HE3	1:A:352:LEU:HD11	1.85	0.59
1:A:56:ALA:HB2	1:A:405:ILE:HD13	1.84	0.59
1:A:758:LYS:O	1:A:762:GLN:NE2	2.36	0.59
1:B:485:LYS:HE3	1:B:766:SER:HB2	1.84	0.58
1:B:56:ALA:HB2	1:B:405:ILE:HD13	1.87	0.57
1:B:800:TYR:O	1:B:804:VAL:HG12	2.05	0.57
1:B:299:PHE:HA	2:B:903:HOH:O	2.05	0.57
1:A:164:GLU:OE1	1:A:189:TYR:OH	2.23	0.56
1:B:485:LYS:HD2	1:B:772:LEU:HB2	1.87	0.56
1:B:627:ASP:HB3	1:B:630:SER:HB2	1.88	0.56
1:B:569:LEU:HD21	1:B:681:VAL:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:PHE:HB3	1:A:563:THR:HG23	1.88	0.55
1:B:140:SER:HB2	1:B:831:VAL:HG12	1.87	0.55
1:B:473:VAL:HG23	1:B:743:ILE:HD12	1.88	0.55
1:A:732:THR:HG23	1:A:737:ILE:HD13	1.88	0.55
1:B:41:SER:OG	1:B:44:ASP:OD1	2.25	0.55
1:B:570:VAL:HG22	1:B:571:LYS:H	1.72	0.54
1:B:226:GLN:HG3	1:B:228:HIS:HE1	1.72	0.54
1:B:616:SER:OG	1:B:617:PHE:N	2.41	0.54
1:B:571:LYS:O	1:B:573:SER:N	2.40	0.54
1:A:79:ALA:HB3	1:A:440:LEU:HD21	1.90	0.53
1:B:250:ASN:HA	1:B:280:LEU:HD21	1.90	0.53
1:B:667:LEU:HB2	1:B:674:ALA:HB2	1.91	0.53
1:A:473:VAL:HG23	1:A:743:ILE:HD12	1.91	0.53
1:A:75:LYS:HG2	1:A:397:LYS:HA	1.91	0.53
1:A:184:ASP:OD1	1:A:188:ASN:N	2.42	0.53
1:A:802:THR:HG22	1:A:807:ALA:HB2	1.91	0.52
1:B:182:GLN:HE22	1:B:194:PHE:H	1.58	0.52
1:A:79:ALA:HB2	1:A:392:THR:HG23	1.92	0.52
1:B:527:MET:HG2	1:B:795:TYR:CE2	2.45	0.52
1:B:609:ASN:HD22	1:B:617:PHE:HE1	1.59	0.51
1:B:94:GLU:OE1	1:B:117:TYR:OH	2.27	0.51
1:B:11:ALA:HB1	1:B:16:GLU:HB3	1.92	0.51
1:B:598:TRP:CZ3	1:B:623:ALA:HB1	2.45	0.51
1:A:542:TYR:CZ	1:A:544:ASN:HB3	2.46	0.51
1:B:450:LEU:HD22	1:B:454:LEU:HD12	1.93	0.50
1:A:560:ASP:OD1	1:A:561:PHE:N	2.44	0.50
1:B:127:GLY:O	1:B:150:ARG:NH2	2.45	0.50
1:A:111:CYS:HB3	2:A:904:HOH:O	2.12	0.50
1:B:195:HIS:CE1	1:B:197:SER:HG	2.30	0.50
1:B:248:GLN:HA	1:B:368:LEU:HD11	1.93	0.50
1:A:569:LEU:HD22	1:A:681:VAL:HG22	1.94	0.49
1:B:15:LEU:HB3	1:B:428:LEU:HD21	1.95	0.49
1:A:539:VAL:HG12	1:A:783:THR:HA	1.94	0.49
1:B:202:TRP:HE3	1:B:215:LYS:HE2	1.77	0.49
1:B:354:SER:HA	1:B:357:LEU:HD13	1.94	0.49
1:A:779:GLN:HB3	2:A:911:HOH:O	2.12	0.49
1:B:578:ASN:HA	1:B:705:LEU:HD11	1.95	0.49
1:B:616:SER:O	1:B:618:PHE:N	2.46	0.49
1:B:790:ASP:OD1	1:B:809:ARG:NH2	2.46	0.48
1:A:708:ASP:N	1:A:708:ASP:OD1	2.47	0.48
1:B:23:LEU:HD13	1:B:419:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:MET:O	1:B:393:VAL:HA	2.14	0.48
1:B:79:ALA:HB3	1:B:440:LEU:HD11	1.96	0.48
1:A:519:ALA:HA	1:A:731:VAL:O	2.14	0.47
1:A:761:PHE:HE2	1:A:763:LEU:HD23	1.78	0.47
1:A:575:LYS:HA	1:A:711:ARG:HH12	1.80	0.47
1:B:695:LYS:HZ2	1:B:695:LYS:HA	1.79	0.47
1:B:748:GLN:O	1:B:752:GLY:N	2.45	0.47
1:B:710:SER:OG	1:B:711:ARG:N	2.48	0.47
1:A:527:MET:HE1	1:A:729:ALA:HB3	1.96	0.46
1:A:567:VAL:HA	1:A:722:LEU:HD13	1.97	0.46
1:A:622:CYS:HB2	1:A:635:LEU:HD12	1.96	0.46
1:B:193:GLN:HB2	1:B:202:TRP:CD1	2.50	0.46
1:B:91:CYS:HB3	1:B:115:GLY:O	2.16	0.46
1:B:598:TRP:HZ3	1:B:623:ALA:HB1	1.81	0.46
1:B:202:TRP:CE3	1:B:215:LYS:HE2	2.50	0.46
1:A:665:ARG:CZ	1:A:669:GLU:HG3	2.46	0.46
1:B:129:CYS:HB2	1:B:150:ARG:HE	1.80	0.46
1:B:259:HIS:CD2	1:B:304:ILE:HG12	2.51	0.46
1:A:248:GLN:HE22	1:A:374:ARG:HG3	1.81	0.45
1:A:527:MET:HG3	1:A:795:TYR:CZ	2.51	0.45
1:B:255:LYS:N	2:B:903:HOH:O	2.50	0.45
1:B:411:GLU:OE2	1:B:414:LYS:NZ	2.49	0.45
1:B:90:LYS:H	1:B:90:LYS:HG2	1.62	0.45
1:B:428:LEU:O	1:B:430:PHE:N	2.45	0.45
1:A:569:LEU:HD11	1:A:702:PHE:HB3	1.98	0.45
1:A:772:LEU:O	1:A:774:PHE:N	2.45	0.45
1:B:359:ASP:N	1:B:359:ASP:OD1	2.50	0.44
1:B:369:CYS:HB2	1:B:371:ASP:OD1	2.17	0.44
1:A:596:ALA:HB2	1:A:725:ILE:HD11	1.99	0.44
1:A:639:ASP:HB3	1:A:642:ASN:HB2	2.00	0.44
1:B:60:ASP:OD1	1:B:61:SER:N	2.51	0.44
1:A:104:ILE:HD12	1:A:104:ILE:HA	1.74	0.44
1:A:488:ASP:O	1:A:492:VAL:HG23	2.18	0.44
1:A:575:LYS:HA	1:A:711:ARG:HH22	1.82	0.44
1:B:804:VAL:HG13	1:B:805:TYR:CD2	2.53	0.44
1:A:522:LEU:HB2	1:A:527:MET:HE2	2.00	0.44
1:B:398:ILE:H	1:B:398:ILE:HD12	1.82	0.43
1:A:259:HIS:CD2	1:A:304:ILE:HG12	2.53	0.43
1:A:160:LYS:HD3	1:A:189:TYR:HE2	1.82	0.43
1:B:301:VAL:HA	1:B:311:ASN:O	2.18	0.43
1:B:567:VAL:HB	1:B:704:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:MET:HB2	1:A:792:MET:HE2	1.66	0.43
1:A:269:LYS:HE2	1:A:458:MET:HE1	1.99	0.43
1:A:589:HIS:CD2	1:A:623:ALA:HB2	2.44	0.43
1:A:650:SER:H	1:A:655:GLU:HG2	1.83	0.43
1:B:199:GLY:HA3	1:B:218:PRO:HB3	1.99	0.43
1:A:22:ASP:OD2	1:A:424:HIS:NE2	2.50	0.42
1:A:65:TYR:HB3	1:A:458:MET:HE2	2.01	0.42
1:B:158:LEU:HD22	1:B:162:LEU:HD23	2.00	0.42
1:B:200:TYR:CD1	1:B:217:PRO:HA	2.53	0.42
1:A:50:LYS:HB3	1:A:50:LYS:HE3	1.84	0.42
1:A:206:ALA:HB2	1:A:228:HIS:HB3	2.00	0.42
1:B:95:ARG:HE	1:B:108:ILE:HG22	1.84	0.42
1:B:162:LEU:HD12	1:B:162:LEU:HA	1.84	0.42
1:A:236:TYR:CE2	1:A:387:THR:HG22	2.55	0.42
1:B:655:GLU:HG3	1:B:657:TYR:H	1.84	0.42
1:B:427:ASP:N	1:B:432:ASP:OD1	2.42	0.42
1:B:73:ASN:HB3	1:B:397:LYS:HE2	2.02	0.42
1:B:461:LEU:HD12	1:B:461:LEU:HA	1.84	0.42
1:A:205:ASN:OD1	1:A:824:HIS:ND1	2.53	0.42
1:B:221:ILE:HD12	1:B:786:ARG:HG3	2.02	0.42
1:A:195:HIS:HB2	1:A:202:TRP:CH2	2.54	0.41
1:A:489:TRP:HE1	1:A:747:GLN:HG2	1.85	0.41
1:B:406:ASN:O	1:B:410:MET:HG2	2.21	0.41
1:A:773:LEU:HD12	1:A:773:LEU:HA	1.88	0.41
1:B:758:LYS:HB2	1:B:758:LYS:HE3	1.81	0.41
1:B:69:LYS:HE2	1:B:69:LYS:HB3	1.79	0.41
1:B:414:LYS:HZ2	1:B:414:LYS:HB2	1.86	0.41
1:A:91:CYS:HB3	2:A:904:HOH:O	2.19	0.41
1:B:592:VAL:HG22	1:B:598:TRP:CZ3	2.56	0.41
1:B:205:ASN:O	1:B:207:ILE:HG13	2.21	0.41
1:A:158:LEU:HD22	1:A:158:LEU:HA	1.86	0.41
1:A:317:LYS:HA	1:A:317:LYS:HD3	1.81	0.41
1:B:622:CYS:SG	1:B:657:TYR:HD2	2.44	0.41
1:B:156:HIS:HA	1:B:163:LYS:NZ	2.36	0.41
1:B:575:LYS:HA	1:B:711:ARG:HH12	1.85	0.41
1:A:691:ALA:HA	1:A:695:LYS:NZ	2.35	0.40
1:B:50:LYS:HE2	1:B:50:LYS:HB3	1.95	0.40
1:B:406:ASN:ND2	1:B:439:LEU:HB2	2.36	0.40
1:B:582:ILE:HG22	1:B:618:PHE:HE1	1.85	0.40
1:B:32:ILE:HG21	1:B:408:PHE:HB2	2.02	0.40
1:B:108:ILE:O	1:B:110:GLN:NE2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:HIS:NE2	1:B:197:SER:OG	2.49	0.40
1:A:78:ILE:HB	1:A:393:VAL:HB	2.03	0.40
1:B:603:SER:OG	1:B:804:VAL:HA	2.21	0.40
1:A:595:ILE:HA	1:A:599:VAL:HB	2.04	0.40
1:B:542:TYR:CZ	1:B:544:ASN:HB3	2.56	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	814/851 (96%)	766 (94%)	46 (6%)	2 (0%)	47	73
1	B	814/851 (96%)	758 (93%)	53 (6%)	3 (0%)	34	60
All	All	1628/1702 (96%)	1524 (94%)	99 (6%)	5 (0%)	41	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	301	VAL
1	B	617	PHE
1	B	828	SER
1	A	639	ASP
1	A	692	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	704/729 (97%)	689 (98%)	15 (2%)	53	80
1	B	704/729 (97%)	687 (98%)	17 (2%)	49	77
All	All	1408/1458 (97%)	1376 (98%)	32 (2%)	50	78

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	132	VAL
1	A	157	GLU
1	A	158	LEU
1	A	352	LEU
1	A	377	LEU
1	A	452	VAL
1	A	561	PHE
1	A	576	ASP
1	A	639	ASP
1	A	649	CYS
1	A	676	VAL
1	A	688	LYS
1	A	773	LEU
1	A	791	ILE
1	B	90	LYS
1	B	144	THR
1	B	185	GLU
1	B	192	GLN
1	B	202	TRP
1	B	215	LYS
1	B	324	CYS
1	B	454	LEU
1	B	558	ILE
1	B	613	ASP
1	B	635	LEU
1	B	670	LYS
1	B	695	LYS
1	B	703	GLU
1	B	704	LEU
1	B	705	LEU
1	B	735	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	A	589	HIS
1	B	89	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 monosaccharides 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	818/851 (96%)	0.40	49 (5%) 21 20	74, 120, 222, 267	0
1	B	818/851 (96%)	0.39	35 (4%) 35 33	82, 124, 205, 309	0
All	All	1636/1702 (96%)	0.40	84 (5%) 28 26	74, 123, 218, 309	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	569	LEU	11.3
1	B	831	VAL	10.5
1	B	830	GLU	7.6
1	A	674	ALA	7.5
1	B	644	ALA	7.3
1	B	832	LEU	6.8
1	B	88	LEU	6.4
1	A	579	TRP	6.3
1	B	615	ASP	6.0
1	A	722	LEU	5.9
1	A	673	VAL	5.3
1	A	704	LEU	5.2
1	A	693	TRP	5.0
1	A	681	VAL	5.0
1	A	570	VAL	4.8
1	A	691	ALA	4.3
1	A	675	PHE	4.2
1	A	639	ASP	4.1
1	A	702	PHE	4.1
1	A	645	ALA	4.1
1	B	614	ILE	4.0
1	A	162	LEU	3.8
1	B	664	PHE	3.8
1	A	618	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	705	LEU	3.7
1	B	829	LEU	3.7
1	A	672	ASP	3.6
1	A	587	SER	3.6
1	B	670	LYS	3.6
1	B	641	LYS	3.5
1	A	574	ASN	3.5
1	B	674	ALA	3.5
1	B	166	GLN	3.5
1	A	647	THR	3.4
1	A	707	LEU	3.4
1	A	582	ILE	3.4
1	B	675	PHE	3.3
1	B	266	ASP	3.3
1	A	688	LYS	3.2
1	A	194	PHE	3.2
1	A	568	ALA	3.1
1	A	637	ILE	3.1
1	B	618	PHE	3.0
1	A	714	VAL	3.0
1	A	670	LYS	2.8
1	A	632	LEU	2.8
1	A	646	ASN	2.8
1	A	197	SER	2.8
1	A	586	LYS	2.7
1	A	684	ASN	2.7
1	B	99	LEU	2.6
1	A	660	ASN	2.6
1	A	696	ASN	2.5
1	A	284	ASP	2.5
1	A	558	ILE	2.5
1	A	641	LYS	2.5
1	B	569	LEU	2.5
1	B	342	LEU	2.4
1	A	692	VAL	2.4
1	A	664	PHE	2.3
1	B	634	LYS	2.3
1	B	620	GLU	2.3
1	B	690	PRO	2.3
1	A	717	TYR	2.3
1	B	117	TYR	2.3
1	B	241	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	192	GLN	2.2
1	A	683	GLU	2.2
1	B	725	ILE	2.2
1	A	781	LEU	2.2
1	B	155	ARG	2.2
1	B	828	SER	2.1
1	B	98	ALA	2.1
1	B	156	HIS	2.1
1	B	288	LYS	2.1
1	B	647	THR	2.1
1	B	586	LYS	2.1
1	A	731	VAL	2.1
1	B	773	LEU	2.1
1	A	644	ALA	2.1
1	B	632	LEU	2.0
1	A	588	CYS	2.0
1	B	816	LEU	2.0
1	A	15	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 monosaccharides 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.