



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:26 am BST

PDB ID : 3TE6  
Title : Crystal Structure of the *S. cerevisiae* Sir3 AAA+ domain  
Authors : Hassler, M.; Ladurner, A.G.  
Deposited on : 2011-08-12  
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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

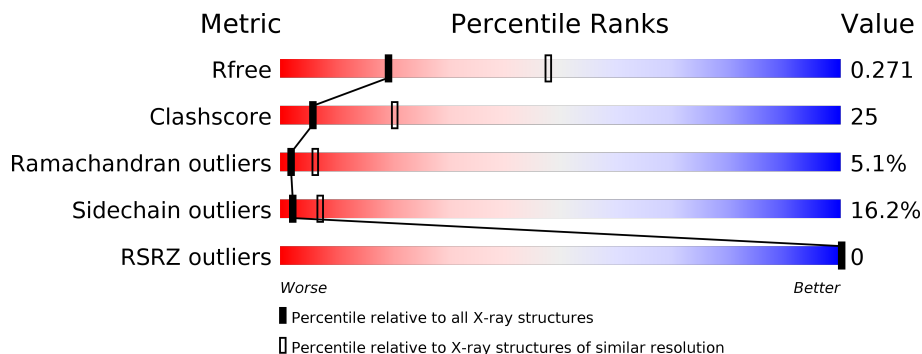
# 1 Overall quality at a glance i

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	318	
1	B	318	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4606 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 Regulatory protein SIR3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	304	2292	1464	391	428	2	7	0	0	0
1	B	303	2310	1482	390	430	2	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	528	GLY	-	EXPRESSION TAG	UNP P06701
A	529	PRO	-	EXPRESSION TAG	UNP P06701
B	528	GLY	-	EXPRESSION TAG	UNP P06701
B	529	PRO	-	EXPRESSION TAG	UNP P06701

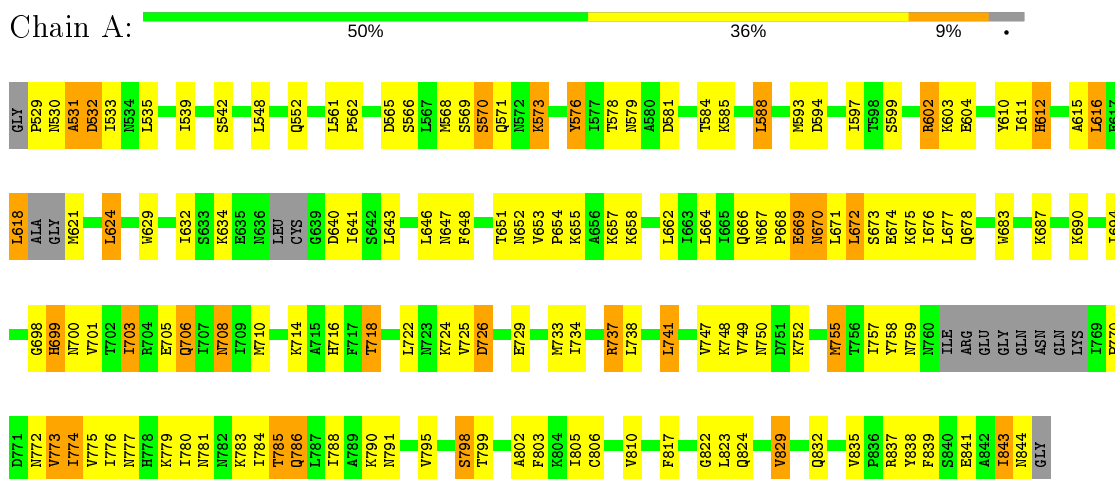
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	O 1	0	0
2	B	3	Total 3	O 3	0	0

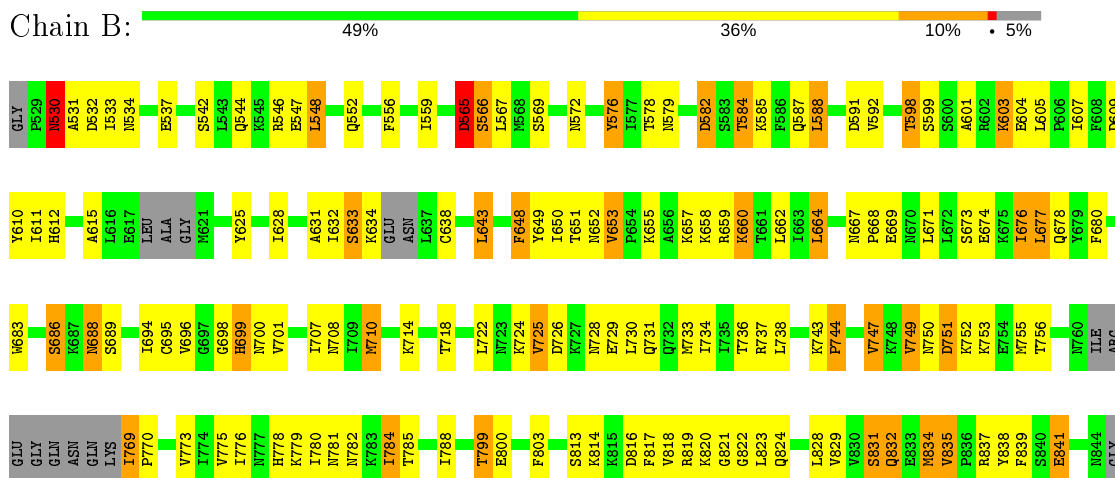
### 3 Residue-property plots

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: Regulatory protein SIR3



- Molecule 1: Regulatory protein SIR3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.59Å 47.02Å 127.85Å 90.00° 95.38° 90.00°	Depositor
Resolution (Å)	43.38 – 2.80 43.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.3 (43.38-2.80) 98.6 (43.38-2.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.219 , 0.276 0.217 , 0.271	Depositor DCC
$R_{free}$ test set	1330 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.8	Xtrriage
Anisotropy	0.411	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 64.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.65% 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	0.49	0/2320	0.62	0/3118
1	B	0.51	0/2339	0.64	0/3149
All	All	0.50	0/4659	0.63	0/6267

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	2292	0	2244	116	0
1	B	2310	0	2281	114	0
2	A	1	0	0	0	0
2	B	3	0	0	1	0
All	All	4606	0	4525	230	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 25.

All (230) 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:654:PRO:HG2	1:A:657:LYS:HG3	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:MSE:HE3	1:B:818:VAL:HA	1.49	0.95
1:B:659:ARG:O	1:B:660:LYS:HB3	1.71	0.90
1:B:674:GLU:O	1:B:678:GLN:HG3	1.71	0.89
1:A:664:LEU:HD12	1:A:694:ILE:HB	1.53	0.88
1:B:729:GLU:O	1:B:733:MSE:HG3	1.74	0.86
1:B:782:ASN:O	1:B:785:THR:HG22	1.75	0.86
1:B:750:ASN:HD22	1:B:752:LYS:H	1.25	0.85
1:A:822:GLY:HA2	1:A:829:VAL:HG22	1.61	0.83
1:A:651:THR:HG23	1:A:652:ASN:HD22	1.45	0.81
1:A:747:VAL:HG21	1:A:755:MSE:HE2	1.63	0.80
1:B:530:ASN:O	1:B:532:ASP:N	2.11	0.80
1:A:654:PRO:HG2	1:A:657:LYS:CG	2.12	0.80
1:A:837:ARG:O	1:A:841:GLU:HG3	1.81	0.79
1:B:747:VAL:HG13	1:B:776:ILE:HD13	1.64	0.78
1:B:819:ARG:HH21	1:B:820:LYS:HG2	1.50	0.75
1:A:530:ASN:O	1:A:532:ASP:N	2.21	0.74
1:A:647:ASN:HD22	1:A:683:TRP:HE1	1.35	0.74
1:A:737:ARG:HD2	1:A:741:LEU:HD22	1.71	0.73
1:B:534:ASN:ND2	1:B:537:GLU:H	1.86	0.72
1:B:689:SER:O	2:B:3:HOH:O	2.06	0.72
1:A:629:TRP:HE3	1:A:646:LEU:HD23	1.55	0.72
1:A:729:GLU:O	1:A:733:MSE:HG3	1.90	0.72
1:B:776:ILE:HG23	1:B:831:SER:HA	1.73	0.71
1:B:655:LYS:HG3	1:B:688:ASN:HA	1.73	0.69
1:B:653:VAL:HG22	1:B:658:LYS:HE3	1.74	0.68
1:B:604:GLU:O	1:B:604:GLU:HG2	1.93	0.68
1:A:725:VAL:O	1:A:726:ASP:HB3	1.94	0.68
1:A:775:VAL:C	1:A:776:ILE:HD12	2.14	0.68
1:B:837:ARG:O	1:B:841:GLU:HG2	1.92	0.68
1:B:659:ARG:O	1:B:660:LYS:CB	2.44	0.66
1:B:784:ILE:O	1:B:788:ILE:HG13	1.96	0.65
1:B:615:ALA:HB3	1:B:667:ASN:O	1.97	0.65
1:B:651:THR:HG22	1:B:686:SER:CB	2.26	0.65
1:B:572:ASN:ND2	1:B:689:SER:HB3	2.12	0.64
1:A:750:ASN:HD22	1:A:752:LYS:H	1.45	0.64
1:B:817:PHE:HB2	1:B:832:GLN:NE2	2.12	0.64
1:A:530:ASN:C	1:A:532:ASP:H	2.00	0.64
1:A:776:ILE:HD12	1:A:776:ILE:N	2.13	0.64
1:A:747:VAL:HG22	1:A:776:ILE:CD1	2.28	0.63
1:B:778:HIS:NE2	1:B:834:MSE:HE1	2.13	0.63
1:A:757:ILE:HG22	1:A:758:TYR:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:ASP:OD1	1:B:584:THR:HG23	2.00	0.62
1:B:755:MSE:HE2	1:B:821:GLY:HA2	1.82	0.61
1:B:534:ASN:HD22	1:B:537:GLU:CB	2.14	0.61
1:A:529:PRO:HB3	1:A:531:ALA:HB3	1.82	0.61
1:B:743:LYS:CD	1:B:744:PRO:HD2	2.30	0.61
1:A:548:LEU:O	1:A:552:GLN:HG3	2.01	0.61
1:A:822:GLY:CA	1:A:829:VAL:HG22	2.31	0.60
1:A:748:LYS:NZ	1:A:772:ASN:HD21	1.99	0.60
1:B:658:LYS:NZ	1:B:688:ASN:O	2.34	0.59
1:B:582:ASP:OD1	1:B:584:THR:N	2.33	0.59
1:B:676:ILE:HD13	1:B:677:LEU:H	1.67	0.59
1:B:676:ILE:HD13	1:B:677:LEU:N	2.18	0.59
1:A:653:VAL:HG13	1:A:654:PRO:HD2	1.85	0.59
1:A:780:ILE:HD13	1:A:785:THR:HG23	1.83	0.58
1:A:747:VAL:HG22	1:A:776:ILE:HD11	1.85	0.58
1:B:530:ASN:C	1:B:532:ASP:H	2.06	0.58
1:A:612:HIS:C	1:A:612:HIS:CD2	2.77	0.58
1:A:817:PHE:HB2	1:A:832:GLN:HE21	1.69	0.58
1:B:747:VAL:HG13	1:B:776:ILE:CD1	2.33	0.58
1:A:699:HIS:CD2	1:A:699:HIS:H	2.22	0.57
1:A:561:LEU:HB2	1:A:562:PRO:HD3	1.86	0.57
1:A:699:HIS:C	1:A:701:VAL:H	2.07	0.57
1:B:674:GLU:HA	1:B:677:LEU:HB2	1.87	0.57
1:A:817:PHE:HB2	1:A:832:GLN:NE2	2.19	0.57
1:A:774:ILE:HG12	1:A:775:VAL:N	2.21	0.56
1:B:655:LYS:CG	1:B:688:ASN:HA	2.36	0.56
1:A:610:TYR:C	1:A:611:ILE:HD12	2.27	0.55
1:A:781:ASN:HD21	1:A:783:LYS:HB2	1.71	0.55
1:A:781:ASN:HD22	1:A:784:ILE:H	1.54	0.55
1:B:609:ASP:OD2	1:B:659:ARG:HD3	2.05	0.55
1:B:743:LYS:HD2	1:B:744:PRO:HD2	1.89	0.55
1:A:790:LYS:HG2	1:A:791:ASN:ND2	2.21	0.55
1:A:568:MSE:HE3	1:A:568:MSE:HA	1.90	0.54
1:A:698:GLY:O	1:A:701:VAL:HG22	2.08	0.54
1:A:737:ARG:HD2	1:A:741:LEU:CD2	2.37	0.54
1:B:648:PHE:CD2	1:B:652:ASN:HB2	2.43	0.54
1:B:747:VAL:CG1	1:B:776:ILE:HD13	2.37	0.53
1:A:647:ASN:O	1:A:651:THR:HG22	2.09	0.53
1:B:578:THR:O	1:B:579:ASN:HB2	2.09	0.53
1:B:673:SER:O	1:B:677:LEU:HB2	2.09	0.53
1:B:725:VAL:HG12	1:B:726:ASP:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ASP:O	1:A:597:ILE:HG13	2.08	0.52
1:B:781:ASN:OD1	1:B:784:ILE:HG23	2.10	0.52
1:B:628:ILE:O	1:B:632:ILE:HG13	2.09	0.52
1:B:728:ASN:O	1:B:731:GLN:HG2	2.10	0.52
1:A:790:LYS:HG2	1:A:791:ASN:HD22	1.74	0.52
1:B:559:ILE:HG22	1:B:592:VAL:HG11	1.92	0.52
1:A:757:ILE:CG2	1:A:758:TYR:N	2.74	0.51
1:B:788:ILE:HD13	1:B:839:PHE:CE1	2.45	0.51
1:B:633:SER:O	1:B:634:LYS:CB	2.58	0.51
1:B:730:LEU:HD12	1:B:730:LEU:O	2.11	0.51
1:B:534:ASN:ND2	1:B:537:GLU:N	2.57	0.51
1:A:737:ARG:O	1:A:741:LEU:HD22	2.11	0.51
1:A:616:LEU:HD13	1:A:616:LEU:N	2.24	0.50
1:B:565:ASP:O	1:B:566:SER:C	2.50	0.50
1:B:724:LYS:O	1:B:725:VAL:O	2.30	0.50
1:B:650:ILE:HG21	1:B:683:TRP:HB3	1.93	0.50
1:A:578:THR:O	1:A:579:ASN:HB2	2.12	0.49
1:B:749:VAL:HG23	1:B:750:ASN:N	2.27	0.49
1:B:770:PRO:O	1:B:773:VAL:HG22	2.13	0.49
1:B:698:GLY:O	1:B:701:VAL:HG23	2.12	0.49
1:B:587:GLN:HA	1:B:587:GLN:OE1	2.12	0.49
1:A:676:ILE:HG23	1:A:677:LEU:N	2.26	0.49
1:B:584:THR:O	1:B:587:GLN:HB3	2.12	0.49
1:B:668:PRO:HG3	1:B:695:CYS:HB3	1.95	0.49
1:A:673:SER:C	1:A:676:ILE:HG22	2.33	0.49
1:A:699:HIS:O	1:A:701:VAL:N	2.45	0.49
1:A:788:ILE:HD13	1:A:839:PHE:CE1	2.48	0.49
1:B:548:LEU:O	1:B:552:GLN:HG3	2.12	0.49
1:B:565:ASP:O	1:B:567:LEU:N	2.45	0.49
1:B:750:ASN:ND2	1:B:752:LYS:H	2.01	0.49
1:A:569:SER:O	1:A:571:GLN:HG2	2.13	0.49
1:A:781:ASN:ND2	1:A:784:ILE:H	2.10	0.49
1:B:778:HIS:NE2	1:B:834:MSE:CE	2.76	0.49
1:A:529:PRO:HA	1:A:530:ASN:C	2.34	0.48
1:B:707:ILE:HA	1:B:710:MSE:HG3	1.96	0.48
1:B:750:ASN:HD22	1:B:752:LYS:N	2.04	0.48
1:A:668:PRO:O	1:A:669:GLU:C	2.52	0.48
1:B:779:LYS:HG2	1:B:780:ILE:N	2.28	0.48
1:A:747:VAL:HG23	1:A:774:ILE:HG23	1.96	0.48
1:B:611:ILE:HG12	1:B:631:ALA:HB1	1.96	0.48
1:A:741:LEU:HB3	1:A:810:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:ASN:HD22	1:A:752:LYS:N	2.11	0.47
1:B:533:ILE:O	1:B:533:ILE:HG22	2.14	0.47
1:A:747:VAL:HG22	1:A:776:ILE:HD13	1.95	0.47
1:B:625:TYR:OH	1:B:676:ILE:HG22	2.15	0.47
1:A:615:ALA:C	1:A:616:LEU:HD13	2.35	0.47
1:B:699:HIS:O	1:B:701:VAL:N	2.47	0.47
1:B:749:VAL:CG2	1:B:750:ASN:N	2.78	0.47
1:B:576:TYR:HE2	1:B:701:VAL:HG13	1.80	0.47
1:A:624:LEU:HD12	1:A:624:LEU:O	2.15	0.47
1:B:799:THR:HG22	1:B:800:GLU:N	2.30	0.47
1:B:820:LYS:NZ	1:B:832:GLN:HE22	2.13	0.46
1:A:629:TRP:CE3	1:A:646:LEU:HD23	2.42	0.46
1:A:581:ASP:HB3	1:A:798:SER:HB3	1.98	0.46
1:A:569:SER:O	1:A:571:GLN:N	2.48	0.46
1:A:569:SER:O	1:A:570:SER:C	2.53	0.46
1:B:588:LEU:HD12	1:B:588:LEU:HA	1.65	0.46
1:A:748:LYS:HZ3	1:A:772:ASN:HD21	1.61	0.46
1:A:785:THR:O	1:A:786:GLN:C	2.54	0.46
1:B:751:ASP:N	1:B:751:ASP:OD2	2.47	0.46
1:A:530:ASN:C	1:A:532:ASP:N	2.63	0.46
1:B:547:GLU:HA	1:B:547:GLU:OE1	2.15	0.46
1:B:556:PHE:HE1	1:B:591:ASP:HB3	1.80	0.46
1:A:533:ILE:CG1	1:A:533:ILE:O	2.64	0.46
1:A:725:VAL:O	1:A:726:ASP:CB	2.63	0.46
1:B:534:ASN:HD22	1:B:537:GLU:H	1.61	0.46
1:A:666:GLN:O	1:A:667:ASN:HB2	2.14	0.45
1:A:576:TYR:OH	1:A:701:VAL:HG11	2.16	0.45
1:A:776:ILE:HG12	1:A:817:PHE:CE2	2.51	0.45
1:B:643:LEU:HD12	1:B:643:LEU:O	2.16	0.45
1:B:813:SER:CB	1:B:834:MSE:CE	2.94	0.45
1:A:648:PHE:O	1:A:652:ASN:HB2	2.16	0.45
1:A:673:SER:O	1:A:676:ILE:HG22	2.16	0.45
1:A:835:VAL:HG22	1:A:838:TYR:CE1	2.52	0.45
1:A:738:LEU:HA	1:A:738:LEU:HD23	1.83	0.45
1:B:813:SER:OG	1:B:834:MSE:CE	2.64	0.45
1:B:834:MSE:HE2	1:B:834:MSE:HA	1.99	0.45
1:A:708:ASN:HD21	1:A:714:LYS:HZ2	1.65	0.45
1:A:654:PRO:O	1:A:657:LYS:HB2	2.17	0.45
1:A:573:LYS:HZ2	1:A:718:THR:HG22	1.81	0.45
1:B:598:THR:HG22	1:B:599:SER:N	2.30	0.45
1:B:680:PHE:CD1	1:B:680:PHE:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:779:LYS:HG2	1:B:780:ILE:H	1.82	0.45
1:A:565:ASP:O	1:A:566:SER:C	2.55	0.45
1:A:817:PHE:HD1	1:A:832:GLN:HE21	1.63	0.45
1:B:707:ILE:HG22	1:B:714:LYS:HG3	1.97	0.45
1:A:670:ASN:O	1:A:672:LEU:N	2.50	0.45
1:A:675:LYS:O	1:A:678:GLN:N	2.50	0.45
1:A:676:ILE:CG2	1:A:677:LEU:N	2.79	0.44
1:A:770:PRO:HB2	1:A:773:VAL:CG1	2.47	0.44
1:B:776:ILE:HG12	1:B:817:PHE:CE2	2.52	0.44
1:B:688:ASN:H	1:B:688:ASN:ND2	2.14	0.44
1:B:813:SER:CB	1:B:834:MSE:HE1	2.48	0.44
1:A:703:ILE:C	1:A:705:GLU:N	2.71	0.44
1:A:535:LEU:HD22	1:A:539:ILE:HD11	1.99	0.44
1:A:624:LEU:HD12	1:A:624:LEU:C	2.38	0.44
1:B:576:TYR:CD1	1:B:695:CYS:HB2	2.53	0.44
1:B:835:VAL:H	1:B:838:TYR:HD1	1.66	0.44
1:A:706:GLN:O	1:A:710:MSE:HG3	2.18	0.44
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.86	0.44
1:A:734:ILE:HG23	1:A:806:CYS:SG	2.58	0.44
1:A:750:ASN:ND2	1:A:752:LYS:H	2.14	0.43
1:A:803:PHE:CD1	1:A:803:PHE:N	2.85	0.43
1:B:607:ILE:HD12	1:B:607:ILE:HA	1.89	0.43
1:A:599:SER:O	1:A:604:GLU:HB3	2.18	0.43
1:B:769:ILE:HG22	1:B:770:PRO:HD3	1.99	0.43
1:B:769:ILE:N	1:B:770:PRO:CD	2.81	0.43
1:A:618:LEU:HD12	1:A:621:MSE:N	2.33	0.43
1:B:751:ASP:C	1:B:753:LYS:H	2.21	0.43
1:B:750:ASN:HB2	1:B:751:ASP:H	1.67	0.43
1:A:776:ILE:N	1:A:776:ILE:CD1	2.81	0.43
1:B:585:LYS:HG3	1:B:722:LEU:HD13	2.00	0.43
1:B:601:ALA:C	1:B:603:LYS:H	2.21	0.43
1:A:632:ILE:HD13	1:A:632:ILE:HA	1.84	0.42
1:B:707:ILE:O	1:B:708:ASN:C	2.57	0.42
1:B:816:ASP:OD2	1:B:838:TYR:OH	2.32	0.42
1:B:649:TYR:HA	1:B:653:VAL:CG1	2.49	0.42
1:A:588:LEU:HD13	1:A:588:LEU:HA	1.69	0.42
1:A:655:LYS:HD3	1:A:687:LYS:O	2.19	0.42
1:A:795:VAL:HG11	1:A:843:ILE:HD12	2.01	0.42
1:B:673:SER:O	1:B:676:ILE:HD13	2.19	0.42
1:B:632:ILE:O	1:B:632:ILE:HG22	2.19	0.42
1:A:593:MSE:HG3	1:A:610:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:PRO:O	1:A:773:VAL:HG13	2.20	0.41
1:B:662:LEU:HD11	1:B:694:ILE:HD11	2.02	0.41
1:B:734:ILE:O	1:B:738:LEU:HB2	2.20	0.41
1:B:775:VAL:C	1:B:776:ILE:HD12	2.41	0.41
1:A:662:LEU:HD11	1:A:694:ILE:HD11	2.02	0.41
1:A:615:ALA:HB3	1:A:667:ASN:O	2.20	0.41
1:A:667:ASN:HA	1:A:669:GLU:OE1	2.21	0.41
1:A:770:PRO:HD2	1:A:773:VAL:HG11	2.03	0.41
1:B:784:ILE:HD12	1:B:788:ILE:HD11	2.02	0.41
1:A:602:ARG:C	1:A:604:GLU:H	2.24	0.41
1:A:655:LYS:CG	1:A:690:LYS:HE3	2.51	0.41
1:A:573:LYS:HG3	1:A:716:HIS:O	2.21	0.41
1:B:610:TYR:CE2	1:B:612:HIS:HB2	2.56	0.41
1:B:655:LYS:H	1:B:688:ASN:HB3	1.86	0.41
1:B:710:MSE:H	1:B:710:MSE:HG2	1.56	0.41
1:B:648:PHE:CD2	1:B:648:PHE:C	2.94	0.40
1:A:602:ARG:C	1:A:604:GLU:N	2.74	0.40
1:A:747:VAL:CG2	1:A:776:ILE:HD11	2.51	0.40
1:A:602:ARG:O	1:A:604:GLU:N	2.55	0.40
1:A:757:ILE:HG22	1:A:758:TYR:H	1.86	0.40
1:B:664:LEU:HD21	1:B:696:VAL:CG2	2.51	0.40
1:B:822:GLY:HA2	1:B:829:VAL:HG23	2.02	0.40
1:A:757:ILE:CG2	1:A:758:TYR:H	2.33	0.40
1:A:802:ALA:O	1:A:805:ILE:HB	2.21	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	296/318 (93%)	251 (85%)	30 (10%)	15 (5%)	<b>2</b> <b>6</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	295/318 (93%)	246 (83%)	34 (12%)	15 (5%)	2	6
All	All	591/636 (93%)	497 (84%)	64 (11%)	30 (5%)	2	6

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	531	ALA
1	A	570	SER
1	A	602	ARG
1	A	670	ASN
1	A	671	LEU
1	A	672	LEU
1	A	759	ASN
1	B	566	SER
1	B	603	LYS
1	B	638	CYS
1	B	669	GLU
1	B	671	LEU
1	B	725	VAL
1	A	634	LYS
1	A	640	ASP
1	A	641	ILE
1	A	669	GLU
1	A	700	ASN
1	B	660	LYS
1	A	603	LYS
1	B	530	ASN
1	B	531	ALA
1	B	565	ASP
1	B	633	SER
1	B	686	SER
1	B	700	ASN
1	B	744	PRO
1	B	803	PHE
1	A	674	GLU
1	A	726	ASP

### 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	242/284 (85%)	205 (85%)	37 (15%)	2	8
1	B	246/284 (87%)	204 (83%)	42 (17%)	2	6
All	All	488/568 (86%)	409 (84%)	79 (16%)	2	7

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	532	ASP
1	A	542	SER
1	A	573	LYS
1	A	576	TYR
1	A	584	THR
1	A	585	LYS
1	A	588	LEU
1	A	612	HIS
1	A	616	LEU
1	A	618	LEU
1	A	624	LEU
1	A	643	LEU
1	A	658	LYS
1	A	699	HIS
1	A	703	ILE
1	A	706	GLN
1	A	708	ASN
1	A	718	THR
1	A	722	LEU
1	A	724	LYS
1	A	737	ARG
1	A	741	LEU
1	A	749	VAL
1	A	755	MSE
1	A	773	VAL
1	A	774	ILE
1	A	777	ASN
1	A	779	LYS
1	A	785	THR
1	A	786	GLN
1	A	798	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	799	THR
1	A	823	LEU
1	A	824	GLN
1	A	829	VAL
1	A	843	ILE
1	A	844	ASN
1	B	530	ASN
1	B	542	SER
1	B	544	GLN
1	B	546	ARG
1	B	548	LEU
1	B	565	ASP
1	B	569	SER
1	B	576	TYR
1	B	582	ASP
1	B	584	THR
1	B	588	LEU
1	B	598	THR
1	B	605	LEU
1	B	643	LEU
1	B	648	PHE
1	B	653	VAL
1	B	657	LYS
1	B	664	LEU
1	B	676	ILE
1	B	677	LEU
1	B	688	ASN
1	B	699	HIS
1	B	710	MSE
1	B	718	THR
1	B	736	THR
1	B	737	ARG
1	B	747	VAL
1	B	749	VAL
1	B	751	ASP
1	B	756	THR
1	B	769	ILE
1	B	784	ILE
1	B	799	THR
1	B	814	LYS
1	B	823	LEU
1	B	824	GLN

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Mol	Chain	Res	Type
1	B	828	LEU
1	B	831	SER
1	B	832	GLN
1	B	834	MSE
1	B	835	VAL
1	B	841	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	571	GLN
1	A	612	HIS
1	A	647	ASN
1	A	652	ASN
1	A	699	HIS
1	A	723	ASN
1	A	746	HIS
1	A	750	ASN
1	A	772	ASN
1	A	781	ASN
1	A	791	ASN
1	A	832	GLN
1	A	844	ASN
1	B	534	ASN
1	B	572	ASN
1	B	666	GLN
1	B	688	ASN
1	B	699	HIS
1	B	746	HIS
1	B	750	ASN
1	B	777	ASN
1	B	791	ASN
1	B	832	GLN

### 5.3.3 RNA

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](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	297/318 (93%)	-0.30	0 <a href="#">100</a> <a href="#">100</a>	56, 73, 98, 112	0
1	B	296/318 (93%)	-0.24	0 <a href="#">100</a> <a href="#">100</a>	54, 72, 99, 113	0
All	All	593/636 (93%)	-0.27	0 <a href="#">100</a> <a href="#">100</a>	54, 72, 98, 113	0

There are no RSRZ outliers to report.

### 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.