



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:23 am BST

PDB ID : 5IW7  
Title : Crystal structure of yeast Tsr1, a pre-40S ribosome synthesis factor  
Authors : McCaughan, U.M.; Jayachandran, U.; Cook, A.G.  
Deposited on : 2016-03-22  
Resolution : 3.60 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  
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

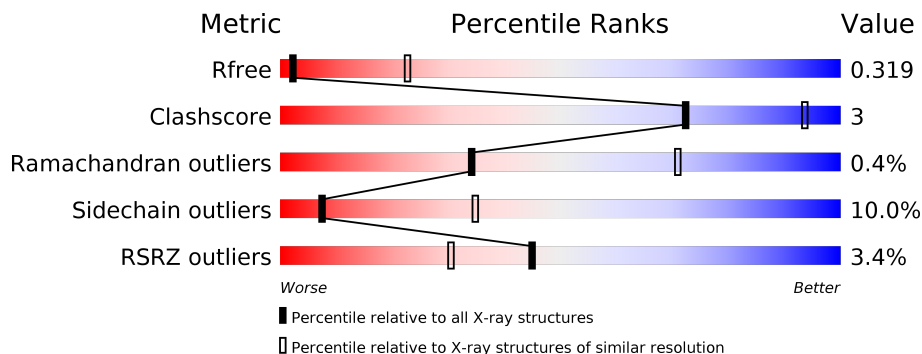
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 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	704	 3% 70% 13% • 15%
1	B	704	 3% 73% 8% • 19%
1	C	704	 3% 69% 10% • 19%
1	D	704	 3% 65% 8% 27%

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 16065 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 Ribosome biogenesis protein TSR1, Ribosome biogenesis protein TSR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	595	4531	2905	771	843	12	0	0	0
1	B	569	4015	2543	691	771	10	0	0	0
1	C	567	4093	2615	697	771	10	0	0	0
1	D	517	3426	2145	604	669	8	0	0	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP Q07381
A	25	LYS	-	expression tag	UNP Q07381
A	26	HIS	-	expression tag	UNP Q07381
A	27	HIS	-	expression tag	UNP Q07381
A	28	HIS	-	expression tag	UNP Q07381
A	29	HIS	-	expression tag	UNP Q07381
A	30	HIS	-	expression tag	UNP Q07381
A	31	HIS	-	expression tag	UNP Q07381
A	32	SER	-	expression tag	UNP Q07381
A	33	ALA	-	expression tag	UNP Q07381
A	34	GLY	-	expression tag	UNP Q07381
A	35	LEU	-	expression tag	UNP Q07381
A	36	GLU	-	expression tag	UNP Q07381
A	37	VAL	-	expression tag	UNP Q07381
A	38	LEU	-	expression tag	UNP Q07381
A	39	PHE	-	expression tag	UNP Q07381
A	40	GLN	-	expression tag	UNP Q07381
A	41	GLY	-	expression tag	UNP Q07381
A	42	PRO	-	expression tag	UNP Q07381
A	43	ASP	-	expression tag	UNP Q07381

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Chain	Residue	Modelled	Actual	Comment	Reference
A	44	SER	-	expression tag	UNP Q07381
A	45	MET	-	expression tag	UNP Q07381
A	471	PRO	-	linker	UNP Q07381
A	472	SER	-	linker	UNP Q07381
A	473	SER	-	linker	UNP Q07381
A	474	GLY	-	linker	UNP Q07381
A	475	SER	-	linker	UNP Q07381
A	476	SER	-	linker	UNP Q07381
B	24	MET	-	initiating methionine	UNP Q07381
B	25	LYS	-	expression tag	UNP Q07381
B	26	HIS	-	expression tag	UNP Q07381
B	27	HIS	-	expression tag	UNP Q07381
B	28	HIS	-	expression tag	UNP Q07381
B	29	HIS	-	expression tag	UNP Q07381
B	30	HIS	-	expression tag	UNP Q07381
B	31	HIS	-	expression tag	UNP Q07381
B	32	SER	-	expression tag	UNP Q07381
B	33	ALA	-	expression tag	UNP Q07381
B	34	GLY	-	expression tag	UNP Q07381
B	35	LEU	-	expression tag	UNP Q07381
B	36	GLU	-	expression tag	UNP Q07381
B	37	VAL	-	expression tag	UNP Q07381
B	38	LEU	-	expression tag	UNP Q07381
B	39	PHE	-	expression tag	UNP Q07381
B	40	GLN	-	expression tag	UNP Q07381
B	41	GLY	-	expression tag	UNP Q07381
B	42	PRO	-	expression tag	UNP Q07381
B	43	ASP	-	expression tag	UNP Q07381
B	44	SER	-	expression tag	UNP Q07381
B	45	MET	-	expression tag	UNP Q07381
B	471	PRO	-	linker	UNP Q07381
B	472	SER	-	linker	UNP Q07381
B	473	SER	-	linker	UNP Q07381
B	474	GLY	-	linker	UNP Q07381
B	475	SER	-	linker	UNP Q07381
B	476	SER	-	linker	UNP Q07381
C	24	MET	-	initiating methionine	UNP Q07381
C	25	LYS	-	expression tag	UNP Q07381
C	26	HIS	-	expression tag	UNP Q07381
C	27	HIS	-	expression tag	UNP Q07381
C	28	HIS	-	expression tag	UNP Q07381
C	29	HIS	-	expression tag	UNP Q07381

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Chain	Residue	Modelled	Actual	Comment	Reference
C	30	HIS	-	expression tag	UNP Q07381
C	31	HIS	-	expression tag	UNP Q07381
C	32	SER	-	expression tag	UNP Q07381
C	33	ALA	-	expression tag	UNP Q07381
C	34	GLY	-	expression tag	UNP Q07381
C	35	LEU	-	expression tag	UNP Q07381
C	36	GLU	-	expression tag	UNP Q07381
C	37	VAL	-	expression tag	UNP Q07381
C	38	LEU	-	expression tag	UNP Q07381
C	39	PHE	-	expression tag	UNP Q07381
C	40	GLN	-	expression tag	UNP Q07381
C	41	GLY	-	expression tag	UNP Q07381
C	42	PRO	-	expression tag	UNP Q07381
C	43	ASP	-	expression tag	UNP Q07381
C	44	SER	-	expression tag	UNP Q07381
C	45	MET	-	expression tag	UNP Q07381
C	471	PRO	-	linker	UNP Q07381
C	472	SER	-	linker	UNP Q07381
C	473	SER	-	linker	UNP Q07381
C	474	GLY	-	linker	UNP Q07381
C	475	SER	-	linker	UNP Q07381
C	476	SER	-	linker	UNP Q07381
D	24	MET	-	initiating methionine	UNP Q07381
D	25	LYS	-	expression tag	UNP Q07381
D	26	HIS	-	expression tag	UNP Q07381
D	27	HIS	-	expression tag	UNP Q07381
D	28	HIS	-	expression tag	UNP Q07381
D	29	HIS	-	expression tag	UNP Q07381
D	30	HIS	-	expression tag	UNP Q07381
D	31	HIS	-	expression tag	UNP Q07381
D	32	SER	-	expression tag	UNP Q07381
D	33	ALA	-	expression tag	UNP Q07381
D	34	GLY	-	expression tag	UNP Q07381
D	35	LEU	-	expression tag	UNP Q07381
D	36	GLU	-	expression tag	UNP Q07381
D	37	VAL	-	expression tag	UNP Q07381
D	38	LEU	-	expression tag	UNP Q07381
D	39	PHE	-	expression tag	UNP Q07381
D	40	GLN	-	expression tag	UNP Q07381
D	41	GLY	-	expression tag	UNP Q07381
D	42	PRO	-	expression tag	UNP Q07381
D	43	ASP	-	expression tag	UNP Q07381

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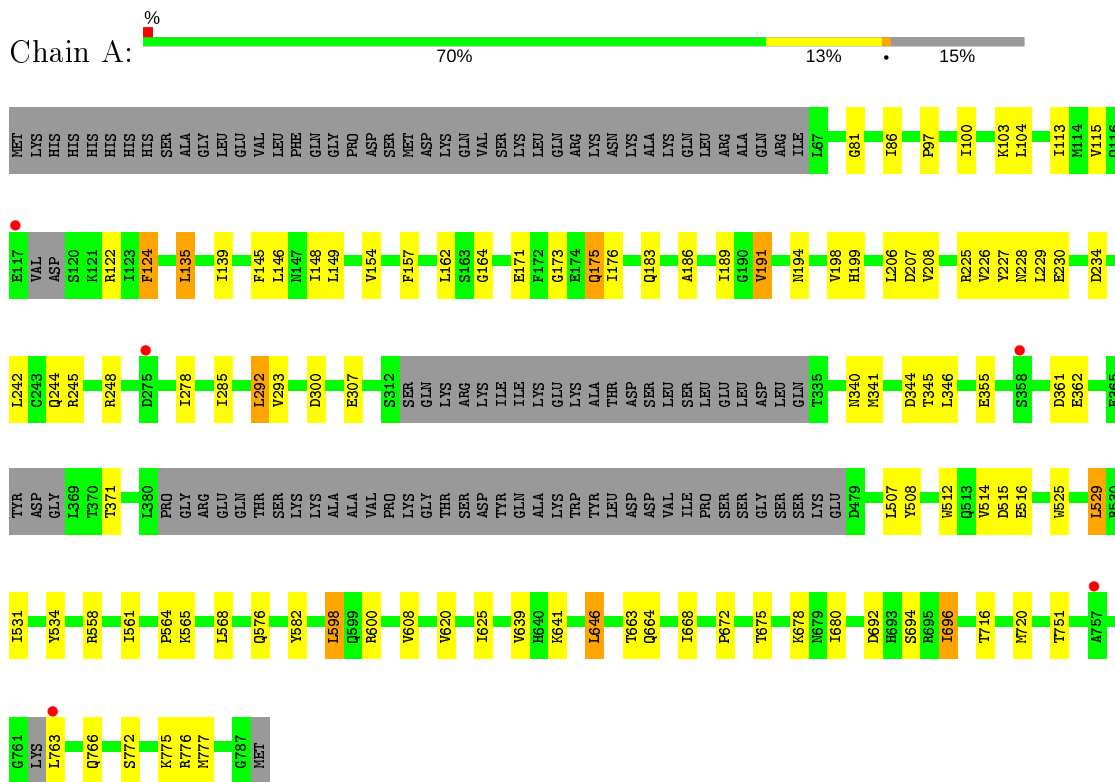
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Chain	Residue	Modelled	Actual	Comment	Reference
D	44	SER	-	expression tag	UNP Q07381
D	45	MET	-	expression tag	UNP Q07381
D	471	PRO	-	linker	UNP Q07381
D	472	SER	-	linker	UNP Q07381
D	473	SER	-	linker	UNP Q07381
D	474	GLY	-	linker	UNP Q07381
D	475	SER	-	linker	UNP Q07381
D	476	SER	-	linker	UNP Q07381

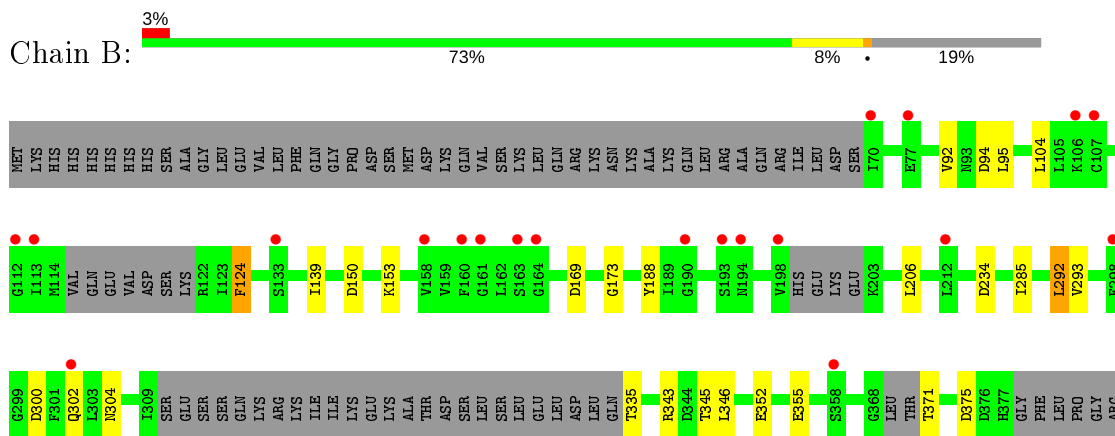
### 3 Residue-property plots [i](#)

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: Ribosome biogenesis protein TSR1,Ribosome biogenesis protein TSR1

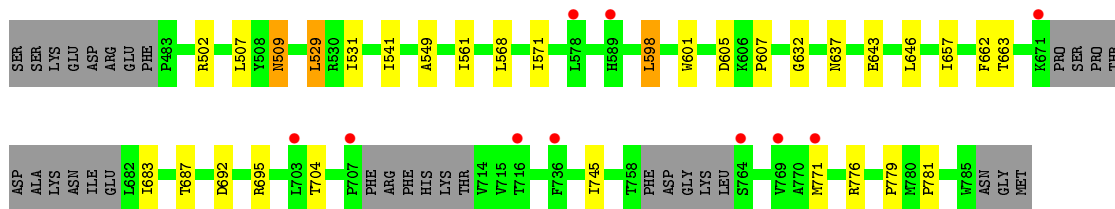


- Molecule 1: Ribosome biogenesis protein TSR1,Ribosome biogenesis protein TSR1









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.69Å 174.20Å 320.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.77 – 3.60 48.77 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.77-3.60) 99.9 (48.77-3.60)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 3.57Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.268 , 0.295 0.288 , 0.319	Depositor DCC
$R_{free}$ test set	2228 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	123.0	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 111.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	16065	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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	0.37	0/4639	0.61	0/6324
1	B	0.36	0/4105	0.58	0/5625
1	C	0.37	0/4193	0.61	0/5740
1	D	0.36	0/3494	0.59	0/4811
All	All	0.36	0/16431	0.60	0/22500

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	4531	0	4160	32	0
1	B	4015	0	3368	18	0
1	C	4093	0	3483	32	0
1	D	3426	0	2669	19	0
All	All	16065	0	13680	100	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 3.

All (100) 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:514:VAL:HA	1:A:776:ARG:HH12	1.44	0.81
1:D:657:ILE:HG23	1:D:779:PRO:HB2	1.68	0.76
1:C:672:PRO:HA	1:C:680:ILE:HA	1.73	0.69
1:B:302:GLN:NE2	1:B:343:ARG:HD2	2.08	0.68
1:D:286:GLY:HA3	1:D:549:ALA:HB1	1.77	0.66
1:C:609:PRO:HG2	1:C:612:GLU:HG3	1.78	0.65
1:C:735:LEU:HD11	1:C:745:ILE:HG22	1.81	0.63
1:A:186:ALA:O	1:A:248:ARG:HB2	1.98	0.62
1:D:90:PRO:HG2	1:D:95:LEU:HD13	1.83	0.61
1:A:198:VAL:HG11	1:A:208:VAL:HG21	1.81	0.61
1:C:538:LYS:HG3	1:C:662:PHE:O	2.00	0.61
1:B:598:LEU:HD21	1:B:646:LEU:HD11	1.85	0.59
1:A:175:GLN:HG2	1:A:678:LYS:HE3	1.84	0.59
1:D:250:ILE:HD12	1:D:253:ARG:HD3	1.84	0.58
1:D:169:ASP:HB3	1:D:173:GLY:H	1.67	0.58
1:A:164:GLY:H	1:A:194:ASN:HB3	1.69	0.57
1:B:572:GLN:HG3	1:B:577:LEU:HB2	1.87	0.56
1:B:150:ASP:HA	1:B:153:LYS:HD2	1.87	0.56
1:A:639:VAL:HG22	1:A:696:ILE:HG12	1.88	0.56
1:C:664:GLN:HA	1:C:688:PHE:HB3	1.88	0.56
1:D:657:ILE:HG13	1:D:781:PRO:HA	1.88	0.56
1:B:302:GLN:HE21	1:B:343:ARG:HD2	1.73	0.54
1:D:605:ASP:O	1:D:607:PRO:HD3	2.08	0.54
1:D:92:VAL:HG22	1:D:142:MET:HB3	1.89	0.54
1:A:514:VAL:HG11	1:A:694:SER:HA	1.91	0.53
1:D:541:ILE:HD11	1:D:662:PHE:HB3	1.90	0.53
1:A:515:ASP:HA	1:A:525:TRP:HE1	1.73	0.52
1:A:122:ARG:HD3	1:A:576:GLN:O	2.09	0.52
1:D:568:LEU:HD23	1:D:571:ILE:HD12	1.91	0.51
1:B:506:ASN:HB3	1:B:509:ASN:HB2	1.91	0.51
1:A:307:GLU:HB2	1:A:558:ARG:HB2	1.92	0.50
1:C:86:ILE:HG12	1:C:242:LEU:HD22	1.93	0.50
1:B:169:ASP:HB3	1:B:173:GLY:H	1.77	0.50
1:D:598:LEU:HD21	1:D:646:LEU:HD11	1.92	0.50
1:B:304:ASN:HB2	1:B:562:ARG:HG3	1.94	0.49
1:C:246:LEU:H	1:C:247:PRO:CD	2.26	0.49
1:A:672:PRO:HA	1:A:680:ILE:HA	1.94	0.49
1:C:164:GLY:H	1:C:194:ASN:HB3	1.77	0.49
1:D:632:GLY:HA2	1:D:695:ARG:HH22	1.76	0.49
1:C:145:PHE:HA	1:C:148:ILE:HD12	1.94	0.49
1:C:185:ILE:HD12	1:C:188:TYR:HD2	1.78	0.49
1:B:565:LYS:HA	1:B:568:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:GLN:OE1	1:C:672:PRO:HD2	2.14	0.48
1:A:565:LYS:HA	1:A:568:LEU:HD12	1.96	0.48
1:C:597:SER:HB3	1:C:689:LEU:HD11	1.95	0.47
1:B:633:SER:O	1:B:640:HIS:CE1	2.67	0.47
1:C:544:GLU:O	1:C:548:GLU:HG2	2.14	0.47
1:B:630:SER:HA	1:B:643:GLU:HG3	1.96	0.47
1:C:246:LEU:H	1:C:247:PRO:HD2	1.80	0.47
1:C:246:LEU:N	1:C:247:PRO:HD2	2.30	0.46
1:A:86:ILE:HG12	1:A:242:LEU:HD22	1.97	0.46
1:C:565:LYS:HA	1:C:568:LEU:HD12	1.97	0.46
1:B:92:VAL:HB	1:B:95:LEU:HD12	1.98	0.46
1:C:582:TYR:CZ	1:C:620:VAL:HG21	2.51	0.46
1:A:146:LEU:HD23	1:A:149:LEU:HD12	1.98	0.46
1:D:529:LEU:HD22	1:D:531:ILE:HG13	1.98	0.46
1:A:145:PHE:HA	1:A:148:ILE:HD12	1.98	0.46
1:B:529:LEU:HD22	1:B:531:ILE:HG13	1.99	0.45
1:C:86:ILE:HD13	1:C:135:LEU:HG	1.97	0.45
1:A:362:GLU:H	1:A:516:GLU:HA	1.80	0.45
1:C:529:LEU:HD22	1:C:531:ILE:HG13	1.97	0.45
1:A:97:PRO:HA	1:A:100:ILE:HD12	1.98	0.45
1:A:103:LYS:HB3	1:A:229:LEU:HB3	1.98	0.45
1:D:252:TRP:HA	1:D:663:THR:HG21	1.99	0.45
1:A:183:GLN:HB3	1:A:668:ILE:HD11	1.98	0.44
1:D:90:PRO:HG2	1:D:95:LEU:CD1	2.47	0.44
1:A:86:ILE:HD13	1:A:135:LEU:HG	1.98	0.44
1:A:124:PHE:HE2	1:A:139:ILE:HD12	1.82	0.44
1:A:162:LEU:HD12	1:A:226:VAL:HG11	2.00	0.44
1:B:292:LEU:HD23	1:B:300:ASP:HB3	2.00	0.44
1:C:608:VAL:HB	1:C:646:LEU:HB3	1.99	0.44
1:C:722:PHE:C	1:C:753:GLY:H	2.21	0.44
1:D:378:GLY:HA2	1:D:509:ASN:HB3	2.00	0.44
1:C:664:GLN:HB2	1:C:688:PHE:O	2.18	0.43
1:C:723:ARG:HB3	1:C:725:GLU:HG3	1.99	0.43
1:A:598:LEU:HD21	1:A:646:LEU:HD11	1.99	0.43
1:C:101:LEU:HD13	1:C:137:ILE:HG21	1.99	0.43
1:A:529:LEU:HD22	1:A:531:ILE:HG13	2.01	0.43
1:A:292:LEU:HD23	1:A:300:ASP:HB3	1.99	0.43
1:B:633:SER:O	1:B:640:HIS:HE1	2.01	0.43
1:A:278:ILE:HD13	1:A:561:ILE:HD12	2.01	0.43
1:A:191:VAL:HA	1:A:227:TYR:O	2.18	0.42
1:A:582:TYR:CE1	1:A:620:VAL:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:LYS:O	1:D:253:ARG:HD2	2.19	0.42
1:D:278:ILE:HD13	1:D:561:ILE:HD12	2.01	0.42
1:C:185:ILE:HD12	1:C:188:TYR:CD2	2.53	0.42
1:B:124:PHE:HE2	1:B:139:ILE:HD12	1.84	0.42
1:C:278:ILE:HD13	1:C:561:ILE:HD12	2.01	0.42
1:A:86:ILE:HG13	1:A:157:PHE:HB2	2.02	0.41
1:C:150:ASP:HA	1:C:153:LYS:HD2	2.01	0.41
1:C:295:ILE:HB	1:C:298:PHE:HB2	2.02	0.41
1:B:670:PHE:HB2	1:B:680:ILE:HG23	2.03	0.41
1:C:246:LEU:N	1:C:247:PRO:CD	2.83	0.41
1:A:534:TYR:HE2	1:A:664:GLN:HE21	1.70	0.40
1:B:582:TYR:CZ	1:B:620:VAL:HG21	2.55	0.40
1:A:173:GLY:HA2	1:A:176:ILE:HD12	2.02	0.40
1:C:182:LEU:O	1:C:666:PRO:HB2	2.22	0.40
1:C:253:ARG:HB3	1:C:253:ARG:HE	1.73	0.40
1:C:292:LEU:HD23	1:C:300:ASP:HB3	2.02	0.40
1:D:153:LYS:HB3	1:D:183:GLN:HE21	1.86	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	583/704 (83%)	550 (94%)	32 (6%)	1 (0%)	47 79
1	B	555/704 (79%)	522 (94%)	31 (6%)	2 (0%)	34 71
1	C	549/704 (78%)	507 (92%)	38 (7%)	4 (1%)	22 61
1	D	493/704 (70%)	462 (94%)	30 (6%)	1 (0%)	47 79
All	All	2180/2816 (77%)	2041 (94%)	131 (6%)	8 (0%)	34 71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	375	ASP
1	C	602	GLU
1	C	753	GLY
1	A	81	GLY
1	B	352	GLU
1	C	246	LEU
1	D	683	ILE
1	C	620	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	449/630 (71%)	397 (88%)	52 (12%)	5 29
1	B	348/630 (55%)	319 (92%)	29 (8%)	11 42
1	C	363/630 (58%)	329 (91%)	34 (9%)	8 38
1	D	264/630 (42%)	237 (90%)	27 (10%)	7 34
All	All	1424/2520 (56%)	1282 (90%)	142 (10%)	7 35

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LEU
1	A	113	ILE
1	A	115	VAL
1	A	124	PHE
1	A	135	LEU
1	A	154	VAL
1	A	171	GLU
1	A	175	GLN
1	A	189	ILE
1	A	191	VAL
1	A	199	HIS
1	A	206	LEU
1	A	207	ASP
1	A	225	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	228	ASN
1	A	230	GLU
1	A	234	ASP
1	A	244	GLN
1	A	245	ARG
1	A	285	ILE
1	A	292	LEU
1	A	293	VAL
1	A	340	ASN
1	A	341	MET
1	A	344	ASP
1	A	345	THR
1	A	346	LEU
1	A	355	GLU
1	A	361	ASP
1	A	371	THR
1	A	507	LEU
1	A	508	TYR
1	A	512	TRP
1	A	529	LEU
1	A	564	PRO
1	A	598	LEU
1	A	600	ARG
1	A	608	VAL
1	A	625	ILE
1	A	641	LYS
1	A	646	LEU
1	A	663	THR
1	A	675	THR
1	A	692	ASP
1	A	696	ILE
1	A	716	THR
1	A	720	MET
1	A	751	THR
1	A	763	LEU
1	A	772	SER
1	A	775	LYS
1	A	777	MET
1	B	94	ASP
1	B	104	LEU
1	B	124	PHE
1	B	188	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	206	LEU
1	B	234	ASP
1	B	285	ILE
1	B	292	LEU
1	B	293	VAL
1	B	335	THR
1	B	345	THR
1	B	346	LEU
1	B	355	GLU
1	B	371	THR
1	B	502	ARG
1	B	529	LEU
1	B	598	LEU
1	B	604	TYR
1	B	610	SER
1	B	621	ARG
1	B	625	ILE
1	B	646	LEU
1	B	663	THR
1	B	678	LYS
1	B	687	THR
1	B	690	ASN
1	B	720	MET
1	B	771	MET
1	B	775	LYS
1	C	102	TYR
1	C	121	LYS
1	C	135	LEU
1	C	153	LYS
1	C	154	VAL
1	C	177	ILE
1	C	234	ASP
1	C	253	ARG
1	C	283	ARG
1	C	292	LEU
1	C	293	VAL
1	C	297	ASP
1	C	345	THR
1	C	346	LEU
1	C	359	ASP
1	C	371	THR
1	C	486	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	507	LEU
1	C	529	LEU
1	C	564	PRO
1	C	598	LEU
1	C	624	THR
1	C	641	LYS
1	C	663	THR
1	C	687	THR
1	C	716	THR
1	C	725	GLU
1	C	742	SER
1	C	752	HIS
1	C	763	LEU
1	C	771	MET
1	C	772	SER
1	C	775	LYS
1	C	777	MET
1	D	145	PHE
1	D	154	VAL
1	D	158	VAL
1	D	206	LEU
1	D	234	ASP
1	D	285	ILE
1	D	292	LEU
1	D	293	VAL
1	D	345	THR
1	D	346	LEU
1	D	356	ASP
1	D	361	ASP
1	D	364	PHE
1	D	502	ARG
1	D	507	LEU
1	D	509	ASN
1	D	529	LEU
1	D	598	LEU
1	D	601	TRP
1	D	637	ASN
1	D	643	GLU
1	D	687	THR
1	D	692	ASP
1	D	704	THR
1	D	745	ILE

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Mol	Chain	Res	Type
1	D	771	MET
1	D	776	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	ASN
1	A	228	ASN
1	A	617	GLN
1	A	647	HIS
1	B	294	HIS
1	B	302	GLN
1	B	377	HIS
1	B	572	GLN
1	B	640	HIS
1	B	690	ASN
1	C	255	ASN
1	C	377	HIS
1	C	587	HIS
1	D	183	GLN
1	D	617	GLN
1	D	637	ASN

### 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 [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	595/704 (84%)	-0.02	5 (0%) 86 75	8, 43, 112, 216	0
1	B	569/704 (80%)	0.13	24 (4%) 36 23	15, 96, 191, 294	0
1	C	567/704 (80%)	0.12	23 (4%) 37 24	18, 89, 193, 291	0
1	D	517/704 (73%)	0.18	24 (4%) 32 20	29, 114, 263, 298	0
All	All	2248/2816 (79%)	0.10	76 (3%) 45 30	8, 85, 191, 298	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	190	GLY	8.7
1	D	192	ILE	6.2
1	D	191	VAL	5.6
1	D	189	ILE	5.0
1	C	191	VAL	4.6
1	D	281	THR	4.4
1	B	161	GLY	4.1
1	D	194	ASN	4.1
1	C	190	GLY	4.0
1	D	707	PRO	4.0
1	B	302	GLN	4.0
1	A	275	ASP	3.8
1	C	163	SER	3.8
1	B	571	ILE	3.7
1	B	194	ASN	3.6
1	B	77	GLU	3.5
1	A	763	LEU	3.4
1	C	194	ASN	3.4
1	B	198	VAL	3.4
1	C	306	ILE	3.3
1	B	70	ILE	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	193	SER	3.2
1	C	192	ILE	3.2
1	D	703	LEU	3.1
1	C	161	GLY	3.1
1	D	188	TYR	3.1
1	C	337	PHE	3.1
1	C	215	TYR	2.9
1	B	190	GLY	2.8
1	C	120	SER	2.8
1	B	568	LEU	2.7
1	B	106	LYS	2.7
1	C	550	GLN	2.7
1	A	117	GLU	2.7
1	B	579	PHE	2.7
1	D	764	SER	2.6
1	C	164	GLY	2.6
1	C	555	ASP	2.6
1	D	123	ILE	2.6
1	D	287	PHE	2.5
1	C	104	LEU	2.5
1	B	163	SER	2.5
1	B	164	GLY	2.5
1	C	310	SER	2.5
1	B	565	LYS	2.4
1	C	90	PRO	2.4
1	D	769	VAL	2.4
1	D	589	HIS	2.4
1	D	303	LEU	2.4
1	C	72	ASN	2.4
1	B	298	PHE	2.4
1	A	757	ALA	2.4
1	B	212	LEU	2.3
1	C	336	VAL	2.3
1	C	227	TYR	2.3
1	B	160	PHE	2.3
1	D	771	MET	2.3
1	D	671	LYS	2.2
1	B	158	VAL	2.2
1	D	736	PHE	2.2
1	C	367	ASP	2.2
1	C	730	PHE	2.1
1	B	193	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	112	GLY	2.1
1	B	113	ILE	2.1
1	B	107	CYS	2.1
1	D	578	LEU	2.1
1	B	133	SER	2.1
1	A	358	SER	2.0
1	D	716	THR	2.0
1	D	153	LYS	2.0
1	B	358	SER	2.0
1	D	259	VAL	2.0
1	C	495	ILE	2.0
1	D	205	GLN	2.0
1	C	73	ARG	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 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.