



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:46 AM EDT

PDB ID : 5IW7 / pdb_00005iw7
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

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

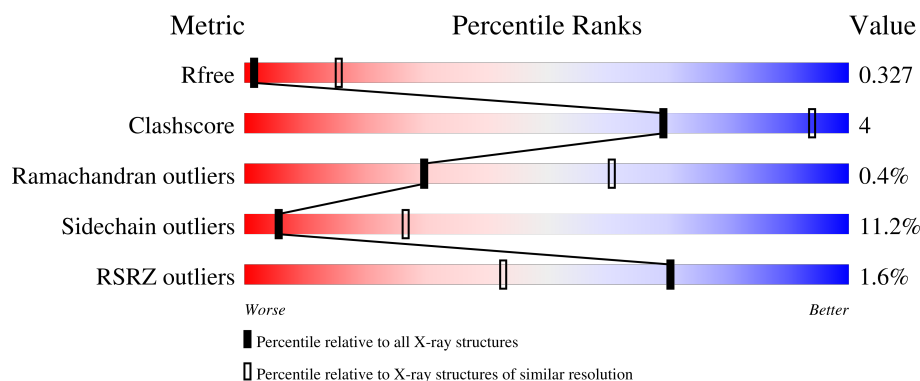
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (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 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	704	
1	B	704	
1	C	704	
1	D	704	

2 Entry composition

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

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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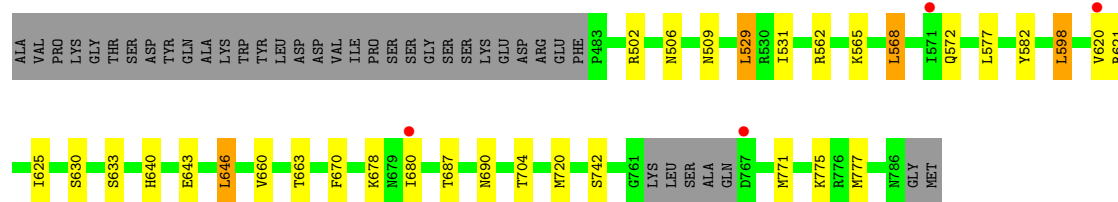
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Chain	Residue	Modelled	Actual	Comment	Reference
C	30	HIS	-	expression tag	UNP Q07381
C	31	HIS	-	expression tag	UNP Q07381
C	32	SER	-	expression tag	UNP Q07381
C	33	ALA	-	expression tag	UNP Q07381
C	34	GLY	-	expression tag	UNP Q07381
C	35	LEU	-	expression 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

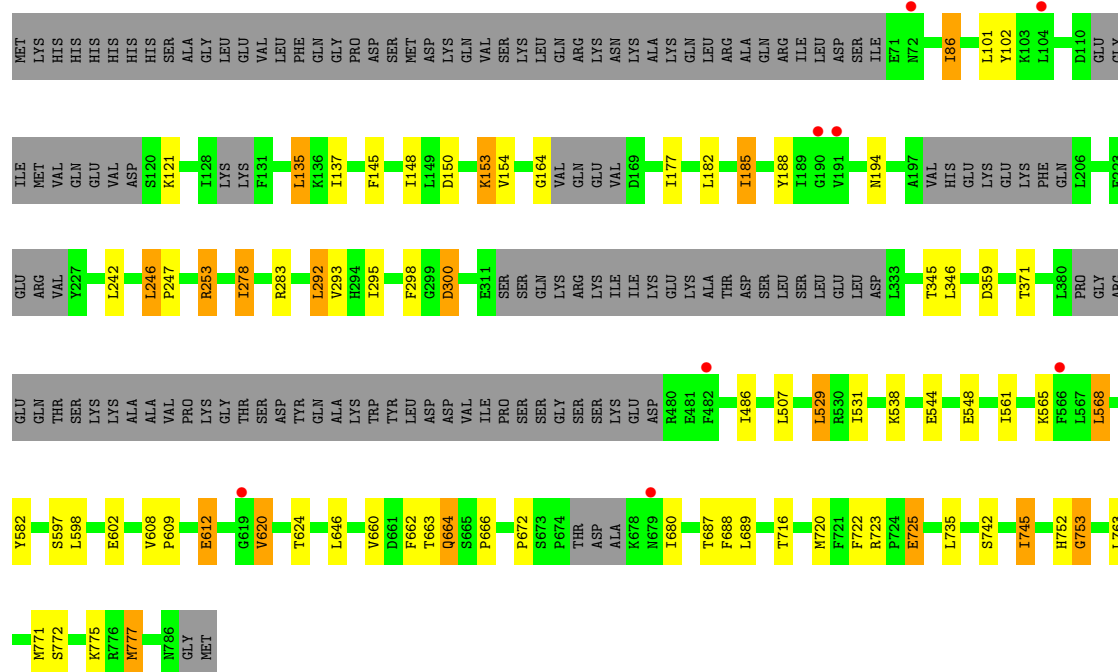
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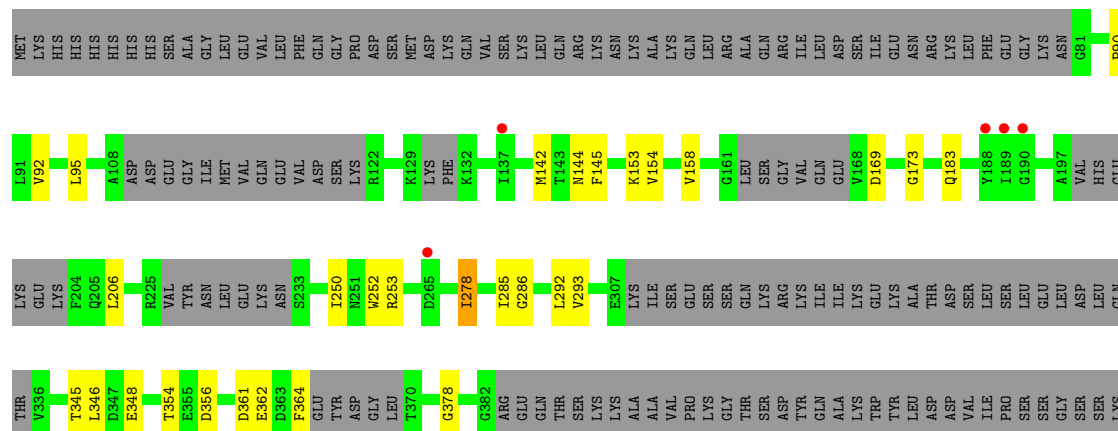
Chain	Residue	Modelled	Actual	Comment	Reference
D	44	SER	-	expression tag	UNP Q07381
D	45	MET	-	expression tag	UNP Q07381
D	471	PRO	-	linker	UNP Q07381
D	472	SER	-	linker	UNP Q07381
D	473	SER	-	linker	UNP Q07381
D	474	GLY	-	linker	UNP Q07381
D	475	SER	-	linker	UNP Q07381
D	476	SER	-	linker	UNP Q07381

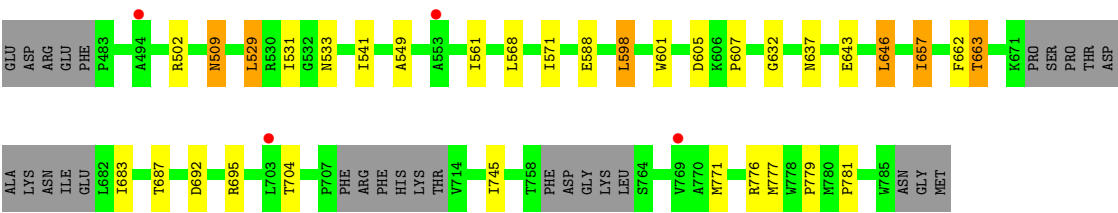


- Molecule 1: Ribosome biogenesis protein TSR1, Ribosome biogenesis protein TSR1



- 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, α , β , γ	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) 99.8 (48.77-3.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.57Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.268 , 0.295 0.293 , 0.327	Depositor DCC
R_{free} test set	2228 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	123.0	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 131.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	16065	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage'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.*

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

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	0.69	0/4639	1.21	7/6324 (0.1%)
1	B	0.69	0/4105	1.20	8/5625 (0.1%)
1	C	0.72	0/4193	1.21	4/5740 (0.1%)
1	D	0.71	0/3494	1.23	6/4811 (0.1%)
All	All	0.70	0/16431	1.21	25/22500 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	92	VAL	CA-C-N	6.07	128.70	120.38
1	A	92	VAL	C-N-CA	6.07	128.70	120.38
1	A	361	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	657	ILE	N-CA-CB	5.82	118.99	111.83
1	C	612	GLU	CB-CG-CD	5.70	122.29	112.60
1	B	152	ALA	CA-C-N	5.46	127.54	120.44
1	B	152	ALA	C-N-CA	5.46	127.54	120.44
1	D	533	ASN	CA-CB-CG	5.43	118.03	112.60
1	B	374	TYR	CA-C-N	5.43	131.91	121.54
1	B	374	TYR	C-N-CA	5.43	131.91	121.54
1	C	664	GLN	CA-C-N	5.42	127.93	120.39
1	C	664	GLN	C-N-CA	5.42	127.93	120.39
1	D	354	THR	CA-C-N	5.33	128.81	120.82
1	D	354	THR	C-N-CA	5.33	128.81	120.82
1	B	300	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	300	ASP	CA-CB-CG	5.28	117.88	112.60
1	D	144	ASN	CA-C-N	5.26	127.28	120.44
1	D	144	ASN	C-N-CA	5.26	127.28	120.44
1	A	692	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	300	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	92	VAL	CA-C-N	5.10	127.06	120.44
1	B	92	VAL	C-N-CA	5.10	127.06	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	515	ASP	CA-CB-CG	5.01	117.61	112.60

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	34	0
1	B	4015	0	3368	19	0
1	C	4093	0	3483	33	0
1	D	3426	0	2669	19	0
All	All	16065	0	13680	104	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 4.

All (104) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:92:VAL:HG22	1:D:142:MET:HB3	1.89	0.54
1:D:605:ASP:O	1:D:607:PRO:HD3	2.08	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
1:C:722:PHE:C	1:C:753:GLY:H	2.21	0.48
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:775:LYS:HE3	1:C:777:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:375:ASP:CG	1:B:377:HIS:HD2	2.26	0.43
1:A:720:MET:HE1	1:A:735:LEU:HD22	2.01	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
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:A:764:SER:C	1:A:766:GLN:H	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE	1:C:253:ARG:HB3	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

5.3.1 Protein backbone

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%)	43	72
1	B	555/704 (79%)	522 (94%)	31 (6%)	2 (0%)	30	61
1	C	549/704 (78%)	507 (92%)	38 (7%)	4 (1%)	18	51
1	D	493/704 (70%)	462 (94%)	30 (6%)	1 (0%)	43	72
All	All	2180/2816 (77%)	2041 (94%)	131 (6%)	8 (0%)	30	61

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

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Mol	Chain	Res	Type
1	C	620	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	449/630 (71%)	392 (87%)	57 (13%)	4	22
1	B	348/630 (55%)	314 (90%)	34 (10%)	7	31
1	C	363/630 (58%)	327 (90%)	36 (10%)	7	31
1	D	264/630 (42%)	232 (88%)	32 (12%)	5	23
All	All	1424/2520 (56%)	1265 (89%)	159 (11%)	6	27

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ILE
1	A	104	LEU
1	A	113	ILE
1	A	115	VAL
1	A	128	ILE
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	230	GLU
1	A	244	GLN
1	A	245	ARG
1	A	259	VAL
1	A	278	ILE
1	A	285	ILE

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Mol	Chain	Res	Type
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	348	GLU
1	A	355	GLU
1	A	356	ASP
1	A	361	ASP
1	A	371	THR
1	A	507	LEU
1	A	508	TYR
1	A	516	GLU
1	A	529	LEU
1	A	557	ILE
1	A	568	LEU
1	A	598	LEU
1	A	600	ARG
1	A	608	VAL
1	A	625	ILE
1	A	646	LEU
1	A	660	VAL
1	A	663	THR
1	A	668	ILE
1	A	675	THR
1	A	692	ASP
1	A	696	ILE
1	A	704	THR
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	86	ILE
1	B	94	ASP
1	B	104	LEU
1	B	128	ILE
1	B	206	LEU

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Mol	Chain	Res	Type
1	B	224	GLU
1	B	259	VAL
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	348	GLU
1	B	355	GLU
1	B	371	THR
1	B	502	ARG
1	B	529	LEU
1	B	568	LEU
1	B	598	LEU
1	B	621	ARG
1	B	625	ILE
1	B	646	LEU
1	B	660	VAL
1	B	663	THR
1	B	678	LYS
1	B	687	THR
1	B	690	ASN
1	B	704	THR
1	B	720	MET
1	B	742	SER
1	B	771	MET
1	B	775	LYS
1	B	777	MET
1	C	86	ILE
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	185	ILE
1	C	253	ARG
1	C	278	ILE
1	C	283	ARG
1	C	292	LEU
1	C	293	VAL

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Mol	Chain	Res	Type
1	C	345	THR
1	C	346	LEU
1	C	359	ASP
1	C	371	THR
1	C	486	ILE
1	C	507	LEU
1	C	529	LEU
1	C	568	LEU
1	C	598	LEU
1	C	624	THR
1	C	660	VAL
1	C	663	THR
1	C	687	THR
1	C	716	THR
1	C	720	MET
1	C	725	GLU
1	C	742	SER
1	C	745	ILE
1	C	752	HIS
1	C	763	LEU
1	C	771	MET
1	C	772	SER
1	C	777	MET
1	D	145	PHE
1	D	154	VAL
1	D	158	VAL
1	D	206	LEU
1	D	278	ILE
1	D	285	ILE
1	D	292	LEU
1	D	293	VAL
1	D	345	THR
1	D	346	LEU
1	D	348	GLU
1	D	356	ASP
1	D	361	ASP
1	D	362	GLU
1	D	364	PHE
1	D	502	ARG
1	D	509	ASN
1	D	529	LEU
1	D	588	GLU

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Mol	Chain	Res	Type
1	D	598	LEU
1	D	601	TRP
1	D	637	ASN
1	D	643	GLU
1	D	646	LEU
1	D	663	THR
1	D	687	THR
1	D	692	ASP
1	D	704	THR
1	D	745	ILE
1	D	771	MET
1	D	776	ARG
1	D	777	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	166	GLN
1	A	183	GLN
1	A	194	ASN
1	A	288	ASN
1	A	340	ASN
1	A	533	ASN
1	A	599	GLN
1	A	647	HIS
1	A	706	HIS
1	B	144	ASN
1	B	166	GLN
1	B	228	ASN
1	B	302	GLN
1	B	377	HIS
1	B	536	ASN
1	B	539	ASN
1	B	690	ASN
1	C	144	ASN
1	C	228	ASN
1	C	255	ASN
1	C	288	ASN
1	C	302	GLN
1	C	377	HIS
1	C	533	ASN

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Mol	Chain	Res	Type
1	C	587	HIS
1	C	690	ASN
1	C	706	HIS
1	C	786	ASN
1	D	144	ASN
1	D	183	GLN
1	D	288	ASN
1	D	294	HIS
1	D	539	ASN
1	D	591	ASN
1	D	617	GLN
1	D	637	ASN
1	D	690	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 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	595/704 (84%)	-0.14	4 (0%) 84 61	8, 43, 112, 216	0
1	B	569/704 (80%)	0.15	15 (2%) 57 33	14, 96, 191, 294	0
1	C	567/704 (80%)	0.15	8 (1%) 73 46	18, 89, 192, 291	0
1	D	517/704 (73%)	0.26	9 (1%) 69 41	29, 114, 263, 298	0
All	All	2248/2816 (79%)	0.10	36 (1%) 70 43	8, 85, 191, 298	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	190	GLY	5.2
1	B	161	GLY	4.3
1	D	703	LEU	4.1
1	D	189	ILE	3.8
1	A	117	GLU	3.6
1	C	104	LEU	3.2
1	B	190	GLY	3.0
1	B	158	VAL	3.0
1	D	494	ALA	3.0
1	B	767	ASP	2.7
1	C	190	GLY	2.6
1	D	188	TYR	2.6
1	D	137	ILE	2.5
1	C	679	ASN	2.5
1	B	83	ALA	2.5
1	B	571	ILE	2.5
1	B	160	PHE	2.4
1	A	765	ALA	2.4
1	B	309	ILE	2.4
1	B	345	THR	2.3
1	B	298	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	363	ASP	2.2
1	B	374	TYR	2.2
1	C	619	GLY	2.2
1	D	265	ASP	2.1
1	C	72	ASN	2.1
1	B	620	VAL	2.1
1	B	680	ILE	2.1
1	D	769	VAL	2.1
1	C	566	PHE	2.1
1	A	761	GLY	2.1
1	B	302	GLN	2.0
1	C	191	VAL	2.0
1	D	553	ALA	2.0
1	A	111	GLU	2.0
1	C	482	PHE	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.