



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:03 PM UTC

PDB ID : 2RBL / pdb_00002rbl
Title : High resolution design of a protein loop
Authors : Hu, X.; Wang, H.; Ke, H.; Kuhlman, B.
Deposited on : 2007-09-19
Resolution : 2.10 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

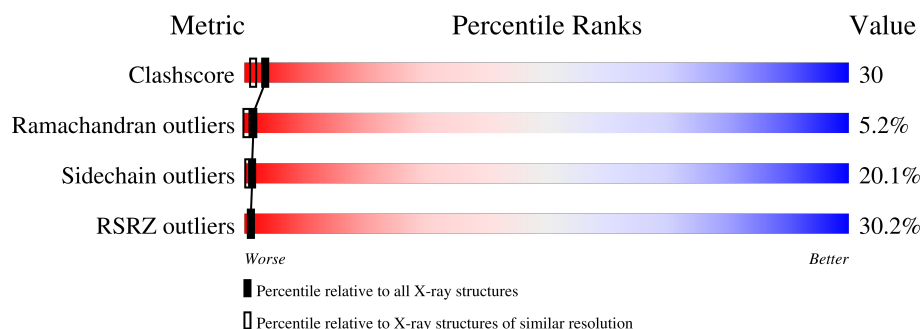
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

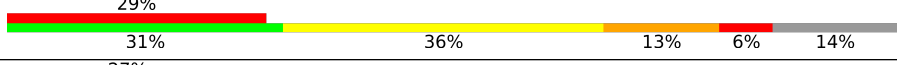
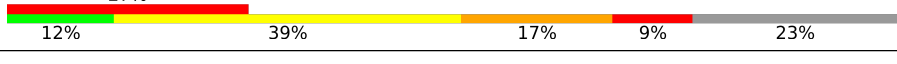
The reported resolution of this entry is 2.10 Å.

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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	104	
1	B	104	
1	M	104	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2009 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 Tenascin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	89	Total	C	N	O	S	0	0	0
			693	428	110	153	2			
1	B	89	Total	C	N	O	S	0	0	0
			693	428	110	153	2			
1	M	80	Total	C	N	O	S	0	0	0
			623	386	99	137	1			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	801	MET	-	initiating methionine	UNP P24821
A	824	SER	PHE	engineered mutation	UNP P24821
A	825	MET	LYS	engineered mutation	UNP P24821
A	826	GLN	PRO	engineered mutation	UNP P24821
A	828	SER	ALA	engineered mutation	UNP P24821
A	829	GLN	GLU	engineered mutation	UNP P24821
A	830	LEU	ILE	engineered mutation	UNP P24821
A	831	GLU	ASP	engineered mutation	UNP P24821
A	894	ALA	-	expression tag	UNP P24821
A	895	ALA	-	expression tag	UNP P24821
A	896	ALA	-	expression tag	UNP P24821
A	897	LEU	-	expression tag	UNP P24821
A	898	GLU	-	expression tag	UNP P24821
A	899	HIS	-	expression tag	UNP P24821
A	900	HIS	-	expression tag	UNP P24821
A	901	HIS	-	expression tag	UNP P24821
A	902	HIS	-	expression tag	UNP P24821
A	903	HIS	-	expression tag	UNP P24821
A	904	HIS	-	expression tag	UNP P24821
B	801	MET	-	initiating methionine	UNP P24821
B	824	SER	PHE	engineered mutation	UNP P24821
B	825	MET	LYS	engineered mutation	UNP P24821
B	826	GLN	PRO	engineered mutation	UNP P24821

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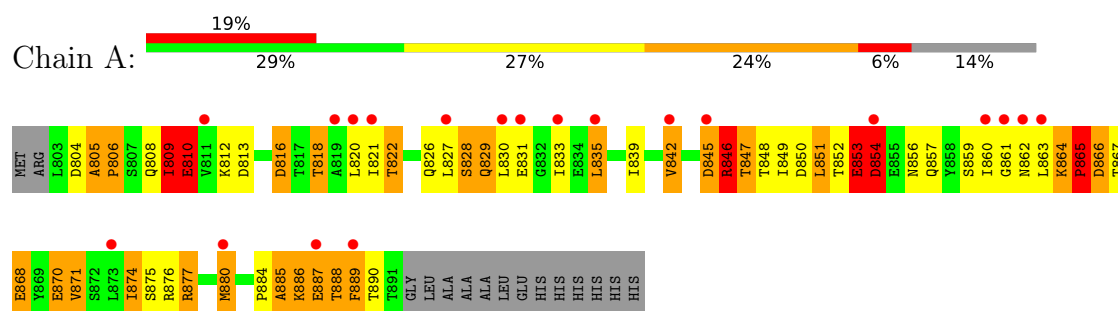
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Chain	Residue	Modelled	Actual	Comment	Reference
B	828	SER	ALA	engineered mutation	UNP P24821
B	829	GLN	GLU	engineered mutation	UNP P24821
B	830	LEU	ILE	engineered mutation	UNP P24821
B	831	GLU	ASP	engineered mutation	UNP P24821
B	894	ALA	-	expression tag	UNP P24821
B	895	ALA	-	expression tag	UNP P24821
B	896	ALA	-	expression tag	UNP P24821
B	897	LEU	-	expression tag	UNP P24821
B	898	GLU	-	expression tag	UNP P24821
B	899	HIS	-	expression tag	UNP P24821
B	900	HIS	-	expression tag	UNP P24821
B	901	HIS	-	expression tag	UNP P24821
B	902	HIS	-	expression tag	UNP P24821
B	903	HIS	-	expression tag	UNP P24821
B	904	HIS	-	expression tag	UNP P24821
M	801	MET	-	initiating methionine	UNP P24821
M	824	SER	PHE	engineered mutation	UNP P24821
M	825	MET	LYS	engineered mutation	UNP P24821
M	826	GLN	PRO	engineered mutation	UNP P24821
M	828	SER	ALA	engineered mutation	UNP P24821
M	829	GLN	GLU	engineered mutation	UNP P24821
M	830	LEU	ILE	engineered mutation	UNP P24821
M	831	GLU	ASP	engineered mutation	UNP P24821
M	894	ALA	-	expression tag	UNP P24821
M	895	ALA	-	expression tag	UNP P24821
M	896	ALA	-	expression tag	UNP P24821
M	897	LEU	-	expression tag	UNP P24821
M	898	GLU	-	expression tag	UNP P24821
M	899	HIS	-	expression tag	UNP P24821
M	900	HIS	-	expression tag	UNP P24821
M	901	HIS	-	expression tag	UNP P24821
M	902	HIS	-	expression tag	UNP P24821
M	903	HIS	-	expression tag	UNP P24821
M	904	HIS	-	expression tag	UNP P24821

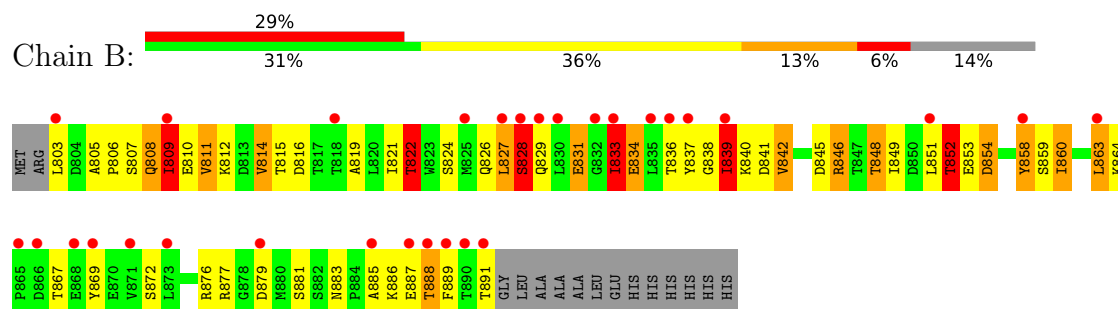
3 Residue-property plots [i](#)

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.

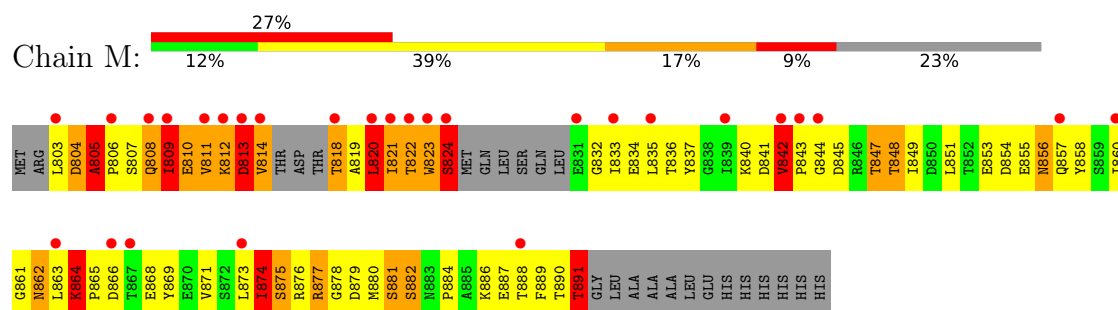
• Molecule 1: Tenascin



• Molecule 1: Tenascin



• Molecule 1: Tenascin



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	137.20Å 137.20Å 86.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 85.8 (50.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.250 , 0.300 0.307 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for $-1/3^*h+1/3^*k+4/3^*l,-k,2/3^*h+1/3^*k+1/3^*l$ 0.024 for $-2/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+4/3^*l,-1/3^*h+1/3^*k+1/3^*l$ 0.017 for $-h,1/3^*h-1/3^*k-4/3^*l,-1/3^*h-2/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2009	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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	2.36	33/702 (4.7%)	2.01	21/955 (2.2%)
1	B	2.38	28/702 (4.0%)	2.04	31/955 (3.2%)
1	M	2.44	25/630 (4.0%)	1.83	20/854 (2.3%)
All	All	2.39	86/2034 (4.2%)	1.97	72/2764 (2.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	M	0	1
All	All	0	3

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	813	ASP	CG-OD2	22.08	1.67	1.25
1	M	813	ASP	CG-OD1	16.35	1.56	1.25
1	B	839	ILE	C-O	-12.32	1.11	1.24
1	M	856	ASN	CG-OD1	12.32	1.47	1.23
1	A	874	ILE	N-CA	9.28	1.56	1.46
1	M	810	GLU	CD-OE1	8.83	1.42	1.25
1	M	810	GLU	CD-OE2	8.82	1.42	1.25
1	B	841	ASP	C-O	8.76	1.35	1.24
1	B	860	ILE	N-CA	-8.72	1.35	1.46
1	M	823	TRP	C-O	8.60	1.32	1.24
1	B	858	TYR	C-O	-8.57	1.13	1.23
1	A	870	GLU	C-O	8.36	1.34	1.23
1	A	857	GLN	CA-C	-8.31	1.42	1.52
1	M	832	GLY	N-CA	7.70	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	886	LYS	CA-C	7.59	1.62	1.52
1	B	808	GLN	C-O	7.53	1.33	1.24
1	A	833	ILE	CA-C	-7.30	1.43	1.52
1	A	889	PHE	N-CA	-7.11	1.37	1.46
1	M	847	THR	C-O	7.01	1.31	1.24
1	B	841	ASP	N-CA	6.83	1.55	1.46
1	A	818	THR	CA-CB	6.68	1.68	1.54
1	B	822	THR	N-CA	-6.66	1.37	1.46
1	M	877	ARG	CA-C	-6.59	1.45	1.52
1	B	859	SER	N-CA	-6.57	1.38	1.46
1	M	874	ILE	C-O	-6.51	1.16	1.23
1	A	875	SER	C-O	6.47	1.31	1.23
1	M	842	VAL	CA-C	6.40	1.59	1.53
1	A	816	ASP	C-O	-6.39	1.15	1.24
1	A	821	ILE	CA-C	-6.34	1.44	1.52
1	A	887	GLU	CA-CB	-6.31	1.41	1.53
1	B	863	LEU	C-O	-6.30	1.15	1.23
1	M	824	SER	CB-OG	6.30	1.54	1.42
1	B	876	ARG	N-CA	6.28	1.54	1.46
1	B	805	ALA	CA-CB	6.28	1.62	1.53
1	M	876	ARG	CA-C	6.18	1.60	1.52
1	A	820	LEU	C-O	6.17	1.31	1.24
1	B	840	LYS	C-O	6.12	1.31	1.24
1	A	820	LEU	CA-CB	-6.05	1.45	1.53
1	A	851	LEU	N-CA	-6.04	1.38	1.45
1	A	890	THR	C-O	-5.98	1.17	1.24
1	M	851	LEU	N-CA	-5.94	1.39	1.45
1	B	888	THR	CA-C	5.87	1.59	1.52
1	A	852	THR	CA-CB	5.85	1.62	1.53
1	M	845	ASP	C-O	5.76	1.30	1.23
1	A	865	PRO	C-O	5.73	1.31	1.24
1	A	846	ARG	N-CA	5.72	1.53	1.46
1	M	847	THR	N-CA	-5.70	1.39	1.46
1	A	877	ARG	CA-C	-5.70	1.46	1.53
1	M	880	MET	C-O	-5.68	1.16	1.23
1	M	805	ALA	CA-C	5.62	1.59	1.52
1	B	860	ILE	CG1-CD1	5.61	1.73	1.51
1	A	810	GLU	C-O	5.60	1.30	1.23
1	B	842	VAL	C-O	-5.57	1.17	1.24
1	M	804	ASP	N-CA	5.53	1.52	1.46
1	A	822	THR	N-CA	-5.51	1.39	1.46
1	B	837	TYR	C-O	5.51	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	820	LEU	C-O	5.50	1.30	1.23
1	B	886	LYS	N-CA	5.49	1.52	1.46
1	A	805	ALA	CA-C	5.48	1.60	1.53
1	B	809	ILE	N-CA	5.47	1.53	1.46
1	A	829	GLN	CA-C	-5.45	1.45	1.52
1	A	809	ILE	CA-CB	5.42	1.61	1.54
1	A	849	ILE	C-O	-5.40	1.18	1.24
1	A	871	VAL	CA-C	-5.39	1.46	1.52
1	B	806	PRO	N-CA	-5.38	1.40	1.47
1	B	809	ILE	C-O	-5.36	1.17	1.24
1	A	842	VAL	CA-CB	5.29	1.61	1.54
1	M	877	ARG	C-O	-5.28	1.17	1.24
1	M	871	VAL	CA-CB	-5.28	1.48	1.54
1	B	872	SER	N-CA	5.27	1.52	1.45
1	B	891	THR	C-O	5.23	1.34	1.23
1	M	855	GLU	CD-OE2	5.22	1.35	1.25
1	A	813	ASP	CA-C	-5.22	1.46	1.53
1	A	845	ASP	N-CA	5.17	1.52	1.46
1	B	839	ILE	N-CA	5.17	1.52	1.46
1	B	879	ASP	CA-CB	5.16	1.60	1.53
1	A	866	ASP	C-O	5.16	1.30	1.24
1	A	850	ASP	C-O	-5.16	1.17	1.24
1	A	848	THR	CA-C	-5.12	1.46	1.52
1	M	890	THR	CA-CB	5.11	1.62	1.53
1	M	866	ASP	CG-OD1	5.06	1.34	1.25
1	A	847	THR	CA-C	-5.06	1.46	1.52
1	B	810	GLU	N-CA	-5.05	1.40	1.46
1	A	888	THR	C-O	-5.04	1.17	1.23
1	B	889	PHE	CB-CG	5.04	1.62	1.50
1	B	845	ASP	C-O	5.01	1.30	1.23

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	842	VAL	N-CA-C	10.70	119.44	108.95
1	M	844	GLY	N-CA-C	10.04	126.62	113.27
1	A	885	ALA	N-CA-C	-9.16	95.02	109.50
1	A	864	LYS	CA-C-N	8.65	130.65	119.84
1	A	864	LYS	C-N-CA	8.65	130.65	119.84
1	M	853	GLU	N-CA-C	8.24	128.34	110.80
1	B	841	ASP	N-CA-C	8.02	122.65	113.02
1	B	834	GLU	CB-CG-CD	-7.98	99.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	853	GLU	N-CA-C	-7.88	103.55	113.01
1	B	854	ASP	N-CA-C	7.88	122.16	112.23
1	M	848	THR	CB-CA-C	-6.76	97.21	109.38
1	B	824	SER	N-CA-C	6.67	119.95	110.14
1	A	865	PRO	N-CA-C	6.62	126.10	112.47
1	B	814	VAL	CB-CA-C	-6.59	104.82	111.80
1	M	877	ARG	CB-CA-C	-6.56	101.05	110.62
1	B	833	ILE	N-CA-C	6.49	117.46	107.99
1	A	809	ILE	N-CA-C	-6.33	96.16	109.34
1	B	811	VAL	N-CA-C	-6.33	99.28	108.71
1	B	859	SER	N-CA-CB	-6.33	99.96	110.47
1	M	834	GLU	CB-CA-C	6.24	120.42	110.19
1	M	845	ASP	CA-C-N	-6.19	111.81	123.27
1	M	845	ASP	C-N-CA	-6.19	111.81	123.27
1	B	869	TYR	N-CA-C	-6.13	99.81	109.50
1	B	876	ARG	NE-CZ-NH1	-6.10	115.40	121.50
1	B	889	PHE	N-CA-C	-6.08	99.90	108.96
1	B	883	ASN	CA-C-N	-6.01	114.08	120.03
1	B	883	ASN	C-N-CA	-6.01	114.08	120.03
1	B	879	ASP	N-CA-C	5.99	119.89	112.59
1	B	812	LYS	N-CA-C	-5.99	100.20	109.24
1	M	821	ILE	N-CA-C	5.93	116.48	108.17
1	A	826	GLN	CA-C-N	5.91	128.51	120.54
1	A	826	GLN	C-N-CA	5.91	128.51	120.54
1	B	833	ILE	CA-C-N	-5.91	114.37	122.93
1	B	833	ILE	C-N-CA	-5.91	114.37	122.93
1	A	854	ASP	CB-CA-C	5.88	120.84	110.85
1	B	867	THR	CA-C-N	-5.87	113.41	122.09
1	B	867	THR	C-N-CA	-5.87	113.41	122.09
1	A	877	ARG	CA-C-N	-5.85	113.81	120.42
1	A	877	ARG	C-N-CA	-5.85	113.81	120.42
1	M	858	TYR	N-CA-C	5.75	118.84	109.06
1	M	849	ILE	N-CA-C	-5.75	99.78	108.17
1	B	852	THR	CB-CA-C	-5.72	100.22	109.72
1	B	842	VAL	CB-CA-C	-5.71	100.97	111.36
1	M	866	ASP	N-CA-C	5.65	119.35	111.90
1	M	891	THR	CA-C-O	5.52	130.19	120.80
1	A	821	ILE	CB-CA-C	-5.52	103.20	110.98
1	B	846	ARG	N-CA-C	5.47	117.31	108.34
1	M	874	ILE	CA-C-N	5.43	130.13	122.09
1	M	874	ILE	C-N-CA	5.43	130.13	122.09
1	A	886	LYS	CG-CD-CE	-5.38	98.93	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	812	LYS	N-CA-C	-5.35	101.22	109.52
1	M	878	GLY	N-CA-C	-5.34	101.03	110.86
1	M	855	GLU	N-CA-C	-5.34	100.20	108.90
1	B	836	THR	OG1-CB-CG2	-5.31	98.69	109.30
1	B	839	ILE	CA-C-O	-5.29	115.09	121.28
1	M	882	SER	N-CA-C	-5.29	101.50	109.85
1	B	887	GLU	N-CA-C	-5.28	101.38	109.41
1	A	870	GLU	N-CA-CB	-5.28	101.76	111.37
1	A	884	PRO	CA-C-O	-5.22	115.64	122.12
1	B	876	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	804	ASP	CA-C-N	-5.22	113.11	121.57
1	A	804	ASP	C-N-CA	-5.22	113.11	121.57
1	A	859	SER	N-CA-CB	-5.21	101.78	110.80
1	B	814	VAL	N-CA-C	5.19	114.74	107.37
1	B	864	LYS	N-CA-C	-5.14	103.29	109.72
1	M	875	SER	N-CA-CB	-5.13	101.92	110.23
1	B	848	THR	CA-C-N	5.10	129.52	123.19
1	B	848	THR	C-N-CA	5.10	129.52	123.19
1	M	813	ASP	OD1-CG-OD2	5.10	135.13	122.90
1	A	806	PRO	CA-C-N	-5.05	114.33	122.82
1	A	806	PRO	C-N-CA	-5.05	114.33	122.82
1	B	891	THR	CA-C-O	5.04	129.38	120.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	885	ALA	Peptide
1	B	858	TYR	Mainchain
1	M	856	ASN	Sidechain

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	693	0	671	44	0
1	B	693	0	671	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	623	0	599	55	0
All	All	2009	0	1941	119	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 30.

All (119) 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:M:813:ASP:CG	1:M:813:ASP:OD2	1.67	1.38
1:B:829:GLN:HG3	1:B:877:ARG:NH2	1.55	1.22
1:A:831:GLU:HB3	1:B:829:GLN:NE2	1.56	1.20
1:B:829:GLN:CG	1:B:877:ARG:HH21	1.58	1.15
1:A:831:GLU:HB3	1:B:829:GLN:HE21	0.93	1.07
1:A:808:GLN:O	1:A:809:ILE:HB	1.61	1.00
1:M:814:VAL:O	1:M:891:THR:HG22	1.69	0.93
1:A:831:GLU:CB	1:B:829:GLN:HE21	1.81	0.93
1:M:874:ILE:HG22	1:M:882:SER:O	1.80	0.81
1:M:835:LEU:O	1:M:848:THR:HA	1.80	0.80
1:B:829:GLN:HG3	1:B:877:ARG:HH21	0.70	0.77
1:M:814:VAL:O	1:M:891:THR:CG2	2.34	0.75
1:M:842:VAL:HG12	1:M:843:PRO:HD2	1.71	0.73
1:M:806:PRO:HG2	1:M:873:LEU:HB3	1.71	0.71
1:A:808:GLN:O	1:A:809:ILE:CB	2.34	0.71
1:M:809:ILE:HG22	1:M:887:GLU:OE1	1.91	0.70
1:M:835:LEU:HD13	1:M:873:LEU:HD11	1.73	0.68
1:M:811:VAL:HG13	1:M:821:ILE:HD13	1.74	0.68
1:B:808:GLN:O	1:B:809:ILE:HB	1.94	0.68
1:M:835:LEU:HD12	1:M:873:LEU:HD12	1.75	0.66
1:M:835:LEU:CD1	1:M:873:LEU:CD1	2.73	0.66
1:A:809:ILE:HD13	1:B:885:ALA:HB1	1.78	0.66
1:B:829:GLN:CG	1:B:877:ARG:NH2	2.35	0.66
1:M:818:THR:HA	1:M:863:LEU:HB2	1.75	0.66
1:B:811:VAL:HG12	1:B:814:VAL:HG22	1.79	0.65
1:A:831:GLU:CD	1:B:829:GLN:HG2	2.22	0.65
1:M:863:LEU:HD22	1:M:869:TYR:CZ	2.33	0.64
1:M:811:VAL:HG13	1:M:821:ILE:CD1	2.28	0.64
1:M:836:THR:HA	1:M:847:THR:O	1.98	0.64
1:M:809:ILE:HA	1:M:822:THR:O	1.98	0.63
1:B:860:ILE:CG2	1:B:863:LEU:HD21	2.28	0.62
1:M:808:GLN:O	1:M:809:ILE:HG13	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:ARG:O	1:A:880:MET:HG2	2.00	0.62
1:A:809:ILE:HA	1:A:822:THR:O	2.00	0.62
1:A:846:ARG:HB2	1:M:881:SER:HB2	1.82	0.61
1:M:835:LEU:CD1	1:M:873:LEU:HD12	2.31	0.61
1:M:863:LEU:CD1	1:M:889:PHE:HZ	2.14	0.60
1:M:840:LYS:HG2	1:M:868:GLU:OE1	2.01	0.60
1:A:839:ILE:HG12	1:A:867:THR:HG21	1.83	0.60
1:B:860:ILE:HG22	1:B:863:LEU:HD21	1.83	0.60
1:A:835:LEU:HD21	1:B:821:ILE:HD13	1.84	0.59
1:M:821:ILE:HG12	1:M:860:ILE:HD12	1.84	0.59
1:A:831:GLU:HA	1:A:876:ARG:O	2.03	0.58
1:A:854:ASP:HB3	1:B:852:THR:HG21	1.85	0.58
1:A:839:ILE:HG21	1:A:842:VAL:HG21	1.86	0.57
1:M:835:LEU:CD1	1:M:873:LEU:HD11	2.34	0.57
1:A:829:GLN:O	1:B:853:GLU:OE2	2.23	0.57
1:M:811:VAL:HG22	1:M:821:ILE:CD1	2.35	0.57
1:A:854:ASP:CB	1:B:852:THR:HG21	2.35	0.56
1:M:809:ILE:HG22	1:M:809:ILE:O	2.06	0.56
1:A:810:GLU:HG3	1:A:822:THR:OG1	2.07	0.55
1:A:860:ILE:HD12	1:A:863:LEU:HD21	1.89	0.55
1:B:829:GLN:CB	1:B:877:ARG:NH2	2.68	0.55
1:A:845:ASP:O	1:M:881:SER:O	2.25	0.55
1:A:831:GLU:CD	1:B:831:GLU:HB3	2.32	0.54
1:A:871:VAL:O	1:A:886:LYS:HA	2.06	0.54
1:A:805:ALA:HB1	1:A:806:PRO:HD2	1.90	0.54
1:B:834:GLU:CG	1:B:848:THR:HG23	2.37	0.54
1:M:863:LEU:HD11	1:M:889:PHE:HZ	1.72	0.54
1:M:861:GLY:O	1:M:862:ASN:C	2.51	0.54
1:M:865:PRO:HA	1:M:891:THR:HB	1.90	0.53
1:B:827:LEU:O	1:B:828:SER:C	2.51	0.52
1:A:846:ARG:HB2	1:M:881:SER:CB	2.39	0.52
1:M:835:LEU:HD13	1:M:873:LEU:CD1	2.35	0.52
1:M:818:THR:O	1:M:819:ALA:HB2	2.10	0.51
1:A:839:ILE:HG21	1:A:842:VAL:CG2	2.41	0.51
1:B:834:GLU:HG3	1:B:848:THR:HG23	1.93	0.51
1:B:839:ILE:O	1:B:846:ARG:NH1	2.44	0.50
1:M:821:ILE:C	1:M:822:THR:CG2	2.85	0.49
1:A:868:GLU:OE2	1:A:888:THR:HG23	2.13	0.48
1:M:869:TYR:O	1:M:888:THR:HA	2.11	0.48
1:A:818:THR:HA	1:B:860:ILE:O	2.12	0.48
1:A:830:LEU:HA	1:B:853:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:813:ASP:N	1:M:813:ASP:OD1	2.46	0.48
1:M:840:LYS:HB3	1:M:868:GLU:HB3	1.96	0.48
1:A:816:ASP:OD1	1:A:816:ASP:N	2.47	0.48
1:A:839:ILE:HG22	1:A:842:VAL:HB	1.95	0.48
1:B:838:GLY:O	1:B:839:ILE:C	2.57	0.47
1:M:884:PRO:HB2	1:M:886:LYS:HE3	1.96	0.47
1:M:812:LYS:HE3	1:M:812:LYS:HB2	1.53	0.47
1:M:814:VAL:HB	1:M:891:THR:O	2.15	0.47
1:B:834:GLU:HG3	1:B:848:THR:CG2	2.45	0.47
1:M:842:VAL:CG1	1:M:843:PRO:HD2	2.42	0.46
1:B:833:ILE:HD12	1:B:853:GLU:HA	1.98	0.46
1:A:809:ILE:CD1	1:B:885:ALA:HB1	2.45	0.46
1:M:804:ASP:O	1:M:805:ALA:HB3	2.16	0.46
1:A:830:LEU:O	1:A:877:ARG:HA	2.16	0.46
1:A:866:ASP:CG	1:A:866:ASP:O	2.59	0.46
1:A:865:PRO:HA	1:B:816:ASP:O	2.15	0.45
1:B:815:THR:OG1	1:B:816:ASP:N	2.48	0.45
1:M:808:GLN:O	1:M:809:ILE:CG1	2.63	0.45
1:A:861:GLY:O	1:A:862:ASN:HB2	2.16	0.45
1:A:831:GLU:OE2	1:B:829:GLN:HG2	2.17	0.45
1:A:864:LYS:HA	1:A:865:PRO:HD3	1.78	0.45
1:A:868:GLU:OE2	1:A:888:THR:CG2	2.65	0.44
1:M:837:TYR:CE2	1:M:847:THR:HG21	2.52	0.44
1:B:854:ASP:C	1:B:854:ASP:OD2	2.60	0.44
1:A:888:THR:HG22	1:A:889:PHE:N	2.33	0.44
1:M:810:GLU:HG3	1:M:812:LYS:HE2	2.00	0.44
1:M:811:VAL:HA	1:M:820:LEU:O	2.18	0.44
1:M:808:GLN:O	1:M:809:ILE:CB	2.66	0.43
1:A:839:ILE:CG2	1:A:842:VAL:CG2	2.97	0.43
1:M:814:VAL:HA	1:M:818:THR:O	2.18	0.43
1:B:809:ILE:HA	1:B:822:THR:O	2.19	0.42
1:B:849:ILE:HG23	1:B:849:ILE:HD12	1.80	0.42
1:M:863:LEU:CD1	1:M:889:PHE:CZ	3.00	0.42
1:A:831:GLU:O	1:A:853:GLU:HG2	2.21	0.41
1:A:877:ARG:HD3	1:A:880:MET:HE2	2.01	0.41
1:M:809:ILE:HG22	1:M:887:GLU:CD	2.46	0.41
1:A:831:GLU:OE1	1:B:829:GLN:O	2.38	0.41
1:A:847:THR:HA	1:M:879:ASP:O	2.20	0.41
1:B:829:GLN:HB2	1:B:877:ARG:NH2	2.35	0.41
1:M:863:LEU:HD22	1:M:869:TYR:CE2	2.56	0.41
1:M:875:SER:HB3	1:M:882:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:807:SER:O	1:B:808:GLN:HB2	2.21	0.40
1:M:863:LEU:O	1:M:864:LYS:C	2.64	0.40
1:B:811:VAL:HG12	1:B:814:VAL:CG2	2.47	0.40
1:B:809:ILE:HG21	1:B:809:ILE:HD13	1.90	0.40
1:M:823:TRP:CD1	1:M:824:SER:N	2.90	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	87/104 (84%)	77 (88%)	6 (7%)	4 (5%)	2	0
1	B	87/104 (84%)	77 (88%)	6 (7%)	4 (5%)	2	0
1	M	74/104 (71%)	59 (80%)	10 (14%)	5 (7%)	1	0
All	All	248/312 (80%)	213 (86%)	22 (9%)	13 (5%)	1	0

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	809	ILE
1	A	828	SER
1	A	846	ARG
1	M	808	GLN
1	M	809	ILE
1	B	809	ILE
1	B	819	ALA
1	M	807	SER
1	B	828	SER
1	M	805	ALA
1	B	842	VAL
1	A	865	PRO

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Mol	Chain	Res	Type
1	M	864	LYS

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	81/92 (88%)	67 (83%)	14 (17%)	2	1
1	B	81/92 (88%)	69 (85%)	12 (15%)	3	1
1	M	72/92 (78%)	51 (71%)	21 (29%)	0	0
All	All	234/276 (85%)	187 (80%)	47 (20%)	1	0

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	810	GLU
1	A	827	LEU
1	A	828	SER
1	A	835	LEU
1	A	846	ARG
1	A	851	LEU
1	A	853	GLU
1	A	854	ASP
1	A	856	ASN
1	A	868	GLU
1	A	870	GLU
1	A	874	ILE
1	A	880	MET
1	A	887	GLU
1	B	803	LEU
1	B	822	THR
1	B	826	GLN
1	B	827	LEU
1	B	828	SER
1	B	831	GLU
1	B	833	ILE

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Mol	Chain	Res	Type
1	B	839	ILE
1	B	851	LEU
1	B	852	THR
1	B	881	SER
1	B	888	THR
1	M	803	LEU
1	M	809	ILE
1	M	811	VAL
1	M	812	LYS
1	M	813	ASP
1	M	814	VAL
1	M	818	THR
1	M	820	LEU
1	M	822	THR
1	M	824	SER
1	M	833	ILE
1	M	841	ASP
1	M	842	VAL
1	M	854	ASP
1	M	857	GLN
1	M	862	ASN
1	M	864	LYS
1	M	874	ILE
1	M	877	ARG
1	M	881	SER
1	M	891	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	829	GLN
1	A	856	ASN
1	B	826	GLN
1	B	829	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 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	89/104 (85%)	1.45	20 (22%)	2 2	40, 54, 70, 74	0
1	B	89/104 (85%)	1.77	30 (33%)	1 1	45, 55, 69, 77	0
1	M	80/104 (76%)	1.82	28 (35%)	1 1	42, 53, 62, 69	0
All	All	258/312 (82%)	1.68	78 (30%)	1 1	40, 54, 69, 77	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	803	LEU	7.1
1	B	818	THR	4.5
1	M	803	LEU	4.4
1	M	814	VAL	4.2
1	B	827	LEU	3.9
1	M	821	ILE	3.8
1	B	891	THR	3.8
1	B	809	ILE	3.7
1	B	828	SER	3.7
1	B	839	ILE	3.7
1	A	845	ASP	3.7
1	B	832	GLY	3.6
1	M	822	THR	3.5
1	A	862	ASN	3.5
1	M	818	THR	3.5
1	A	827	LEU	3.4
1	B	829	GLN	3.4
1	M	844	GLY	3.4
1	M	860	ILE	3.3
1	B	873	LEU	3.3
1	M	863	LEU	3.3
1	A	861	GLY	3.3
1	M	842	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	833	ILE	3.2
1	M	824	SER	3.2
1	B	830	LEU	3.1
1	B	889	PHE	3.1
1	M	820	LEU	3.0
1	M	811	VAL	2.9
1	A	889	PHE	2.9
1	M	833	ILE	2.9
1	B	869	TYR	2.9
1	B	868	GLU	2.8
1	A	833	ILE	2.8
1	B	871	VAL	2.7
1	B	851	LEU	2.7
1	A	863	LEU	2.6
1	B	836	THR	2.6
1	B	885	ALA	2.6
1	M	806	PRO	2.6
1	M	866	ASP	2.5
1	M	809	ILE	2.5
1	A	854	ASP	2.5
1	M	867	THR	2.5
1	M	831	GLU	2.4
1	A	835	LEU	2.4
1	B	866	ASP	2.4
1	A	880	MET	2.4
1	A	811	VAL	2.4
1	M	839	ILE	2.4
1	M	812	LYS	2.4
1	M	843	PRO	2.3
1	B	835	LEU	2.3
1	M	857	GLN	2.3
1	B	879	ASP	2.3
1	A	820	LEU	2.3
1	B	863	LEU	2.2
1	M	808	GLN	2.2
1	A	819	ALA	2.2
1	A	831	GLU	2.2
1	M	873	LEU	2.2
1	A	821	ILE	2.1
1	M	835	LEU	2.1
1	B	837	TYR	2.1
1	A	830	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	825	MET	2.1
1	B	887	GLU	2.1
1	M	813	ASP	2.1
1	B	865	PRO	2.1
1	A	860	ILE	2.1
1	A	873	LEU	2.1
1	A	887	GLU	2.1
1	B	858	TYR	2.1
1	B	890	THR	2.1
1	M	823	TRP	2.1
1	A	842	VAL	2.0
1	B	888	THR	2.0
1	M	888	THR	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.