Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 08:58 AM EDT

PDB ID	:	2RBL
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 (i) 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 (1)) were used in the production of this report:

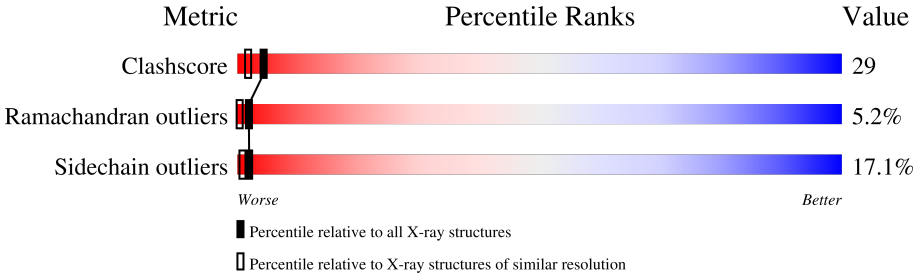
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	104	36% 34% 12% 5% 14%
1	B	104	40% 31% 12% • 14%
1	M	104	20% 34% 20% • 23%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	89	693	428	110	153	2	0	0	0
1	B	89	693	428	110	153	2	0	0	0
1	M	80	623	386	99	137	1	0	0	0

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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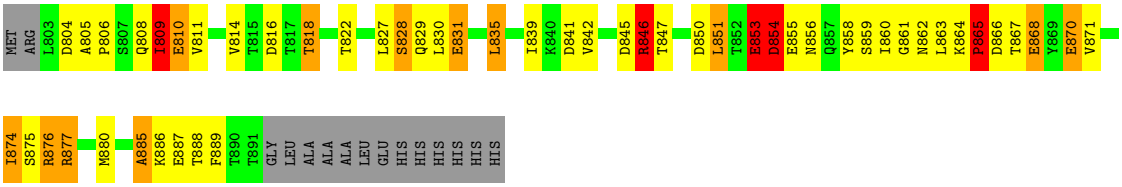
Chain	Residue	Modelled	Actual	Comment	Reference
B	828	SER	ALA	engineered mutation	UNP P24821
B	829	GLN	GLU	engineered mutation	UNP P24821
B	830	LEU	ILE	engineered mutation	UNP P24821
B	831	GLU	ASP	engineered mutation	UNP P24821
B	894	ALA	-	expression tag	UNP P24821
B	895	ALA	-	expression tag	UNP P24821
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. 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. 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.

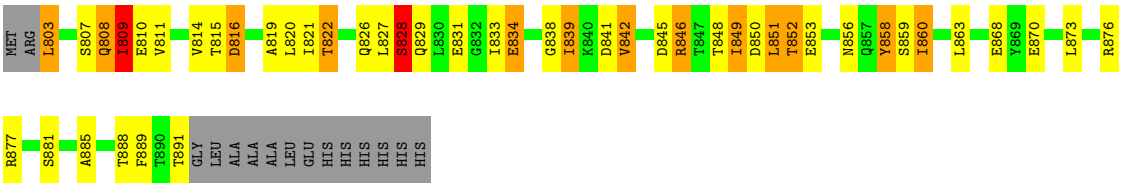
• Molecule 1: Tenascin

Chain A: 36% 34% 12% 5% 14%



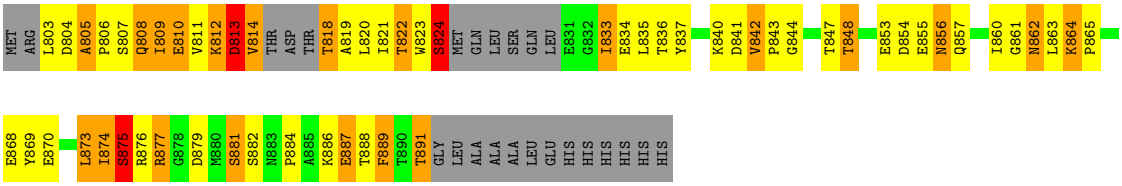
• Molecule 1: Tenascin

Chain B: 40% 31% 12% • 14%



• Molecule 1: Tenascin

Chain M: 20% 34% 20% • 23%



4 Data and refinement statistics (i)

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 49.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 85.7 (49.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	1.93	18/702 (2.6%)	1.78	19/955 (2.0%)
1	B	1.88	12/702 (1.7%)	1.78	18/955 (1.9%)
1	M	2.15	12/630 (1.9%)	1.51	13/854 (1.5%)
All	All	1.99	42/2034 (2.1%)	1.70	50/2764 (1.8%)

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 (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	813	ASP	CG-OD2	18.24	1.67	1.25
1	M	810	GLU	CD-OE1	14.98	1.42	1.25
1	M	810	GLU	CD-OE2	14.96	1.42	1.25
1	M	813	ASP	CG-OD1	13.50	1.56	1.25
1	M	856	ASN	CG-OD1	10.46	1.47	1.24
1	M	824	SER	CB-OG	9.62	1.54	1.42
1	M	855	GLU	CD-OE2	8.74	1.35	1.25
1	A	858	TYR	CE1-CZ	-8.21	1.27	1.38
1	A	855	GLU	CD-OE2	7.88	1.34	1.25
1	M	855	GLU	CD-OE1	7.71	1.34	1.25
1	B	810	GLU	CG-CD	-7.07	1.41	1.51
1	B	868	GLU	CG-CD	-6.80	1.41	1.51
1	A	858	TYR	CB-CG	6.76	1.61	1.51
1	M	810	GLU	CG-CD	6.54	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	831	GLU	CD-OE2	6.53	1.32	1.25
1	B	841	ASP	C-O	6.47	1.35	1.23
1	B	889	PHE	CB-CG	6.41	1.62	1.51
1	A	810	GLU	CD-OE2	6.39	1.32	1.25
1	A	858	TYR	CE2-CZ	6.34	1.46	1.38
1	A	858	TYR	CD2-CE2	6.29	1.48	1.39
1	B	839	ILE	C-O	-6.12	1.11	1.23
1	A	853	GLU	CD-OE2	5.99	1.32	1.25
1	M	870	GLU	CD-OE2	5.94	1.32	1.25
1	A	854	ASP	CB-CG	5.93	1.64	1.51
1	A	870	GLU	C-O	5.81	1.34	1.23
1	B	846	ARG	CG-CD	5.80	1.66	1.51
1	M	855	GLU	CG-CD	5.78	1.60	1.51
1	M	887	GLU	CD-OE1	5.66	1.31	1.25
1	A	858	TYR	CD1-CE1	5.62	1.47	1.39
1	B	891	THR	C-O	5.61	1.34	1.23
1	A	818	THR	CA-CB	5.61	1.68	1.53
1	A	810	GLU	CD-OE1	5.54	1.31	1.25
1	A	887	GLU	CA-CB	-5.49	1.41	1.53
1	B	860	ILE	N-CA	-5.43	1.35	1.46
1	B	870	GLU	CB-CG	-5.41	1.41	1.52
1	B	808	GLN	C-O	5.32	1.33	1.23
1	A	876	ARG	CG-CD	-5.27	1.38	1.51
1	B	858	TYR	C-O	-5.24	1.13	1.23
1	B	810	GLU	CB-CG	5.23	1.62	1.52
1	A	874	ILE	N-CA	5.22	1.56	1.46
1	A	855	GLU	CG-CD	5.09	1.59	1.51
1	A	875	SER	CB-OG	-5.01	1.35	1.42

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	877	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	B	876	ARG	NE-CZ-NH1	-9.80	115.40	120.30
1	A	854	ASP	CB-CG-OD1	9.09	126.48	118.30
1	M	876	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	B	816	ASP	CB-CG-OD1	-8.32	110.81	118.30
1	M	813	ASP	CB-CG-OD1	-8.07	111.03	118.30
1	B	845	ASP	CB-CG-OD2	8.00	125.50	118.30
1	A	858	TYR	CB-CG-CD2	7.98	125.79	121.00
1	B	850	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	B	876	ARG	NE-CZ-NH2	7.20	123.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	859	SER	N-CA-CB	-7.03	99.96	110.50
1	A	846	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	M	833	ILE	CG1-CB-CG2	-6.71	96.64	111.40
1	A	876	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	877	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	809	ILE	CG1-CB-CG2	-6.46	97.18	111.40
1	M	853	GLU	N-CA-C	6.42	128.34	111.00
1	B	816	ASP	CB-CG-OD2	6.34	124.01	118.30
1	B	820	LEU	CB-CG-CD2	6.33	121.77	111.00
1	B	851	LEU	CA-CB-CG	6.25	129.67	115.30
1	M	813	ASP	OD1-CG-OD2	6.23	135.13	123.30
1	A	846	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	803	LEU	CB-CG-CD2	6.20	121.54	111.00
1	B	870	GLU	OE1-CD-OE2	6.13	130.66	123.30
1	B	849	ILE	CG1-CB-CG2	-5.95	98.32	111.40
1	A	885	ALA	N-CA-C	-5.92	95.02	111.00
1	B	809	ILE	CG1-CB-CG2	-5.82	98.60	111.40
1	A	859	SER	N-CA-CB	-5.81	101.78	110.50
1	M	834	GLU	OE1-CD-OE2	-5.75	116.39	123.30
1	M	875	SER	N-CA-CB	-5.72	101.92	110.50
1	M	873	LEU	CB-CG-CD2	-5.66	101.39	111.00
1	B	834	GLU	CB-CG-CD	-5.62	99.03	114.20
1	M	877	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	804	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	873	LEU	CB-CG-CD2	-5.56	101.54	111.00
1	A	809	ILE	N-CA-C	-5.50	96.16	111.00
1	B	842	VAL	CB-CA-C	-5.49	100.97	111.40
1	M	844	GLY	N-CA-C	5.41	126.62	113.10
1	A	865	PRO	N-CA-C	5.38	126.10	112.10
1	M	848	THR	CB-CA-C	-5.33	97.21	111.60
1	A	814	VAL	CG1-CB-CG2	-5.28	102.45	110.90
1	B	841	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	846	ARG	CD-NE-CZ	5.24	130.93	123.60
1	A	854	ASP	CB-CA-C	5.22	120.84	110.40
1	M	876	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	850	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	841	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	851	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	A	811	VAL	CA-CB-CG1	-5.01	103.38	110.90
1	M	834	GLU	CB-CA-C	5.01	120.42	110.40

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 (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	693	0	671	43	0
1	B	693	0	671	39	0
1	M	623	0	599	53	0
All	All	2009	0	1941	115	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 29.

All (115) 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	1.33
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:831:GLU:CD	1:B:829:GLN:HG2	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:863:LEU:HD11	1:M:889:PHE:HZ	1.72	0.54
1:M:865:PRO:HA	1:M:891:THR:HB	1.90	0.53
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:A:831:GLU:CD	1:B:831:GLU:HB3	2.32	0.50
1:M:861:GLY:O	1:M:862:ASN:C	2.51	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
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:827:LEU:O	1:B:828:SER:C	2.51	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: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:M:821:ILE:C	1:M:822:THR:CG2	2.85	0.44
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ILE:CG2	1:A:842:VAL:CG2	2.97	0.43
1:B:838:GLY:O	1:B:839:ILE:C	2.57	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:866:ASP:CG	1:A:866:ASP:O	2.59	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
1:B:807:SER:O	1:B:808:GLN:HB2	2.21	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%)	2 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
1	M	864	LYS

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	81/92 (88%)	70 (86%)	11 (14%)	3 2
1	B	81/92 (88%)	72 (89%)	9 (11%)	6 3
1	M	72/92 (78%)	52 (72%)	20 (28%)	0 0
All	All	234/276 (85%)	194 (83%)	40 (17%)	2 1

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
1	A	874	ILE
1	B	803	LEU
1	B	822	THR
1	B	826	GLN
1	B	828	SER
1	B	851	LEU
1	B	852	THR
1	B	856	ASN
1	B	881	SER
1	B	888	THR
1	M	803	LEU
1	M	812	LYS
1	M	813	ASP
1	M	814	VAL
1	M	818	THR
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	875	SER
1	M	877	ARG
1	M	881	SER
1	M	889	PHE
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	856	ASN
1	B	826	GLN
1	B	829	GLN
1	M	857	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.