Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:40 am BST

PDB ID	:	4XI0
Title	:	MamA 41-end from Desulfovibrio magneticus RS-1
Authors	:	Zarivach, R.; Zeytuni, N.; Cronin, S.; Davidov, G.; Baran, D.; Stein, T.
Deposited on	:	2015-01-06
Resolution	:	2.88 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 following versions of software and data (see references ①) were used in the production of this report:

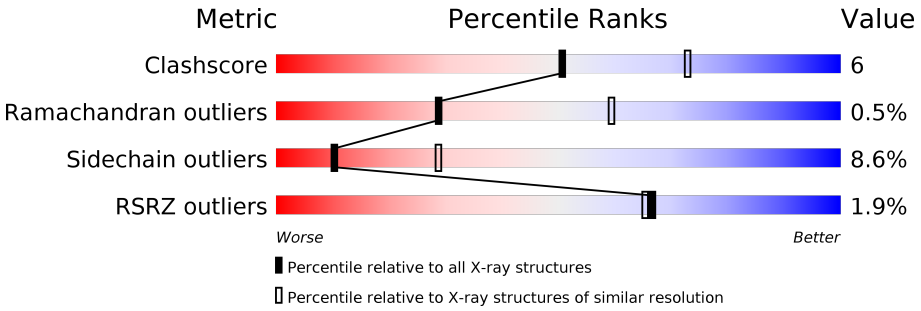
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 >=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% 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	202	68% 18% • 12%
1	B	202	67% 19% 13%
1	C	202	67% 15% • 13%
1	D	202	71% 13% • 13%
1	E	202	72% 14% • 12%
1	F	202	3% 71% 15% • 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8530 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 Magnetosome protein MamA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1426	904	255	260	7			
1	B	175	Total	C	N	O	S	0	0	0
			1412	897	253	255	7			
1	C	175	Total	C	N	O	S	0	0	0
			1412	897	253	255	7			
1	D	176	Total	C	N	O	S	0	0	0
			1420	901	254	258	7			
1	E	177	Total	C	N	O	S	0	0	0
			1426	904	255	260	7			
1	F	178	Total	C	N	O	S	0	0	0
			1434	908	256	263	7			

There are 174 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	initiating methionine	UNP C4XPQ7
A	38	ALA	-	expression tag	UNP C4XPQ7
A	39	MET	-	expression tag	UNP C4XPQ7
A	40	GLY	-	expression tag	UNP C4XPQ7
A	124	ILE	MET	engineered mutation	UNP C4XPQ7
A	140	ALA	GLU	engineered mutation	UNP C4XPQ7
A	141	ALA	LYS	engineered mutation	UNP C4XPQ7
A	143	ALA	GLU	engineered mutation	UNP C4XPQ7
A	218	GLU	-	expression tag	UNP C4XPQ7
A	219	LEU	-	expression tag	UNP C4XPQ7
A	220	ALA	-	expression tag	UNP C4XPQ7
A	221	LEU	-	expression tag	UNP C4XPQ7
A	222	VAL	-	expression tag	UNP C4XPQ7
A	223	PRO	-	expression tag	UNP C4XPQ7
A	224	ARG	-	expression tag	UNP C4XPQ7
A	225	GLY	-	expression tag	UNP C4XPQ7
A	226	SER	-	expression tag	UNP C4XPQ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	SER	-	expression tag	UNP C4XPQ7
A	228	ALA	-	expression tag	UNP C4XPQ7
A	229	HIS	-	expression tag	UNP C4XPQ7
A	230	HIS	-	expression tag	UNP C4XPQ7
A	231	HIS	-	expression tag	UNP C4XPQ7
A	232	HIS	-	expression tag	UNP C4XPQ7
A	233	HIS	-	expression tag	UNP C4XPQ7
A	234	HIS	-	expression tag	UNP C4XPQ7
A	235	HIS	-	expression tag	UNP C4XPQ7
A	236	HIS	-	expression tag	UNP C4XPQ7
A	237	HIS	-	expression tag	UNP C4XPQ7
A	238	HIS	-	expression tag	UNP C4XPQ7
B	37	MET	-	initiating methionine	UNP C4XPQ7
B	38	ALA	-	expression tag	UNP C4XPQ7
B	39	MET	-	expression tag	UNP C4XPQ7
B	40	GLY	-	expression tag	UNP C4XPQ7
B	124	ILE	MET	engineered mutation	UNP C4XPQ7
B	140	ALA	GLU	engineered mutation	UNP C4XPQ7
B	141	ALA	LYS	engineered mutation	UNP C4XPQ7
B	143	ALA	GLU	engineered mutation	UNP C4XPQ7
B	218	GLU	-	expression tag	UNP C4XPQ7
B	219	LEU	-	expression tag	UNP C4XPQ7
B	220	ALA	-	expression tag	UNP C4XPQ7
B	221	LEU	-	expression tag	UNP C4XPQ7
B	222	VAL	-	expression tag	UNP C4XPQ7
B	223	PRO	-	expression tag	UNP C4XPQ7
B	224	ARG	-	expression tag	UNP C4XPQ7
B	225	GLY	-	expression tag	UNP C4XPQ7
B	226	SER	-	expression tag	UNP C4XPQ7
B	227	SER	-	expression tag	UNP C4XPQ7
B	228	ALA	-	expression tag	UNP C4XPQ7
B	229	HIS	-	expression tag	UNP C4XPQ7
B	230	HIS	-	expression tag	UNP C4XPQ7
B	231	HIS	-	expression tag	UNP C4XPQ7
B	232	HIS	-	expression tag	UNP C4XPQ7
B	233	HIS	-	expression tag	UNP C4XPQ7
B	234	HIS	-	expression tag	UNP C4XPQ7
B	235	HIS	-	expression tag	UNP C4XPQ7
B	236	HIS	-	expression tag	UNP C4XPQ7
B	237	HIS	-	expression tag	UNP C4XPQ7
B	238	HIS	-	expression tag	UNP C4XPQ7
C	37	MET	-	initiating methionine	UNP C4XPQ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	38	ALA	-	expression tag	UNP C4XPQ7
C	39	MET	-	expression tag	UNP C4XPQ7
C	40	GLY	-	expression tag	UNP C4XPQ7
C	124	ILE	MET	engineered mutation	UNP C4XPQ7
C	140	ALA	GLU	engineered mutation	UNP C4XPQ7
C	141	ALA	LYS	engineered mutation	UNP C4XPQ7
C	143	ALA	GLU	engineered mutation	UNP C4XPQ7
C	218	GLU	-	expression tag	UNP C4XPQ7
C	219	LEU	-	expression tag	UNP C4XPQ7
C	220	ALA	-	expression tag	UNP C4XPQ7
C	221	LEU	-	expression tag	UNP C4XPQ7
C	222	VAL	-	expression tag	UNP C4XPQ7
C	223	PRO	-	expression tag	UNP C4XPQ7
C	224	ARG	-	expression tag	UNP C4XPQ7
C	225	GLY	-	expression tag	UNP C4XPQ7
C	226	SER	-	expression tag	UNP C4XPQ7
C	227	SER	-	expression tag	UNP C4XPQ7
C	228	ALA	-	expression tag	UNP C4XPQ7
C	229	HIS	-	expression tag	UNP C4XPQ7
C	230	HIS	-	expression tag	UNP C4XPQ7
C	231	HIS	-	expression tag	UNP C4XPQ7
C	232	HIS	-	expression tag	UNP C4XPQ7
C	233	HIS	-	expression tag	UNP C4XPQ7
C	234	HIS	-	expression tag	UNP C4XPQ7
C	235	HIS	-	expression tag	UNP C4XPQ7
C	236	HIS	-	expression tag	UNP C4XPQ7
C	237	HIS	-	expression tag	UNP C4XPQ7
C	238	HIS	-	expression tag	UNP C4XPQ7
D	37	MET	-	initiating methionine	UNP C4XPQ7
D	38	ALA	-	expression tag	UNP C4XPQ7
D	39	MET	-	expression tag	UNP C4XPQ7
D	40	GLY	-	expression tag	UNP C4XPQ7
D	124	ILE	MET	engineered mutation	UNP C4XPQ7
D	140	ALA	GLU	engineered mutation	UNP C4XPQ7
D	141	ALA	LYS	engineered mutation	UNP C4XPQ7
D	143	ALA	GLU	engineered mutation	UNP C4XPQ7
D	218	GLU	-	expression tag	UNP C4XPQ7
D	219	LEU	-	expression tag	UNP C4XPQ7
D	220	ALA	-	expression tag	UNP C4XPQ7
D	221	LEU	-	expression tag	UNP C4XPQ7
D	222	VAL	-	expression tag	UNP C4XPQ7
D	223	PRO	-	expression tag	UNP C4XPQ7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	224	ARG	-	expression tag	UNP C4XPQ7
D	225	GLY	-	expression tag	UNP C4XPQ7
D	226	SER	-	expression tag	UNP C4XPQ7
D	227	SER	-	expression tag	UNP C4XPQ7
D	228	ALA	-	expression tag	UNP C4XPQ7
D	229	HIS	-	expression tag	UNP C4XPQ7
D	230	HIS	-	expression tag	UNP C4XPQ7
D	231	HIS	-	expression tag	UNP C4XPQ7
D	232	HIS	-	expression tag	UNP C4XPQ7
D	233	HIS	-	expression tag	UNP C4XPQ7
D	234	HIS	-	expression tag	UNP C4XPQ7
D	235	HIS	-	expression tag	UNP C4XPQ7
D	236	HIS	-	expression tag	UNP C4XPQ7
D	237	HIS	-	expression tag	UNP C4XPQ7
D	238	HIS	-	expression tag	UNP C4XPQ7
E	37	MET	-	initiating methionine	UNP C4XPQ7
E	38	ALA	-	expression tag	UNP C4XPQ7
E	39	MET	-	expression tag	UNP C4XPQ7
E	40	GLY	-	expression tag	UNP C4XPQ7
E	124	ILE	MET	engineered mutation	UNP C4XPQ7
E	140	ALA	GLU	engineered mutation	UNP C4XPQ7
E	141	ALA	LYS	engineered mutation	UNP C4XPQ7
E	143	ALA	GLU	engineered mutation	UNP C4XPQ7
E	218	GLU	-	expression tag	UNP C4XPQ7
E	219	LEU	-	expression tag	UNP C4XPQ7
E	220	ALA	-	expression tag	UNP C4XPQ7
E	221	LEU	-	expression tag	UNP C4XPQ7
E	222	VAL	-	expression tag	UNP C4XPQ7
E	223	PRO	-	expression tag	UNP C4XPQ7
E	224	ARG	-	expression tag	UNP C4XPQ7
E	225	GLY	-	expression tag	UNP C4XPQ7
E	226	SER	-	expression tag	UNP C4XPQ7
E	227	SER	-	expression tag	UNP C4XPQ7
E	228	ALA	-	expression tag	UNP C4XPQ7
E	229	HIS	-	expression tag	UNP C4XPQ7
E	230	HIS	-	expression tag	UNP C4XPQ7
E	231	HIS	-	expression tag	UNP C4XPQ7
E	232	HIS	-	expression tag	UNP C4XPQ7
E	233	HIS	-	expression tag	UNP C4XPQ7
E	234	HIS	-	expression tag	UNP C4XPQ7
E	235	HIS	-	expression tag	UNP C4XPQ7
E	236	HIS	-	expression tag	UNP C4XPQ7

Continued on next page...

Continued from previous page...

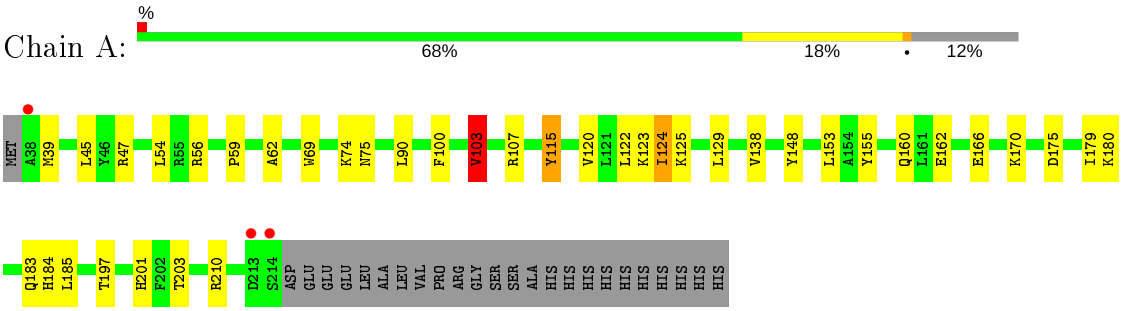
Chain	Residue	Modelled	Actual	Comment	Reference
E	237	HIS	-	expression tag	UNP C4XPQ7
E	238	HIS	-	expression tag	UNP C4XPQ7
F	37	MET	-	initiating methionine	UNP C4XPQ7
F	38	ALA	-	expression tag	UNP C4XPQ7
F	39	MET	-	expression tag	UNP C4XPQ7
F	40	GLY	-	expression tag	UNP C4XPQ7
F	124	ILE	MET	engineered mutation	UNP C4XPQ7
F	140	ALA	GLU	engineered mutation	UNP C4XPQ7
F	141	ALA	LYS	engineered mutation	UNP C4XPQ7
F	143	ALA	GLU	engineered mutation	UNP C4XPQ7
F	218	GLU	-	expression tag	UNP C4XPQ7
F	219	LEU	-	expression tag	UNP C4XPQ7
F	220	ALA	-	expression tag	UNP C4XPQ7
F	221	LEU	-	expression tag	UNP C4XPQ7
F	222	VAL	-	expression tag	UNP C4XPQ7
F	223	PRO	-	expression tag	UNP C4XPQ7
F	224	ARG	-	expression tag	UNP C4XPQ7
F	225	GLY	-	expression tag	UNP C4XPQ7
F	226	SER	-	expression tag	UNP C4XPQ7
F	227	SER	-	expression tag	UNP C4XPQ7
F	228	ALA	-	expression tag	UNP C4XPQ7
F	229	HIS	-	expression tag	UNP C4XPQ7
F	230	HIS	-	expression tag	UNP C4XPQ7
F	231	HIS	-	expression tag	UNP C4XPQ7
F	232	HIS	-	expression tag	UNP C4XPQ7
F	233	HIS	-	expression tag	UNP C4XPQ7
F	234	HIS	-	expression tag	UNP C4XPQ7
F	235	HIS	-	expression tag	UNP C4XPQ7
F	236	HIS	-	expression tag	UNP C4XPQ7
F	237	HIS	-	expression tag	UNP C4XPQ7
F	238	HIS	-	expression tag	UNP C4XPQ7

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.

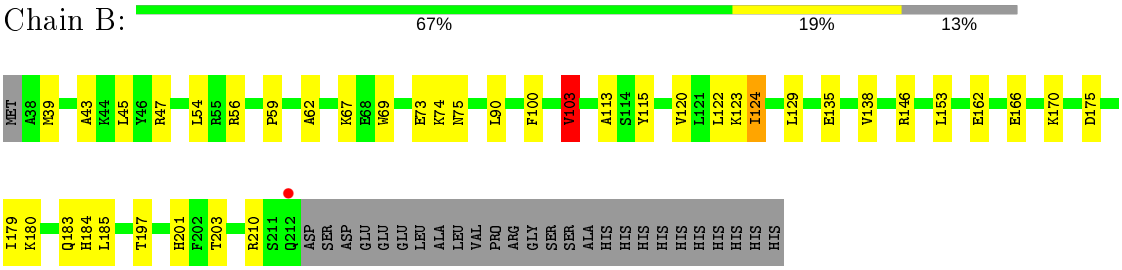
- Molecule 1: Magnetosome protein MamA

Chain A:



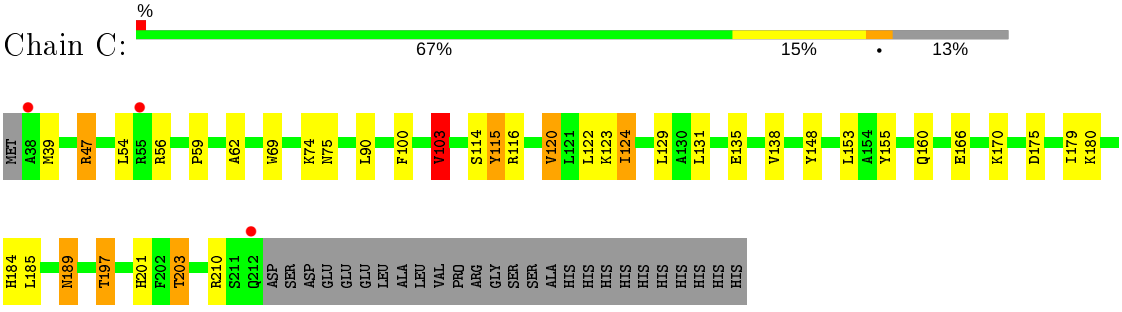
- Molecule 1: Magnetosome protein MamA

Chain B:



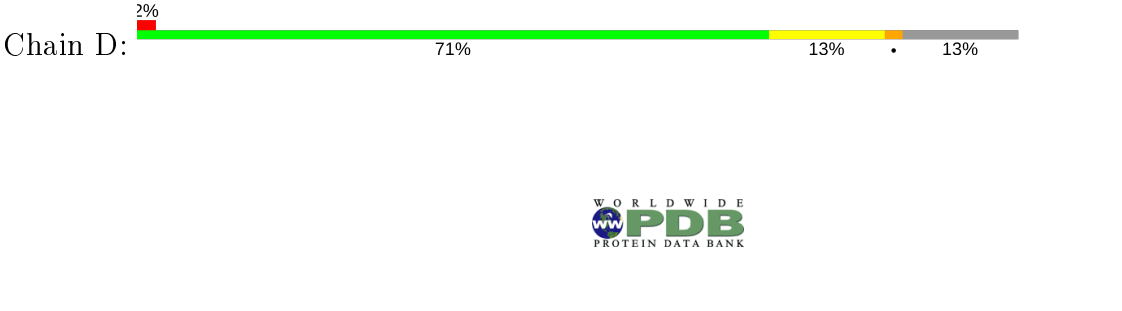
- Molecule 1: Magnetosome protein MamA

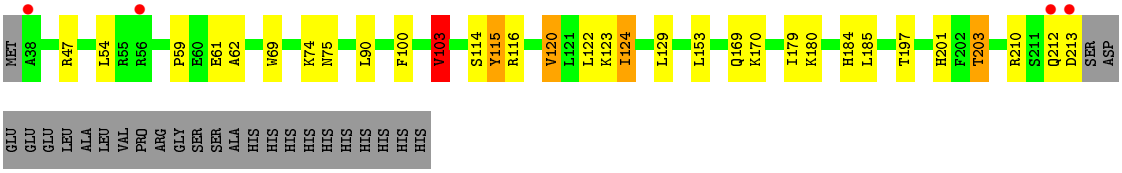
Chain C:



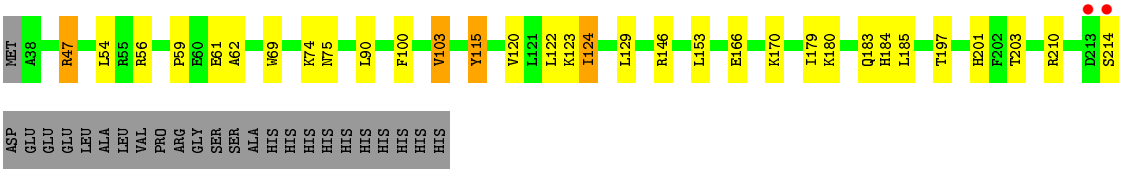
- Molecule 1: Magnetosome protein MamA

Chain D:

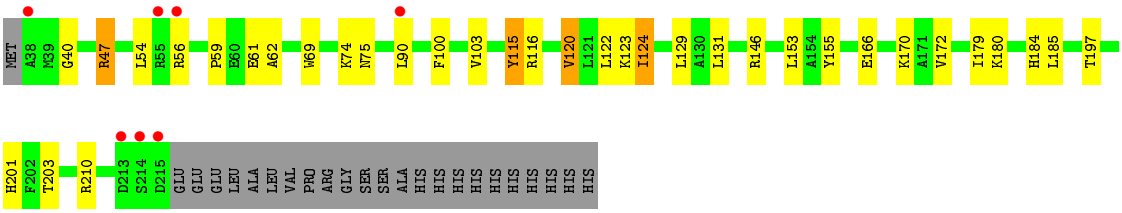




• Molecule 1: Magnetosome protein MamA



• Molecule 1: Magnetosome protein MamA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	151.09Å 151.09Å 204.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.00 – 2.88 21.65 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.4 (22.00-2.88) 95.9 (21.65-2.88)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.08 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.209 , 0.220 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	75.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.000 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.002 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.000 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k 0.019 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8530	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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

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	1.31	8/1454 (0.6%)	1.04	7/1956 (0.4%)
1	B	1.24	5/1440 (0.3%)	1.04	7/1937 (0.4%)
1	C	1.12	5/1440 (0.3%)	0.96	5/1937 (0.3%)
1	D	1.01	3/1448 (0.2%)	0.91	2/1948 (0.1%)
1	E	1.05	2/1454 (0.1%)	0.93	4/1956 (0.2%)
1	F	0.96	1/1462 (0.1%)	0.91	2/1967 (0.1%)
All	All	1.12	24/8698 (0.3%)	0.97	27/11701 (0.2%)

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	F	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	GLU	CG-CD	8.98	1.65	1.51
1	A	155	TYR	CE1-CZ	-8.26	1.27	1.38
1	A	138	VAL	CB-CG1	-7.66	1.36	1.52
1	E	166	GLU	CG-CD	7.42	1.63	1.51
1	B	162	GLU	CG-CD	7.36	1.62	1.51
1	A	148	TYR	CE1-CZ	-7.03	1.29	1.38
1	D	169	GLN	CD-NE2	-7.01	1.15	1.32
1	D	169	GLN	CD-OE1	-6.98	1.08	1.24
1	A	160	GLN	CD-OE1	-6.97	1.08	1.24
1	C	160	GLN	CD-NE2	-6.73	1.16	1.32
1	B	138	VAL	CB-CG1	-6.68	1.38	1.52
1	E	103	VAL	CB-CG1	-6.51	1.39	1.52
1	A	166	GLU	CG-CD	6.35	1.61	1.51
1	B	103	VAL	CB-CG1	-6.32	1.39	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	VAL	CB-CG1	-5.92	1.40	1.52
1	C	135	GLU	CG-CD	5.88	1.60	1.51
1	A	160	GLN	CD-NE2	-5.77	1.18	1.32
1	C	166	GLU	CG-CD	5.74	1.60	1.51
1	C	103	VAL	CB-CG1	-5.72	1.40	1.52
1	C	160	GLN	CD-OE1	-5.65	1.11	1.24
1	A	162	GLU	CG-CD	5.50	1.60	1.51
1	F	166	GLU	CG-CD	5.39	1.60	1.51
1	B	113	ALA	CA-CB	-5.23	1.41	1.52
1	D	103	VAL	CB-CG1	-5.18	1.42	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	103	VAL	CG1-CB-CG2	-8.18	97.82	110.90
1	E	47	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	C	103	VAL	CG1-CB-CG2	-7.22	99.34	110.90
1	B	124	ILE	CB-CA-C	-6.65	98.31	111.60
1	E	47	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	E	124	ILE	CB-CA-C	-6.49	98.62	111.60
1	F	124	ILE	CB-CA-C	-6.47	98.66	111.60
1	A	175	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	D	124	ILE	CB-CA-C	-6.36	98.88	111.60
1	C	124	ILE	CB-CA-C	-6.31	98.98	111.60
1	A	124	ILE	CB-CG1-CD1	-6.26	96.38	113.90
1	A	103	VAL	CG1-CB-CG2	-6.16	101.05	110.90
1	C	175	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	175	ASP	CB-CG-OD1	6.03	123.72	118.30
1	E	103	VAL	CG1-CB-CG2	-6.02	101.26	110.90
1	D	103	VAL	CG1-CB-CG2	-5.86	101.52	110.90
1	B	124	ILE	CB-CG1-CD1	-5.83	97.58	113.90
1	A	124	ILE	CB-CA-C	-5.81	99.97	111.60
1	C	47	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	115	TYR	CB-CG-CD2	5.73	124.44	121.00
1	A	107	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	135	GLU	CB-CA-C	5.58	121.55	110.40
1	C	47	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	175	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	175	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	146	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	F	47	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	40	GLY	Peptide

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	1426	0	1434	13	0
1	B	1412	0	1425	15	0
1	C	1412	0	1425	21	0
1	D	1420	0	1429	19	0
1	E	1426	0	1434	15	0
1	F	1434	0	1438	19	0
All	All	8530	0	8585	97	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 6.

All (97) 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:F:124:ILE:CG2	1:F:124:ILE:O	2.09	0.99
1:B:124:ILE:O	1:B:124:ILE:HG22	1.63	0.97
1:D:124:ILE:O	1:D:124:ILE:CG2	2.10	0.97
1:B:124:ILE:CG2	1:B:124:ILE:O	2.11	0.96
1:E:124:ILE:O	1:E:124:ILE:CG2	2.11	0.96
1:D:124:ILE:O	1:D:124:ILE:HG22	1.66	0.96
1:F:124:ILE:O	1:F:124:ILE:HG22	1.66	0.95
1:C:124:ILE:CG2	1:C:124:ILE:O	2.18	0.90
1:E:124:ILE:O	1:E:124:ILE:HG22	1.69	0.90
1:C:124:ILE:HG22	1:C:124:ILE:O	1.73	0.89
1:D:59:PRO:HB2	1:D:90:LEU:HD21	1.64	0.80
1:A:124:ILE:HG22	1:A:124:ILE:O	1.83	0.78
1:B:153:LEU:HD21	1:B:184:HIS:CD2	2.19	0.78
1:A:124:ILE:CG2	1:A:124:ILE:O	2.32	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:PRO:HB2	1:F:90:LEU:HD21	1.68	0.76
1:A:59:PRO:HB2	1:A:90:LEU:HD21	1.67	0.73
1:F:100:PHE:O	1:F:103:VAL:HG12	1.88	0.73
1:D:212:GLN:O	1:D:213:ASP:C	2.28	0.72
1:E:100:PHE:O	1:E:103:VAL:HG12	1.93	0.68
1:B:183:GLN:NE2	1:F:61:GLU:OE2	2.29	0.66
1:C:59:PRO:HB2	1:C:90:LEU:HD21	1.77	0.65
1:D:61:GLU:OE2	1:E:183:GLN:NE2	2.29	0.65
1:F:54:LEU:CD2	1:F:62:ALA:CB	2.75	0.65
1:C:100:PHE:O	1:C:103:VAL:HG12	1.97	0.65
1:E:59:PRO:HB2	1:E:90:LEU:HD21	1.77	0.65
1:E:124:ILE:O	1:E:124:ILE:HG23	1.98	0.64
1:A:100:PHE:O	1:A:103:VAL:HG12	1.99	0.63
1:D:124:ILE:O	1:D:124:ILE:HG23	1.99	0.63
1:D:100:PHE:O	1:D:103:VAL:HG12	1.99	0.62
1:B:59:PRO:HB2	1:B:90:LEU:HD21	1.82	0.61
1:D:153:LEU:HD21	1:D:184:HIS:CD2	2.35	0.61
1:F:124:ILE:HG23	1:F:124:ILE:O	1.97	0.59
1:D:54:LEU:CD2	1:D:62:ALA:CB	2.81	0.58
1:B:54:LEU:CD2	1:B:62:ALA:CB	2.82	0.58
1:E:54:LEU:CD2	1:E:62:ALA:CB	2.82	0.57
1:A:185:LEU:HD13	1:A:201:HIS:CE1	2.40	0.57
1:D:74:LYS:O	1:D:75:ASN:HB2	2.05	0.56
1:B:124:ILE:HG23	1:B:124:ILE:O	2.03	0.55
1:C:39:MET:HE1	1:C:47:ARG:NH2	2.21	0.55
1:C:54:LEU:CD2	1:C:62:ALA:CB	2.84	0.55
1:B:74:LYS:O	1:B:75:ASN:HB2	2.07	0.55
1:B:100:PHE:O	1:B:103:VAL:HG12	2.07	0.54
1:F:54:LEU:CD2	1:F:62:ALA:HB1	2.37	0.54
1:E:153:LEU:HD21	1:E:184:HIS:CD2	2.42	0.54
1:C:153:LEU:HD21	1:C:184:HIS:CD2	2.43	0.53
1:B:45:LEU:HD22	1:C:203:THR:HG23	1.91	0.53
1:C:74:LYS:O	1:C:75:ASN:HB2	2.08	0.53
1:F:74:LYS:O	1:F:75:ASN:HB2	2.09	0.53
1:D:185:LEU:HD13	1:D:201:HIS:CE1	2.43	0.52
1:E:74:LYS:O	1:E:75:ASN:HB2	2.08	0.52
1:C:124:ILE:HG23	1:C:124:ILE:O	2.09	0.52
1:A:183:GLN:NE2	1:E:61:GLU:OE2	2.44	0.51
1:A:74:LYS:O	1:A:75:ASN:HB2	2.11	0.51
1:C:47:ARG:HG3	1:C:69:TRP:CH2	2.46	0.51
1:F:172:VAL:HG21	1:F:185:LEU:HD12	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:ARG:HG3	1:F:69:TRP:CH2	2.47	0.49
1:A:54:LEU:CD2	1:A:62:ALA:CB	2.90	0.49
1:E:185:LEU:HD13	1:E:201:HIS:CE1	2.47	0.49
1:E:47:ARG:HG3	1:E:69:TRP:CH2	2.47	0.49
1:C:185:LEU:HD13	1:C:201:HIS:CE1	2.49	0.48
1:E:124:ILE:HD13	1:E:124:ILE:HG21	1.58	0.48
1:F:153:LEU:HD21	1:F:184:HIS:CD2	2.49	0.48
1:D:54:LEU:CD2	1:D:62:ALA:HB1	2.44	0.47
1:A:47:ARG:HG3	1:A:69:TRP:CH2	2.50	0.46
1:F:115:TYR:OH	1:F:146:ARG:HB3	2.15	0.46
1:B:47:ARG:HG3	1:B:69:TRP:CH2	2.51	0.46
1:B:54:LEU:CD2	1:B:62:ALA:HB1	2.45	0.46
1:A:153:LEU:HD21	1:A:184:HIS:CD2	2.51	0.46
1:D:47:ARG:HG3	1:D:69:TRP:CH2	2.51	0.45
1:B:185:LEU:HD13	1:B:201:HIS:CE1	2.52	0.44
1:C:39:MET:CE	1:C:47:ARG:NH2	2.79	0.44
1:C:124:ILE:HG21	1:C:124:ILE:HD13	1.45	0.44
1:F:54:LEU:HD22	1:F:62:ALA:CB	2.47	0.44
1:B:124:ILE:HG21	1:B:124:ILE:HD13	1.48	0.44
1:C:189:ASN:HD22	1:C:189:ASN:N	2.16	0.44
1:E:54:LEU:CD2	1:E:62:ALA:HB1	2.48	0.43
1:C:138:VAL:HG13	1:C:148:TYR:CZ	2.54	0.43
1:F:116:ARG:O	1:F:120:VAL:HG13	2.18	0.43
1:C:54:LEU:CD2	1:C:62:ALA:HB1	2.48	0.43
1:D:54:LEU:HD22	1:D:62:ALA:CB	2.48	0.42
1:A:124:ILE:O	1:A:125:LYS:HB2	2.19	0.42
1:A:124:ILE:HG21	1:A:124:ILE:HD13	1.22	0.42
1:B:43:ALA:HB2	1:B:73:GLU:HG2	2.01	0.42
1:C:131:LEU:HD22	1:C:155:TYR:CE1	2.55	0.42
1:D:124:ILE:HG21	1:D:124:ILE:HD13	1.66	0.42
1:E:115:TYR:OH	1:E:146:ARG:HB3	2.20	0.41
1:C:189:ASN:OD1	1:C:197:THR:HB	2.20	0.41
1:F:124:ILE:HG21	1:F:124:ILE:HD13	1.63	0.41
1:F:54:LEU:HD23	1:F:62:ALA:HB1	2.02	0.41
1:F:131:LEU:HD22	1:F:155:TYR:CE1	2.56	0.41
1:C:116:ARG:O	1:C:120:VAL:HG13	2.21	0.41
1:D:114:SER:O	1:D:115:TYR:C	2.59	0.41
1:A:45:LEU:HD22	1:D:203:THR:HG23	2.03	0.41
1:D:116:ARG:O	1:D:120:VAL:HG13	2.21	0.41
1:F:185:LEU:HD13	1:F:201:HIS:CE1	2.56	0.40
1:C:114:SER:O	1:C:115:TYR:C	2.58	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:LEU:HA	1:D:185:LEU:HD23	1.89	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	175/202 (87%)	168 (96%)	6 (3%)	1 (1%)	25	55
1	B	173/202 (86%)	167 (96%)	5 (3%)	1 (1%)	25	55
1	C	173/202 (86%)	168 (97%)	4 (2%)	1 (1%)	25	55
1	D	174/202 (86%)	168 (97%)	6 (3%)	0	100	100
1	E	175/202 (87%)	169 (97%)	5 (3%)	1 (1%)	25	55
1	F	176/202 (87%)	167 (95%)	8 (4%)	1 (1%)	25	55
All	All	1046/1212 (86%)	1007 (96%)	34 (3%)	5 (0%)	29	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	56	ARG
1	E	56	ARG
1	A	56	ARG
1	B	56	ARG
1	F	56	ARG

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	146/168 (87%)	133 (91%)	13 (9%)	9 27
1	B	144/168 (86%)	130 (90%)	14 (10%)	8 23
1	C	144/168 (86%)	131 (91%)	13 (9%)	9 26
1	D	145/168 (86%)	133 (92%)	12 (8%)	11 30
1	E	146/168 (87%)	134 (92%)	12 (8%)	11 31
1	F	147/168 (88%)	136 (92%)	11 (8%)	13 35
All	All	872/1008 (86%)	797 (91%)	75 (9%)	10 29

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	MET
1	A	103	VAL
1	A	115	TYR
1	A	120	VAL
1	A	122	LEU
1	A	123	LYS
1	A	129	LEU
1	A	170	LYS
1	A	179	ILE
1	A	180	LYS
1	A	197	THR
1	A	203	THR
1	A	210	ARG
1	B	39	MET
1	B	67	LYS
1	B	103	VAL
1	B	115	TYR
1	B	120	VAL
1	B	122	LEU
1	B	123	LYS
1	B	129	LEU
1	B	170	LYS
1	B	179	ILE
1	B	180	LYS
1	B	197	THR
1	B	203	THR
1	B	210	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	103	VAL
1	C	115	TYR
1	C	120	VAL
1	C	122	LEU
1	C	123	LYS
1	C	129	LEU
1	C	170	LYS
1	C	179	ILE
1	C	180	LYS
1	C	189	ASN
1	C	197	THR
1	C	203	THR
1	C	210	ARG
1	D	103	VAL
1	D	115	TYR
1	D	120	VAL
1	D	122	LEU
1	D	123	LYS
1	D	129	LEU
1	D	170	LYS
1	D	179	ILE
1	D	180	LYS
1	D	197	THR
1	D	203	THR
1	D	210	ARG
1	E	115	TYR
1	E	120	VAL
1	E	122	LEU
1	E	123	LYS
1	E	129	LEU
1	E	170	LYS
1	E	179	ILE
1	E	180	LYS
1	E	197	THR
1	E	203	THR
1	E	210	ARG
1	E	214	SER
1	F	115	TYR
1	F	120	VAL
1	F	122	LEU
1	F	123	LYS
1	F	129	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	170	LYS
1	F	179	ILE
1	F	180	LYS
1	F	197	THR
1	F	203	THR
1	F	210	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	89	ASN
1	A	94	GLN
1	A	126	GLN
1	A	201	HIS
1	A	212	GLN
1	B	51	GLN
1	B	89	ASN
1	B	94	GLN
1	B	126	GLN
1	B	184	HIS
1	B	201	HIS
1	C	51	GLN
1	C	89	ASN
1	C	94	GLN
1	C	126	GLN
1	C	201	HIS
1	D	51	GLN
1	D	89	ASN
1	D	201	HIS
1	E	51	GLN
1	E	89	ASN
1	E	201	HIS
1	E	212	GLN
1	F	89	ASN
1	F	201	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	177/202 (87%)	-0.18	3 (1%)	70	70	36, 64, 116, 139	1 (0%)
1	B	175/202 (86%)	-0.28	1 (0%)	89	89	37, 62, 113, 144	1 (0%)
1	C	175/202 (86%)	-0.20	3 (1%)	70	70	43, 69, 114, 130	0
1	D	176/202 (87%)	-0.22	4 (2%)	60	59	51, 80, 123, 142	0
1	E	177/202 (87%)	-0.21	2 (1%)	80	80	48, 71, 126, 147	0
1	F	178/202 (88%)	-0.07	7 (3%)	39	35	54, 79, 132, 145	0
All	All	1058/1212 (87%)	-0.19	20 (1%)	66	65	36, 72, 123, 147	2 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	ALA	4.7
1	F	214	SER	4.3
1	E	214	SER	3.8
1	F	38	ALA	3.4
1	B	212	GLN	3.4
1	F	215	ASP	3.3
1	E	213	ASP	3.3
1	A	214	SER	3.1
1	F	213	ASP	2.8
1	F	56	ARG	2.7
1	D	212	GLN	2.7
1	D	213	ASP	2.6
1	A	213	ASP	2.4
1	C	55	ARG	2.3
1	F	90	LEU	2.3
1	F	55	ARG	2.2
1	C	38	ALA	2.2
1	D	38	ALA	2.1
1	C	212	GLN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	56	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.