



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:48 PM UTC

PDB ID : 2P9M / pdb_00002p9m
Title : Crystal structure of conserved hypothetical protein MJ0922 from Methanocaldococcus jannaschii DSM 2661
Authors : Zhao, M.; Ebihara, A.; Shinkai, A.; Kuramitsu, S.; Yokoyama, S.; Zhu, J.; Swindell II, J.T.; Chen, L.; Fu, Z.-Q.; Charz, J.; Rose, J.P.; Wang, B.-C.; Southeast Collaboratory for Structural Genomics (SECSG); RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-03-26
Resolution : 2.59 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
Mogul	:	2022.3.0, CSD as543be (2022)
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)

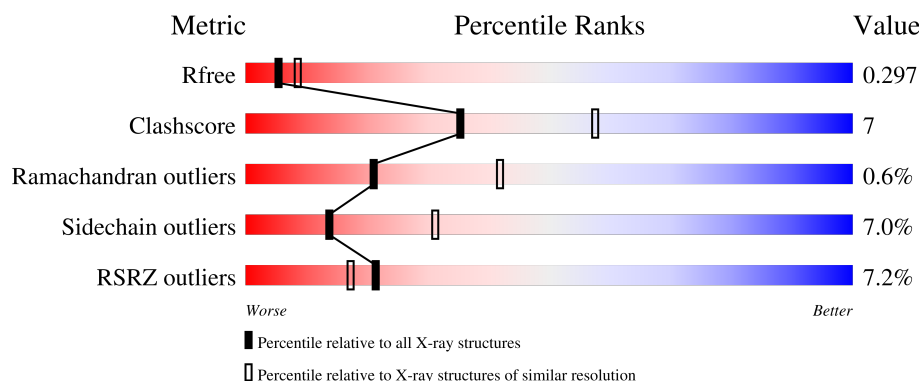
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	138	3% 63% 21% 8% 7%
1	B	138	7% 57% 30% 7% 7%
1	C	138	% 70% 17% • • 7%
1	D	138	15% 67% 20% 6% 7%

Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4070 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 Hypothetical protein MJ0922.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	Se	49	0	0
			1002	639	165	194	4			
1	B	129	Total	C	N	O	Se	55	1	0
			1018	649	168	197	4			
1	C	129	Total	C	N	O	Se	53	2	0
			1019	649	170	196	4			
1	D	128	Total	C	N	O	Se	74	1	0
			1009	642	166	197	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q58332
A	14	MSE	MET	modified residue	UNP Q58332
A	34	MSE	MET	modified residue	UNP Q58332
A	79	MSE	MET	modified residue	UNP Q58332
A	99	MSE	MET	modified residue	UNP Q58332
B	1	MSE	MET	modified residue	UNP Q58332
B	14	MSE	MET	modified residue	UNP Q58332
B	34	MSE	MET	modified residue	UNP Q58332
B	79	MSE	MET	modified residue	UNP Q58332
B	99	MSE	MET	modified residue	UNP Q58332
C	1	MSE	MET	modified residue	UNP Q58332
C	14	MSE	MET	modified residue	UNP Q58332
C	34	MSE	MET	modified residue	UNP Q58332
C	79	MSE	MET	modified residue	UNP Q58332
C	99	MSE	MET	modified residue	UNP Q58332
D	1	MSE	MET	modified residue	UNP Q58332
D	14	MSE	MET	modified residue	UNP Q58332
D	34	MSE	MET	modified residue	UNP Q58332
D	79	MSE	MET	modified residue	UNP Q58332
D	99	MSE	MET	modified residue	UNP Q58332

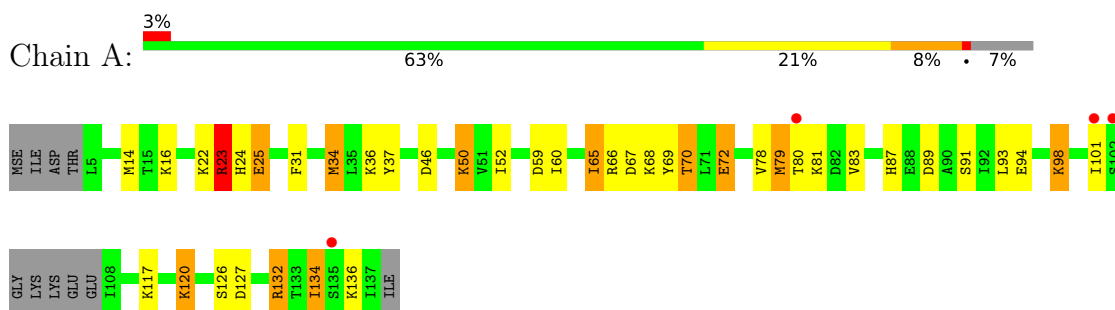
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total 5	O 5	0	0
2	B	2	Total 2	O 2	0	0
2	C	7	Total 7	O 7	0	0
2	D	8	Total 8	O 8	0	0

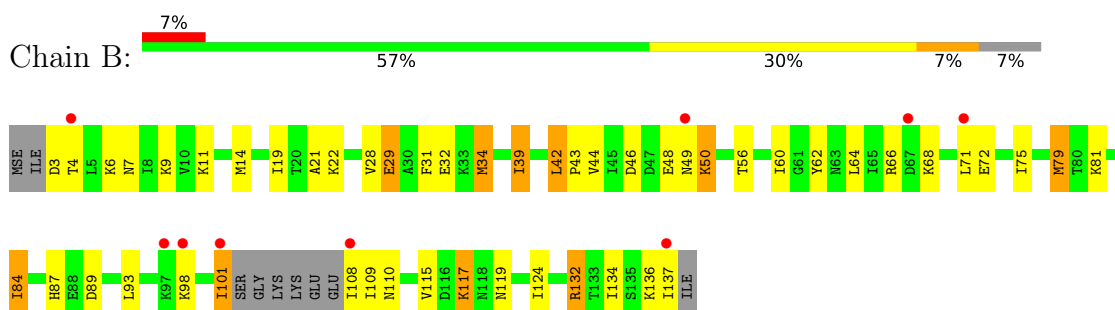
3 Residue-property plots [i](#)

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.

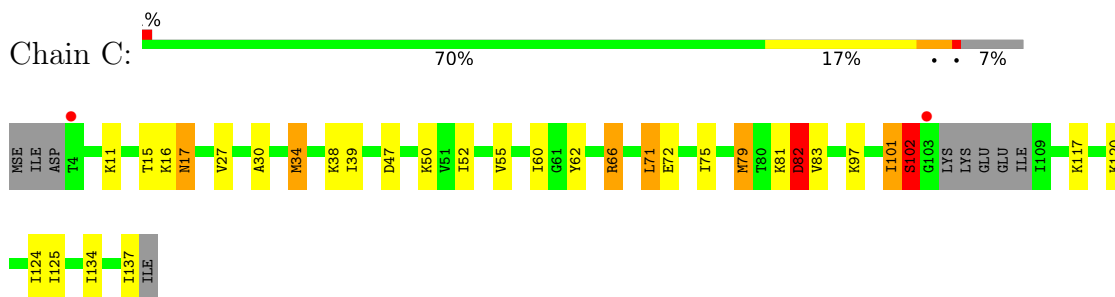
- Molecule 1: Hypothetical protein MJ0922



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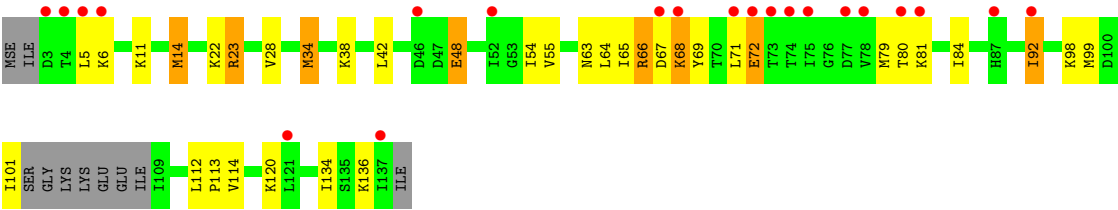


- Molecule 1: Hypothetical protein MJ0922



- Molecule 1: Hypothetical protein MJ0922





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.21Å 94.69Å 102.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.47 – 2.59 36.47 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.0 (36.47-2.59) 99.1 (36.47-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.292 0.239 , 0.297	Depositor DCC
R_{free} test set	907 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4070	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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	1.90	20/1004 (2.0%)	1.73	19/1345 (1.4%)
1	B	1.67	17/1024 (1.7%)	1.46	21/1373 (1.5%)
1	C	3.11	23/1029 (2.2%)	2.51	21/1379 (1.5%)
1	D	2.18	20/1014 (2.0%)	1.88	13/1359 (1.0%)
All	All	2.29	80/4071 (2.0%)	1.94	74/5456 (1.4%)

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	3
1	B	1	1
1	C	1	3
1	D	1	2
All	All	3	9

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	ARG	NE-CZ	85.25	2.26	1.33
1	D	48	GLU	CD-OE1	42.54	2.06	1.25
1	A	68	LYS	CE-NZ	-25.44	0.73	1.49
1	B	22	LYS	CG-CD	-24.88	0.77	1.52
1	A	23	ARG	CD-NE	-24.57	1.11	1.46
1	D	72	GLU	CA-CB	-23.27	1.17	1.53
1	B	117	LYS	CA-CB	-22.29	1.15	1.53
1	D	66	ARG	NE-CZ	21.52	1.56	1.33
1	D	23	ARG	CB-CG	-20.03	0.92	1.52
1	A	81	LYS	CB-CG	18.18	2.06	1.52
1	A	59	ASP	CG-OD2	-16.80	0.93	1.25
1	B	136	LYS	CD-CE	-15.54	1.05	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	LYS	CG-CD	-15.02	1.07	1.52
1	D	6	LYS	CD-CE	14.83	1.97	1.52
1	C	16	LYS	CG-CD	-14.39	1.09	1.52
1	C	102	SER	CA-CB	-14.38	1.29	1.53
1	C	66	ARG	CZ-NH1	13.94	1.52	1.32
1	C	71	LEU	CG-CD2	-13.67	1.07	1.52
1	D	6	LYS	CE-NZ	-13.64	1.08	1.49
1	A	136	LYS	CD-CE	-12.68	1.14	1.52
1	C	72	GLU	CB-CG	12.68	1.90	1.52
1	B	101	ILE	CB-CG2	-12.60	1.10	1.52
1	C	101	ILE	CB-CG1	12.02	1.77	1.53
1	B	49	ASN	CG-OD1	-11.44	1.01	1.23
1	B	11	LYS	CB-CG	-11.17	1.19	1.52
1	A	132	ARG	CD-NE	10.65	1.61	1.46
1	C	38	LYS	CD-CE	-10.50	1.21	1.52
1	A	72	GLU	CA-CB	-9.48	1.38	1.53
1	B	6	LYS	CG-CD	-9.47	1.24	1.52
1	C	66	ARG	CD-NE	-9.43	1.33	1.46
1	A	50	LYS	CG-CD	-9.21	1.24	1.52
1	A	23	ARG	CB-CG	-8.84	1.25	1.52
1	C	17	ASN	CB-CG	8.80	1.74	1.52
1	C	117	LYS	CA-CB	8.51	1.68	1.53
1	B	72	GLU	CG-CD	8.44	1.73	1.52
1	D	84	ILE	CB-CG1	-8.32	1.36	1.53
1	D	11	LYS	CB-CG	-8.20	1.27	1.52
1	C	82	ASP	CG-OD2	8.11	1.40	1.25
1	C	66	ARG	CZ-NH2	8.06	1.44	1.33
1	C	81	LYS	CE-NZ	-7.87	1.25	1.49
1	C	71	LEU	CG-CD1	7.62	1.77	1.52
1	A	93	LEU	CB-CG	-7.39	1.38	1.53
1	C	11	LYS	CG-CD	-7.28	1.30	1.52
1	D	68	LYS	CB-CG	-7.22	1.30	1.52
1	C	97	LYS	CG-CD	-7.06	1.31	1.52
1	B	34	MSE	SE-CE	-6.84	1.75	1.95
1	C	50	LYS	CG-CD	-6.64	1.32	1.52
1	A	120	LYS	CD-CE	-6.62	1.32	1.52
1	A	66	ARG	CZ-NH2	-6.57	1.25	1.33
1	B	68	LYS	CG-CD	-6.43	1.33	1.52
1	A	72	GLU	CG-CD	-6.36	1.36	1.52
1	D	22	LYS	CD-CE	-6.36	1.33	1.52
1	B	108	ILE	CA-CB	-6.22	1.37	1.54
1	B	71	LEU	CB-CG	-6.21	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	17	ASN	CG-OD1	6.20	1.35	1.23
1	D	98	LYS	CE-NZ	-6.18	1.30	1.49
1	B	101	ILE	CB-CG1	6.16	1.65	1.53
1	A	34	MSE	SE-CE	-6.00	1.77	1.95
1	C	79	MSE	SE-CE	-5.97	1.77	1.95
1	A	14	MSE	SE-CE	-5.94	1.77	1.95
1	B	98	LYS	CE-NZ	-5.92	1.31	1.49
1	C	34	MSE	SE-CE	-5.87	1.77	1.95
1	A	79	MSE	SE-CE	-5.86	1.77	1.95
1	A	24	HIS	CB-CG	5.71	1.58	1.50
1	C	79	MSE	CG-SE	-5.68	1.78	1.95
1	C	17	ASN	CA-CB	-5.63	1.45	1.52
1	B	14	MSE	SE-CE	-5.63	1.78	1.95
1	D	67	ASP	CB-CG	-5.56	1.38	1.52
1	D	120	LYS	CB-CG	-5.51	1.35	1.52
1	D	79	MSE	SE-CE	-5.45	1.79	1.95
1	D	34	MSE	CG-SE	-5.32	1.79	1.95
1	B	14	MSE	CG-SE	-5.31	1.79	1.95
1	D	14	MSE	SE-CE	-5.26	1.79	1.95
1	A	132	ARG	CG-CD	-5.25	1.36	1.52
1	D	79	MSE	CG-SE	-5.18	1.79	1.95
1	D	34	MSE	SE-CE	-5.18	1.79	1.95
1	B	79	MSE	SE-CE	-5.10	1.80	1.95
1	D	14	MSE	CG-SE	-5.07	1.80	1.95
1	A	70	THR	CB-CG2	-5.06	1.35	1.52
1	D	66	ARG	CZ-NH1	-5.03	1.25	1.32

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	ARG	NE-CZ-NH2	-51.03	73.27	119.20
1	C	66	ARG	NE-CZ-NH1	-49.24	72.26	121.50
1	D	66	ARG	NE-CZ-NH1	-39.55	81.94	121.50
1	A	23	ARG	CD-NE-CZ	24.43	158.60	124.40
1	A	22	LYS	CB-CG-CD	21.68	161.16	111.30
1	D	66	ARG	NE-CZ-NH2	-21.36	99.98	119.20
1	D	72	GLU	CB-CA-C	19.47	141.13	110.95
1	C	82	ASP	OD1-CG-OD2	-18.80	77.78	122.90
1	D	23	ARG	CA-CB-CG	17.79	149.67	114.10
1	C	16	LYS	CB-CG-CD	17.02	150.44	111.30
1	B	11	LYS	CA-CB-CG	16.55	147.20	114.10
1	A	81	LYS	CA-CB-CG	-16.21	81.68	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	LYS	CG-CD-CE	15.46	146.86	111.30
1	C	66	ARG	NH1-CZ-NH2	-13.52	101.72	119.30
1	C	17	ASN	CA-CB-CG	13.40	126.00	112.60
1	C	17	ASN	CB-CG-ND2	-13.31	96.44	116.40
1	A	66	ARG	NE-CZ-NH1	-12.69	108.81	121.50
1	A	23	ARG	CG-CD-NE	12.48	139.46	112.00
1	B	101	ILE	CA-CB-CG1	-11.12	91.50	110.40
1	D	72	GLU	CA-CB-CG	11.00	136.09	114.10
1	A	66	ARG	NE-CZ-NH2	10.99	129.09	119.20
1	D	101	ILE	CB-CA-C	-10.94	89.72	111.60
1	A	22	LYS	CG-CD-CE	10.69	135.89	111.30
1	B	22	LYS	CB-CG-CD	10.59	135.67	111.30
1	C	17	ASN	OD1-CG-ND2	-10.54	112.06	122.60
1	C	72	GLU	CA-CB-CG	-10.46	93.17	114.10
1	B	6	LYS	CG-CD-CE	9.99	134.27	111.30
1	B	132	ARG	CA-CB-CG	9.39	132.88	114.10
1	D	66	ARG	CG-CD-NE	9.21	132.26	112.00
1	B	117	LYS	CB-CA-C	9.14	128.61	110.42
1	D	136	LYS	CB-CG-CD	-9.04	90.51	111.30
1	A	24	HIS	CA-CB-CG	-9.02	104.78	113.80
1	C	71	LEU	CB-CG-CD2	8.89	137.38	110.70
1	C	97	LYS	CB-CG-CD	8.89	131.74	111.30
1	B	101	ILE	CG1-CB-CG2	8.83	137.18	110.70
1	A	59	ASP	CB-CG-OD2	8.71	138.44	118.40
1	B	9	LYS	CD-CE-NZ	8.59	139.38	111.90
1	A	132	ARG	CG-CD-NE	8.58	130.87	112.00
1	A	23	ARG	CA-CB-CG	8.41	130.91	114.10
1	A	59	ASP	OD1-CG-OD2	-8.17	103.28	122.90
1	C	101	ILE	CA-CB-CG1	-8.04	96.74	110.40
1	B	50	LYS	CG-CD-CE	7.52	128.60	111.30
1	B	101	ILE	CA-CB-CG2	7.28	122.88	110.50
1	B	117	LYS	CA-CB-CG	7.27	128.65	114.10
1	A	120	LYS	CG-CD-CE	7.26	128.01	111.30
1	C	66	ARG	CD-NE-CZ	-7.19	114.33	124.40
1	B	11	LYS	CB-CG-CD	7.15	127.74	111.30
1	B	6	LYS	CB-CG-CD	7.11	127.66	111.30
1	C	120	LYS	CG-CD-CE	7.06	127.55	111.30
1	B	101	ILE	CB-CG1-CD1	6.96	128.41	113.80
1	B	108	ILE	CB-CA-C	6.94	125.47	111.60
1	B	108	ILE	CA-CB-CG2	6.67	121.84	110.50
1	C	71	LEU	CB-CG-CD1	-6.56	91.01	110.70
1	A	120	LYS	CD-CE-NZ	6.38	132.33	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	102	SER	N-CA-CB	6.38	121.28	110.49
1	A	70	THR	CA-CB-CG2	6.28	121.18	110.50
1	D	67	ASP	CA-CB-CG	6.27	118.87	112.60
1	D	66	ARG	CA-CB-CG	-6.21	101.67	114.10
1	C	11	LYS	CB-CG-CD	6.18	125.51	111.30
1	C	38	LYS	CG-CD-CE	6.16	125.47	111.30
1	D	23	ARG	CB-CG-CD	6.16	125.47	111.30
1	B	68	LYS	CB-CG-CD	6.15	125.44	111.30
1	B	132	ARG	CB-CG-CD	6.05	125.21	111.30
1	C	17	ASN	CB-CG-OD1	-5.99	108.82	120.80
1	A	136	LYS	CG-CD-CE	5.99	125.07	111.30
1	D	120	LYS	CA-CB-CG	5.99	126.07	114.10
1	B	49	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	B	50	LYS	CB-CG-CD	5.66	124.33	111.30
1	B	110	ASN	N-CA-CB	-5.58	101.04	110.41
1	C	11	LYS	CG-CD-CE	5.46	123.87	111.30
1	A	117	LYS	CB-CG-CD	-5.27	99.19	111.30
1	A	25	GLU	N-CA-C	5.25	117.64	110.55
1	A	83	VAL	N-CA-C	5.12	115.84	108.93
1	D	23	ARG	CD-NE-CZ	5.05	131.47	124.40

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	117	LYS	CA
1	C	102	SER	CA
1	D	72	GLU	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	SER	Peptide
1	A	132	ARG	Sidechain
1	A	23	ARG	Sidechain
1	B	132	ARG	Sidechain
1	C	17	ASN	Sidechain
1	C	66	ARG	Sidechain
1	C	82	ASP	Sidechain
1	D	48	GLU	Sidechain
1	D	66	ARG	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	1002	0	1077	21	0
1	B	1018	0	1090	20	0
1	C	1019	0	1090	11	0
1	D	1009	0	1080	12	0
2	A	5	0	0	1	0
2	B	2	0	0	0	0
2	C	7	0	0	0	0
2	D	8	0	0	0	0
All	All	4070	0	4337	57	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 7.

All (57) 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:98:LYS:O	1:A:101:ILE:HG12	1.82	0.78
1:A:50:LYS:HG3	1:A:120:LYS:HE2	1.71	0.72
1:A:134:ILE:HD12	1:B:134:ILE:HD13	1.74	0.69
1:A:46:ASP:HB3	1:A:52:ILE:HD11	1.75	0.68
1:B:31:PHE:HA	1:B:34:MSE:HE3	1.76	0.68
1:A:87:HIS:CE1	1:A:89:ASP:HB2	2.30	0.67
1:A:46:ASP:HB3	1:A:52:ILE:CD1	2.23	0.67
1:A:36:LYS:O	1:B:66:ARG:NH1	2.26	0.65
1:D:42:LEU:HB3	1:D:55:VAL:HG22	1.82	0.62
1:A:52:ILE:HG22	1:A:79:MSE:HE1	1.82	0.61
1:B:21:ALA:HB2	1:B:42:LEU:HD23	1.81	0.61
1:B:4:THR:H	1:B:7:ASN:HB2	1.68	0.59
1:C:34:MSE:HG2	1:C:39:ILE:HG13	1.86	0.56
1:A:87:HIS:HE1	1:A:89:ASP:HB2	1.68	0.56
1:D:34:MSE:HG3	1:D:42:LEU:HD22	1.88	0.56
1:D:14:MSE:SE	1:D:114:VAL:HG11	2.57	0.55
1:B:56:THR:O	1:B:60:ILE:HG12	2.06	0.55
1:A:52:ILE:HG22	1:A:79:MSE:CE	2.39	0.53
1:A:36:LYS:HE3	1:A:37:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:TYR:CE1	1:A:78:VAL:HG11	2.45	0.52
1:A:31:PHE:HB2	1:A:60:ILE:HG21	1.94	0.50
1:D:63:ASN:HB2	1:D:69:TYR:CE2	2.48	0.49
1:A:31:PHE:HA	1:A:34:MSE:HE3	1.94	0.49
1:A:52:ILE:HG22	1:A:52:ILE:O	2.12	0.48
1:B:28:VAL:HG22	1:B:64:LEU:HD21	1.95	0.48
1:A:67:ASP:HB2	2:A:140:HOH:O	2.13	0.47
1:D:23:ARG:CB	1:D:23:ARG:NE	2.77	0.47
1:D:99:MSE:HG2	1:D:112:LEU:HG	1.95	0.47
1:C:34:MSE:HA	1:C:39:ILE:HG12	1.97	0.47
1:B:29:GLU:H	1:B:29:GLU:HG2	1.54	0.47
1:C:52:ILE:HG22	1:C:79:MSE:HE1	1.95	0.46
1:A:87:HIS:CE1	1:A:89:ASP:H	2.32	0.46
1:D:5:LEU:HD22	1:D:92:ILE:HG21	1.98	0.46
1:A:36:LYS:HG3	1:B:66:ARG:NH1	2.30	0.46
1:B:19:ILE:HD11	1:B:39:ILE:CD1	2.46	0.46
1:A:65:ILE:HD11	1:B:32:GLU:HG2	1.98	0.45
1:B:87[A]:HIS:CD2	1:B:89:ASP:HB2	2.52	0.45
1:B:115:VAL:HB	1:B:119:ASN:HA	1.98	0.45
1:B:109:ILE:O	1:B:109:ILE:HG13	2.16	0.45
1:B:46:ASP:OD2	1:B:50:LYS:HB3	2.18	0.44
1:C:27:VAL:CG2	1:C:60:ILE:HD12	2.47	0.44
1:B:43:PRO:CG	1:B:124:ILE:HD11	2.48	0.44
1:A:50:LYS:CG	1:A:120:LYS:HE2	2.44	0.43
1:C:34:MSE:HA	1:C:39:ILE:CG1	2.48	0.43
1:B:62:TYR:CE1	1:B:66:ARG:NH1	2.87	0.42
1:C:55:VAL:HB	1:C:60:ILE:HD11	2.01	0.42
1:B:48:GLU:HG2	1:C:47:ASP:HB3	2.01	0.41
1:D:54:ILE:HD12	1:D:113:PRO:HG3	2.01	0.41
1:C:30:ALA:CB	1:C:75:ILE:HD11	2.50	0.41
1:B:44:VAL:HG11	1:B:79:MSE:SE	2.71	0.41
1:D:28:VAL:HG22	1:D:64:LEU:HD11	2.03	0.41
1:C:124:ILE:HG22	1:C:125:ILE:N	2.36	0.41
1:B:84:ILE:H	1:B:84:ILE:HG12	1.54	0.41
1:C:134:ILE:HD13	1:D:134:ILE:HD13	2.03	0.40
1:C:62:TYR:CG	1:D:38:LYS:HE3	2.56	0.40
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.89	0.40
1:A:91:SER:O	1:A:94:GLU:HB2	2.22	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	124/138 (90%)	119 (96%)	4 (3%)	1 (1%)	16	34
1	B	126/138 (91%)	122 (97%)	3 (2%)	1 (1%)	16	34
1	C	127/138 (92%)	119 (94%)	7 (6%)	1 (1%)	16	34
1	D	125/138 (91%)	119 (95%)	6 (5%)	0	100	100
All	All	502/552 (91%)	479 (95%)	20 (4%)	3 (1%)	21	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	ASP
1	C	102	SER
1	B	117	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	118/122 (97%)	109 (92%)	9 (8%)	12	27
1	B	120/122 (98%)	110 (92%)	10 (8%)	10	23
1	C	120/122 (98%)	113 (94%)	7 (6%)	18	39
1	D	119/122 (98%)	112 (94%)	7 (6%)	18	38
All	All	477/488 (98%)	444 (93%)	33 (7%)	14	32

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	23	ARG
1	A	25	GLU
1	A	65	ILE
1	A	70	THR
1	A	72	GLU
1	A	80	THR
1	A	98	LYS
1	A	134	ILE
1	B	3	ASP
1	B	29	GLU
1	B	39	ILE
1	B	42	LEU
1	B	75	ILE
1	B	81	LYS
1	B	84	ILE
1	B	93	LEU
1	B	101	ILE
1	B	137	ILE
1	C	15	THR
1	C	71	LEU
1	C	82	ASP
1	C	83	VAL
1	C	101	ILE
1	C	102	SER
1	C	137	ILE
1	D	65	ILE
1	D	68	LYS
1	D	71	LEU
1	D	72	GLU
1	D	80	THR
1	D	81	LYS
1	D	92	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	110	ASN
1	B	63	ASN
1	B	111	GLN
1	B	119	ASN
1	D	63	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	124/138 (89%)	0.29	4 (3%)	50	44	12, 23, 33, 44	20 (16%)
1	B	125/138 (90%)	0.37	9 (7%)	21	17	11, 24, 35, 61	26 (20%)
1	C	125/138 (90%)	0.17	2 (1%)	70	66	8, 22, 29, 49	23 (18%)
1	D	124/138 (89%)	0.84	21 (16%)	4	3	12, 26, 50, 68	25 (20%)
All	All	498/552 (90%)	0.42	36 (7%)	21	17	8, 24, 40, 68	94 (18%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	74	THR	4.6
1	C	103	GLY	4.2
1	B	108	ILE	3.9
1	D	71	LEU	3.8
1	D	73	THR	3.7
1	B	137	ILE	3.6
1	D	80	THR	3.5
1	A	102	SER	3.5
1	D	4	THR	3.4
1	A	101	ILE	3.3
1	D	5	LEU	3.1
1	D	67	ASP	3.1
1	B	101	ILE	3.1
1	B	98	LYS	2.8
1	D	92	ILE	2.8
1	D	68	LYS	2.8
1	D	72	GLU	2.8
1	D	52	ILE	2.7
1	B	67	ASP	2.6
1	B	4	THR	2.6
1	B	71	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	137	ILE	2.5
1	A	135	SER	2.4
1	D	81	LYS	2.4
1	D	75	ILE	2.4
1	D	46	ASP	2.4
1	D	77	ASP	2.4
1	D	78	VAL	2.3
1	B	49	ASN	2.3
1	D	87	HIS	2.3
1	C	4	THR	2.2
1	A	80	THR	2.2
1	D	3	ASP	2.2
1	B	97	LYS	2.2
1	D	121	LEU	2.1
1	D	6	LYS	2.1

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.