Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 08:49 am BST

PDB ID	:	2P9M
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

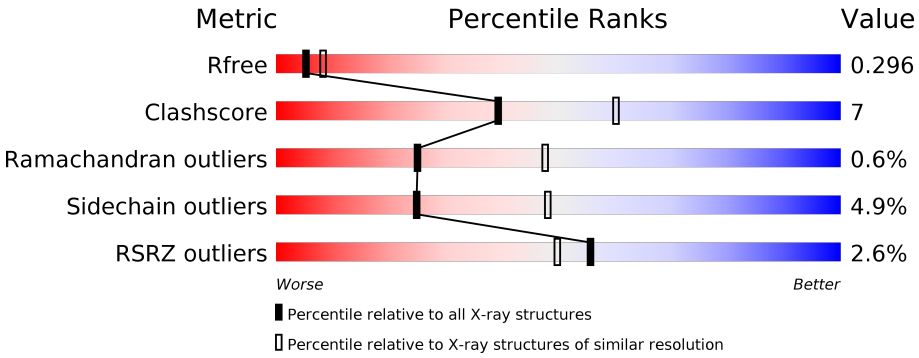
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.59 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 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	138	3% 64% 23% • • 7%
1	B	138	% 59% 29% 6% 7%
1	C	138	% 72% 17% • • 7%
1	D	138	4% 68% 22% • 7%

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.

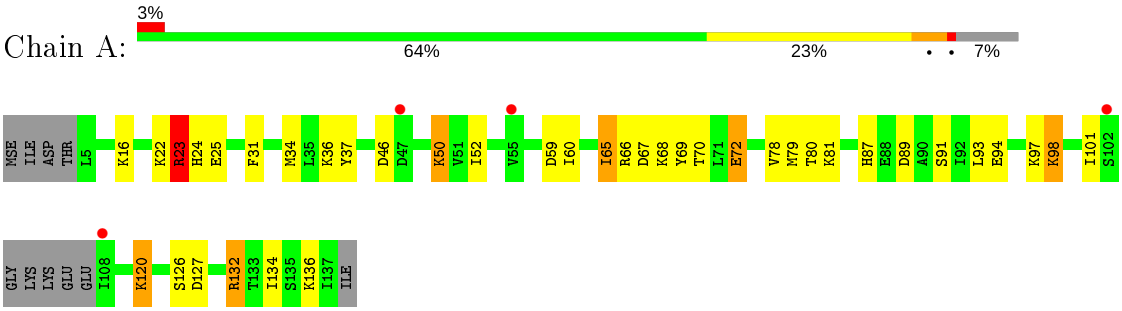
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total O 5 5	0	0
2	B	2	Total O 2 2	0	0
2	C	7	Total O 7 7	0	0
2	D	8	Total O 8 8	0	0

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.

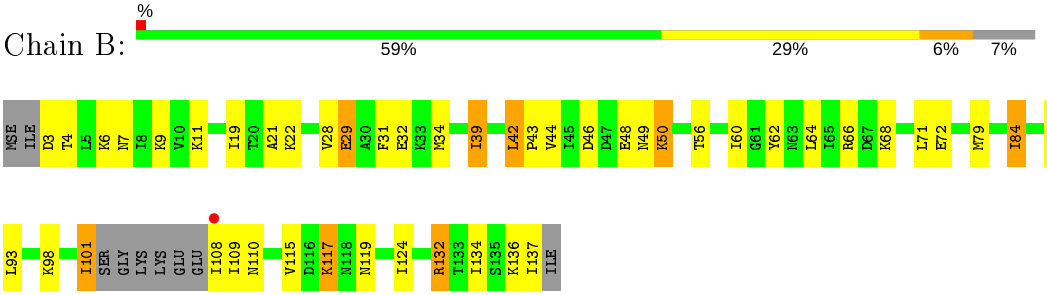
- Molecule 1: Hypothetical protein MJ0922

Chain A:



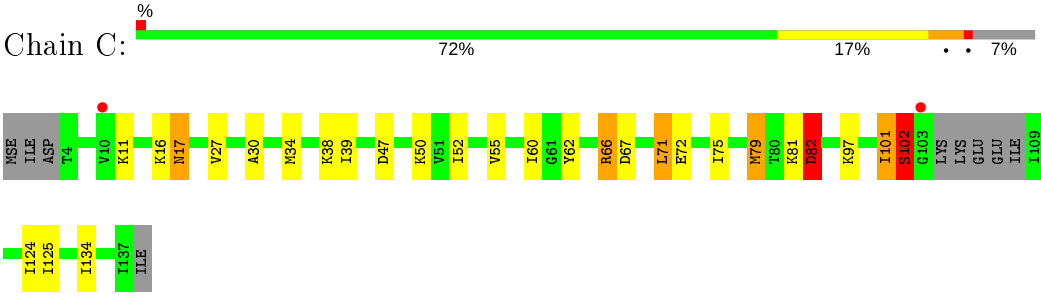
- Molecule 1: Hypothetical protein MJ0922

Chain B:



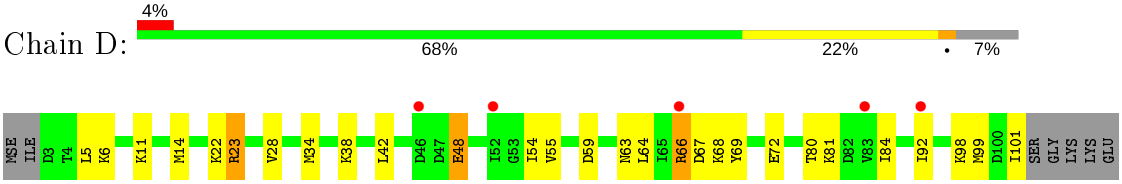
- Molecule 1: Hypothetical protein MJ0922

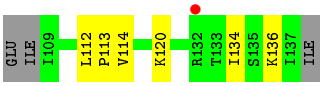
Chain C:



- Molecule 1: Hypothetical protein MJ0922

Chain D:




GLU
ILE
I109
L112
P113
V114
K120
R132
T133
I134
S135
K136
I137
ILE

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.48 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.292 0.239 , 0.296	Depositor DCC
R_{free} test set	907 reflections (5.12%)	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)	0.28 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[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	1.82	15/1004 (1.5%)	1.76	17/1345 (1.3%)
1	B	1.54	11/1024 (1.1%)	1.24	20/1373 (1.5%)
1	C	2.73	21/1029 (2.0%)	3.91	21/1379 (1.5%)
1	D	2.82	16/1014 (1.6%)	2.63	13/1359 (1.0%)
All	All	2.30	63/4071 (1.5%)	2.60	71/5456 (1.3%)

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 (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	48	GLU	CD-OE1	73.20	2.06	1.25
1	C	66	ARG	NE-CZ	72.14	2.26	1.33
1	A	68	LYS	CE-NZ	-30.41	0.73	1.49
1	D	23	ARG	CB-CG	-22.30	0.92	1.52
1	B	22	LYS	CG-CD	-21.95	0.77	1.52
1	A	23	ARG	CD-NE	-20.35	1.11	1.46
1	C	72	GLU	CB-CG	20.17	1.90	1.52
1	A	81	LYS	CB-CG	20.16	2.06	1.52
1	D	6	LYS	CD-CE	18.28	1.97	1.51
1	D	66	ARG	NE-CZ	18.21	1.56	1.33
1	B	136	LYS	CD-CE	-18.17	1.05	1.51
1	B	117	LYS	CA-CB	-17.34	1.15	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	72	GLU	CA-CB	-16.84	1.17	1.53
1	D	6	LYS	CE-NZ	-16.25	1.08	1.49
1	C	102	SER	CA-CB	-15.86	1.29	1.52
1	C	66	ARG	CZ-NH1	14.78	1.52	1.33
1	A	136	LYS	CD-CE	-14.74	1.14	1.51
1	B	72	GLU	CG-CD	14.14	1.73	1.51
1	A	59	ASP	CG-OD2	-13.88	0.93	1.25
1	B	101	ILE	CB-CG2	-13.51	1.10	1.52
1	A	22	LYS	CG-CD	-13.26	1.07	1.52
1	C	16	LYS	CG-CD	-12.70	1.09	1.52
1	B	11	LYS	CB-CG	-12.45	1.19	1.52
1	C	38	LYS	CD-CE	-12.12	1.21	1.51
1	C	71	LEU	CG-CD2	-12.00	1.07	1.51
1	A	72	GLU	CG-CD	-10.54	1.36	1.51
1	B	49	ASN	CG-OD1	-10.07	1.01	1.24
1	C	17	ASN	CB-CG	10.00	1.74	1.51
1	A	23	ARG	CB-CG	-9.86	1.25	1.52
1	C	81	LYS	CE-NZ	-9.32	1.25	1.49
1	D	11	LYS	CB-CG	-9.14	1.27	1.52
1	A	132	ARG	CD-NE	8.66	1.61	1.46
1	C	101	ILE	CB-CG1	8.37	1.77	1.54
1	C	66	ARG	CZ-NH2	8.37	1.44	1.33
1	B	6	LYS	CG-CD	-8.36	1.24	1.52
1	A	50	LYS	CG-CD	-8.13	1.24	1.52
1	D	68	LYS	CB-CG	-8.05	1.30	1.52
1	C	66	ARG	CD-NE	-7.88	1.33	1.46
1	B	108	ILE	CA-CB	-7.48	1.37	1.54
1	A	120	LYS	CD-CE	-7.46	1.32	1.51
1	D	98	LYS	CE-NZ	-7.30	1.30	1.49
1	A	72	GLU	CA-CB	-7.28	1.38	1.53
1	D	22	LYS	CD-CE	-7.15	1.33	1.51
1	C	71	LEU	CG-CD1	6.98	1.77	1.51
1	B	98	LYS	CE-NZ	-6.98	1.31	1.49
1	C	82	ASP	CG-OD2	6.70	1.40	1.25
1	C	117	LYS	CA-CB	6.63	1.68	1.53
1	D	67	ASP	CB-CG	-6.48	1.38	1.51
1	D	48	GLU	CB-CG	-6.48	1.39	1.52
1	C	11	LYS	CG-CD	-6.42	1.30	1.52
1	A	66	ARG	CZ-NH2	-6.26	1.25	1.33
1	C	97	LYS	CG-CD	-6.23	1.31	1.52
1	D	84	ILE	CB-CG1	-6.16	1.36	1.54
1	D	120	LYS	CB-CG	-6.16	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ARG	CG-CD	-6.11	1.36	1.51
1	C	50	LYS	CG-CD	-5.86	1.32	1.52
1	B	68	LYS	CG-CD	-5.68	1.33	1.52
1	D	66	ARG	CZ-NH1	-5.65	1.25	1.33
1	D	59	ASP	CB-CG	-5.30	1.40	1.51
1	C	17	ASN	CG-OD1	5.17	1.35	1.24
1	C	120	LYS	CD-CE	-5.06	1.38	1.51
1	C	79	MSE	CG-SE	-5.01	1.78	1.95
1	A	66	ARG	CZ-NH1	5.00	1.39	1.33

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	66	ARG	NE-CZ-NH1	-96.08	72.26	120.30
1	C	66	ARG	NE-CZ-NH2	-94.06	73.27	120.30
1	D	66	ARG	NE-CZ-NH1	-76.71	81.94	120.30
1	D	66	ARG	NE-CZ-NH2	-40.64	99.98	120.30
1	A	23	ARG	CD-NE-CZ	25.00	158.60	123.60
1	C	82	ASP	OD1-CG-OD2	-23.96	77.78	123.30
1	A	66	ARG	NE-CZ-NH1	-22.98	108.81	120.30
1	A	59	ASP	CB-CG-OD2	22.38	138.44	118.30
1	A	22	LYS	CB-CG-CD	19.06	161.16	111.60
1	A	66	ARG	NE-CZ-NH2	17.59	129.09	120.30
1	D	23	ARG	CA-CB-CG	16.49	149.67	113.40
1	C	66	ARG	NH1-CZ-NH2	-16.07	101.72	119.40
1	C	71	LEU	CB-CG-CD2	15.52	137.38	111.00
1	D	72	GLU	CB-CA-C	15.37	141.13	110.40
1	B	11	LYS	CA-CB-CG	15.36	147.20	113.40
1	C	16	LYS	CB-CG-CD	14.94	150.44	111.60
1	A	81	LYS	CA-CB-CG	-14.42	81.68	113.40
1	A	23	ARG	CG-CD-NE	13.17	139.46	111.80
1	B	9	LYS	CD-CE-NZ	12.04	139.38	111.70
1	C	71	LEU	CB-CG-CD1	-11.76	91.01	111.00
1	B	101	ILE	CG1-CB-CG2	11.72	137.18	111.40
1	C	16	LYS	CG-CD-CE	11.65	146.86	111.90
1	D	101	ILE	CB-CA-C	-10.94	89.72	111.60
1	A	59	ASP	OD1-CG-OD2	-10.54	103.28	123.30
1	D	72	GLU	CA-CB-CG	10.31	136.09	113.40
1	B	101	ILE	CA-CB-CG1	-10.26	91.50	111.00
1	D	66	ARG	CG-CD-NE	9.74	132.26	111.80
1	B	22	LYS	CB-CG-CD	9.26	135.67	111.60
1	C	72	GLU	CA-CB-CG	-9.20	93.17	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	117	LYS	CB-CA-C	9.10	128.61	110.40
1	A	132	ARG	CG-CD-NE	9.08	130.87	111.80
1	A	120	LYS	CD-CE-NZ	8.97	132.33	111.70
1	B	132	ARG	CA-CB-CG	8.85	132.88	113.40
1	C	17	ASN	CB-CG-ND2	-8.44	96.44	116.70
1	D	136	LYS	CB-CG-CD	-8.11	90.51	111.60
1	A	22	LYS	CG-CD-CE	8.00	135.89	111.90
1	A	23	ARG	CA-CB-CG	7.96	130.91	113.40
1	A	93	LEU	CA-CB-CG	7.83	133.31	115.30
1	C	97	LYS	CB-CG-CD	7.75	131.74	111.60
1	C	101	ILE	CA-CB-CG1	-7.50	96.74	111.00
1	B	6	LYS	CG-CD-CE	7.46	134.27	111.90
1	C	102	SER	N-CA-CB	7.18	121.28	110.50
1	B	108	ILE	CB-CA-C	6.94	125.47	111.60
1	B	117	LYS	CA-CB-CG	6.93	128.65	113.40
1	C	82	ASP	CB-CG-OD2	6.70	124.33	118.30
1	C	66	ARG	CD-NE-CZ	-6.62	114.33	123.60
1	C	17	ASN	CB-CG-OD1	-6.39	108.82	121.60
1	A	70	THR	CA-CB-CG2	6.27	121.18	112.40
1	B	11	LYS	CB-CG-CD	6.21	127.74	111.60
1	B	6	LYS	CB-CG-CD	6.18	127.66	111.60
1	B	101	ILE	CA-CB-CG2	5.99	122.88	110.90
1	A	68	LYS	CD-CE-NZ	5.99	125.47	111.70
1	D	120	LYS	CA-CB-CG	5.76	126.07	113.40
1	B	71	LEU	CA-CB-CG	5.73	128.47	115.30
1	C	17	ASN	CA-CB-CG	5.73	126.00	113.40
1	D	23	ARG	CD-NE-CZ	5.62	131.47	123.60
1	B	50	LYS	CG-CD-CE	5.57	128.60	111.90
1	D	48	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	B	108	ILE	CA-CB-CG2	5.47	121.84	110.90
1	A	120	LYS	CG-CD-CE	5.37	128.01	111.90
1	C	11	LYS	CB-CG-CD	5.35	125.51	111.60
1	C	102	SER	CB-CA-C	5.34	120.25	110.10
1	D	23	ARG	CB-CG-CD	5.33	125.47	111.60
1	D	66	ARG	CA-CB-CG	-5.33	101.67	113.40
1	B	68	LYS	CB-CG-CD	5.32	125.44	111.60
1	B	110	ASN	N-CA-CB	-5.31	101.04	110.60
1	B	132	ARG	CB-CG-CD	5.23	125.21	111.60
1	C	120	LYS	CG-CD-CE	5.21	127.55	111.90
1	A	24	HIS	CA-CB-CG	-5.19	104.78	113.60
1	B	101	ILE	CB-CG1-CD1	5.18	128.41	113.90
1	C	66	ARG	CG-CD-NE	5.09	122.50	111.80

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 (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	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
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:O	1:A:52:ILE:HG22	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:NE	1:D:23:ARG:CB	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:B:115:VAL:HB	1:B:119:ASN:HA	1.98	0.45
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:109:ILE:HG13	1:B:109:ILE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:112:LEU:HD23	1:D:112:LEU:HA	1.89	0.40
1:C:62:TYR:CG	1:D:38:LYS:HE3	2.56	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 (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	124/138 (90%)	119 (96%)	4 (3%)	1 (1%)	19	39
1	B	126/138 (91%)	122 (97%)	3 (2%)	1 (1%)	19	39
1	C	127/138 (92%)	119 (94%)	7 (6%)	1 (1%)	19	39
1	D	125/138 (91%)	119 (95%)	6 (5%)	0	100	100
All	All	502/552 (91%)	479 (95%)	20 (4%)	3 (1%)	25	47

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 (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	118/122 (97%)	110 (93%)	8 (7%)	16	32
1	B	120/122 (98%)	112 (93%)	8 (7%)	16	33
1	C	120/122 (98%)	115 (96%)	5 (4%)	30	55
1	D	119/122 (98%)	117 (98%)	2 (2%)	60	81
All	All	477/488 (98%)	454 (95%)	23 (5%)	25	49

All (23) 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	72	GLU
1	A	80	THR
1	A	97	LYS
1	A	98	LYS
1	B	3	ASP
1	B	29	GLU
1	B	39	ILE
1	B	42	LEU
1	B	84	ILE
1	B	93	LEU
1	B	101	ILE
1	B	137	ILE
1	C	67	ASP
1	C	71	LEU
1	C	82	ASP

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Mol	Chain	Res	Type
1	C	101	ILE
1	C	102	SER
1	D	80	THR
1	D	81	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	111	GLN

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	124/138 (89%)	0.21	4 (3%)	47	40	16, 25, 33, 44	20 (16%)
1	B	125/138 (90%)	0.10	1 (0%)	86	84	18, 25, 35, 61	25 (20%)
1	C	125/138 (90%)	0.12	2 (1%)	72	68	16, 22, 32, 49	21 (16%)
1	D	124/138 (89%)	0.28	6 (4%)	30	24	19, 27, 50, 68	24 (19%)
All	All	498/552 (90%)	0.18	13 (2%)	56	50	16, 25, 43, 68	90 (18%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	ILE	7.1
1	A	102	SER	5.2
1	A	108	ILE	2.8
1	C	103	GLY	2.7
1	D	92	ILE	2.6
1	D	52	ILE	2.5
1	A	55	VAL	2.4
1	D	83	VAL	2.4
1	D	46	ASP	2.1
1	D	66	ARG	2.1
1	A	47	ASP	2.1
1	D	132	ARG	2.1
1	C	10	VAL	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.