



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:37 PM UTC

PDB ID : 4P7T / pdb_00004p7t
Title : Structural insights into higher-order assembly and function of the bacterial microcompartment protein PduA
Authors : Pickersgill, R.W.; Frank, S.; Pang, A.; Warren, M.J.
Deposited on : 2014-03-27
Resolution : 1.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

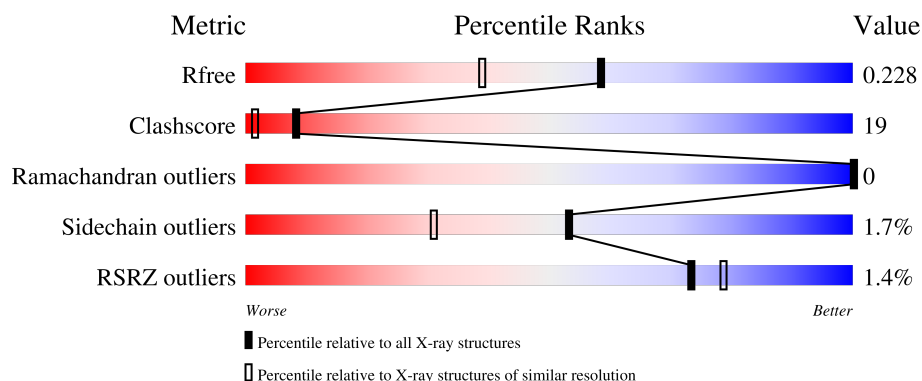
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	115	2% 43% 28% . 26%
1	B	115	% 60% 11% . 25%
1	C	115	2% 49% 15% . 36%
1	D	115	% 47% 23% . 25%
1	E	115	55% 17% . 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	115	% 54% 16% • 27%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3837 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 Polyhedral bodies.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	S	0	0	0
			600	373	106	118	3			
1	B	86	Total	C	N	O	S	0	0	0
			606	379	106	118	3			
1	C	74	Total	C	N	O	S	0	0	0
			512	319	91	99	3			
1	D	86	Total	C	N	O	S	0	0	0
			606	379	106	118	3			
1	E	86	Total	C	N	O	S	0	0	0
			606	379	106	118	3			
1	F	84	Total	C	N	O	S	0	0	0
			590	369	104	114	3			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B1VB62
A	0	SER	-	expression tag	UNP B1VB62
A	26	ASP	LYS	engineered mutation	UNP B1VB62
A	93	ARG	-	expression tag	UNP B1VB62
A	94	LEU	-	expression tag	UNP B1VB62
A	95	VAL	-	expression tag	UNP B1VB62
A	96	LYS	-	expression tag	UNP B1VB62
A	97	ASP	-	expression tag	UNP B1VB62
A	98	PRO	-	expression tag	UNP B1VB62
A	99	ALA	-	expression tag	UNP B1VB62
A	100	ALA	-	expression tag	UNP B1VB62
A	101	ASN	-	expression tag	UNP B1VB62
A	102	LYS	-	expression tag	UNP B1VB62
A	103	ALA	-	expression tag	UNP B1VB62
A	104	ARG	-	expression tag	UNP B1VB62
A	105	LYS	-	expression tag	UNP B1VB62
A	106	GLU	-	expression tag	UNP B1VB62

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ALA	-	expression tag	UNP B1VB62
A	108	GLU	-	expression tag	UNP B1VB62
A	109	LEU	-	expression tag	UNP B1VB62
A	110	ALA	-	expression tag	UNP B1VB62
A	111	ALA	-	expression tag	UNP B1VB62
A	112	ALA	-	expression tag	UNP B1VB62
A	113	THR	-	expression tag	UNP B1VB62
B	-1	GLY	-	expression tag	UNP B1VB62
B	0	SER	-	expression tag	UNP B1VB62
B	26	ASP	LYS	engineered mutation	UNP B1VB62
B	93	ARG	-	expression tag	UNP B1VB62
B	94	LEU	-	expression tag	UNP B1VB62
B	95	VAL	-	expression tag	UNP B1VB62
B	96	LYS	-	expression tag	UNP B1VB62
B	97	ASP	-	expression tag	UNP B1VB62
B	98	PRO	-	expression tag	UNP B1VB62
B	99	ALA	-	expression tag	UNP B1VB62
B	100	ALA	-	expression tag	UNP B1VB62
B	101	ASN	-	expression tag	UNP B1VB62
B	102	LYS	-	expression tag	UNP B1VB62
B	103	ALA	-	expression tag	UNP B1VB62
B	104	ARG	-	expression tag	UNP B1VB62
B	105	LYS	-	expression tag	UNP B1VB62
B	106	GLU	-	expression tag	UNP B1VB62
B	107	ALA	-	expression tag	UNP B1VB62
B	108	GLU	-	expression tag	UNP B1VB62
B	109	LEU	-	expression tag	UNP B1VB62
B	110	ALA	-	expression tag	UNP B1VB62
B	111	ALA	-	expression tag	UNP B1VB62
B	112	ALA	-	expression tag	UNP B1VB62
B	113	THR	-	expression tag	UNP B1VB62
C	-1	GLY	-	expression tag	UNP B1VB62
C	0	SER	-	expression tag	UNP B1VB62
C	26	ASP	LYS	engineered mutation	UNP B1VB62
C	93	ARG	-	expression tag	UNP B1VB62
C	94	LEU	-	expression tag	UNP B1VB62
C	95	VAL	-	expression tag	UNP B1VB62
C	96	LYS	-	expression tag	UNP B1VB62
C	97	ASP	-	expression tag	UNP B1VB62
C	98	PRO	-	expression tag	UNP B1VB62
C	99	ALA	-	expression tag	UNP B1VB62
C	100	ALA	-	expression tag	UNP B1VB62

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	101	ASN	-	expression tag	UNP B1VB62
C	102	LYS	-	expression tag	UNP B1VB62
C	103	ALA	-	expression tag	UNP B1VB62
C	104	ARG	-	expression tag	UNP B1VB62
C	105	LYS	-	expression tag	UNP B1VB62
C	106	GLU	-	expression tag	UNP B1VB62
C	107	ALA	-	expression tag	UNP B1VB62
C	108	GLU	-	expression tag	UNP B1VB62
C	109	LEU	-	expression tag	UNP B1VB62
C	110	ALA	-	expression tag	UNP B1VB62
C	111	ALA	-	expression tag	UNP B1VB62
C	112	ALA	-	expression tag	UNP B1VB62
C	113	THR	-	expression tag	UNP B1VB62
D	-1	GLY	-	expression tag	UNP B1VB62
D	0	SER	-	expression tag	UNP B1VB62
D	26	ASP	LYS	engineered mutation	UNP B1VB62
D	93	ARG	-	expression tag	UNP B1VB62
D	94	LEU	-	expression tag	UNP B1VB62
D	95	VAL	-	expression tag	UNP B1VB62
D	96	LYS	-	expression tag	UNP B1VB62
D	97	ASP	-	expression tag	UNP B1VB62
D	98	PRO	-	expression tag	UNP B1VB62
D	99	ALA	-	expression tag	UNP B1VB62
D	100	ALA	-	expression tag	UNP B1VB62
D	101	ASN	-	expression tag	UNP B1VB62
D	102	LYS	-	expression tag	UNP B1VB62
D	103	ALA	-	expression tag	UNP B1VB62
D	104	ARG	-	expression tag	UNP B1VB62
D	105	LYS	-	expression tag	UNP B1VB62
D	106	GLU	-	expression tag	UNP B1VB62
D	107	ALA	-	expression tag	UNP B1VB62
D	108	GLU	-	expression tag	UNP B1VB62
D	109	LEU	-	expression tag	UNP B1VB62
D	110	ALA	-	expression tag	UNP B1VB62
D	111	ALA	-	expression tag	UNP B1VB62
D	112	ALA	-	expression tag	UNP B1VB62
D	113	THR	-	expression tag	UNP B1VB62
E	-1	GLY	-	expression tag	UNP B1VB62
E	0	SER	-	expression tag	UNP B1VB62
E	26	ASP	LYS	engineered mutation	UNP B1VB62
E	93	ARG	-	expression tag	UNP B1VB62
E	94	LEU	-	expression tag	UNP B1VB62

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	95	VAL	-	expression tag	UNP B1VB62
E	96	LYS	-	expression tag	UNP B1VB62
E	97	ASP	-	expression tag	UNP B1VB62
E	98	PRO	-	expression tag	UNP B1VB62
E	99	ALA	-	expression tag	UNP B1VB62
E	100	ALA	-	expression tag	UNP B1VB62
E	101	ASN	-	expression tag	UNP B1VB62
E	102	LYS	-	expression tag	UNP B1VB62
E	103	ALA	-	expression tag	UNP B1VB62
E	104	ARG	-	expression tag	UNP B1VB62
E	105	LYS	-	expression tag	UNP B1VB62
E	106	GLU	-	expression tag	UNP B1VB62
E	107	ALA	-	expression tag	UNP B1VB62
E	108	GLU	-	expression tag	UNP B1VB62
E	109	LEU	-	expression tag	UNP B1VB62
E	110	ALA	-	expression tag	UNP B1VB62
E	111	ALA	-	expression tag	UNP B1VB62
E	112	ALA	-	expression tag	UNP B1VB62
E	113	THR	-	expression tag	UNP B1VB62
F	-1	GLY	-	expression tag	UNP B1VB62
F	0	SER	-	expression tag	UNP B1VB62
F	26	ASP	LYS	engineered mutation	UNP B1VB62
F	93	ARG	-	expression tag	UNP B1VB62
F	94	LEU	-	expression tag	UNP B1VB62
F	95	VAL	-	expression tag	UNP B1VB62
F	96	LYS	-	expression tag	UNP B1VB62
F	97	ASP	-	expression tag	UNP B1VB62
F	98	PRO	-	expression tag	UNP B1VB62
F	99	ALA	-	expression tag	UNP B1VB62
F	100	ALA	-	expression tag	UNP B1VB62
F	101	ASN	-	expression tag	UNP B1VB62
F	102	LYS	-	expression tag	UNP B1VB62
F	103	ALA	-	expression tag	UNP B1VB62
F	104	ARG	-	expression tag	UNP B1VB62
F	105	LYS	-	expression tag	UNP B1VB62
F	106	GLU	-	expression tag	UNP B1VB62
F	107	ALA	-	expression tag	UNP B1VB62
F	108	GLU	-	expression tag	UNP B1VB62
F	109	LEU	-	expression tag	UNP B1VB62
F	110	ALA	-	expression tag	UNP B1VB62
F	111	ALA	-	expression tag	UNP B1VB62
F	112	ALA	-	expression tag	UNP B1VB62

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	113	THR	-	expression tag	UNP B1VB62

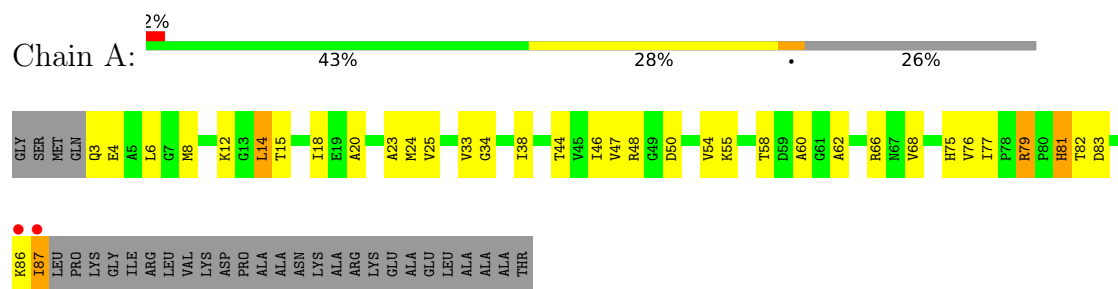
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	52	Total O 52 52	0	0
2	B	41	Total O 41 41	0	0
2	C	35	Total O 35 35	0	0
2	D	53	Total O 53 53	0	0
2	E	76	Total O 76 76	0	0
2	F	60	Total O 60 60	0	0

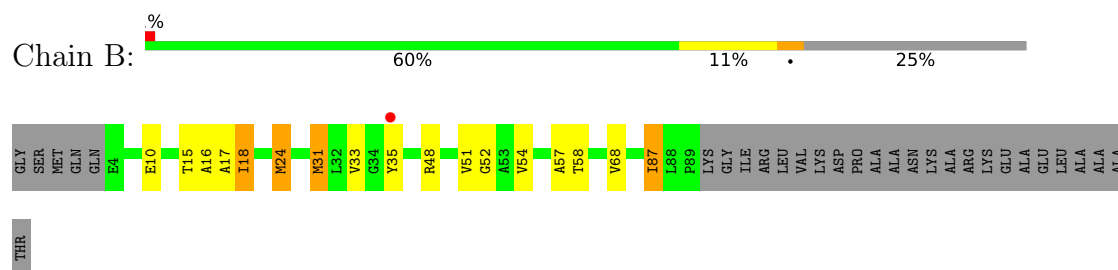
3 Residue-property plots [i](#)

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.

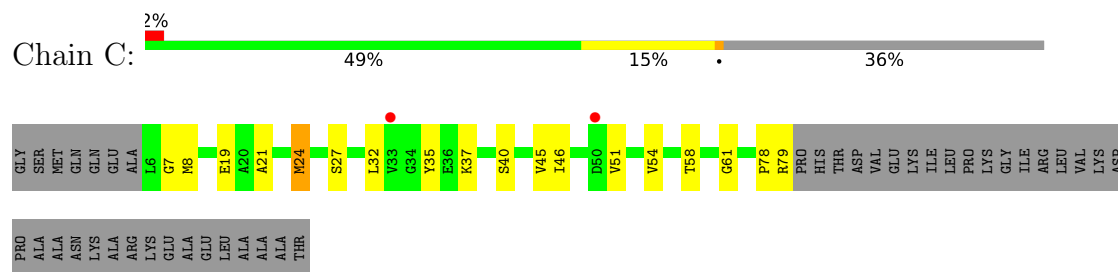
• Molecule 1: Polyhedral bodies



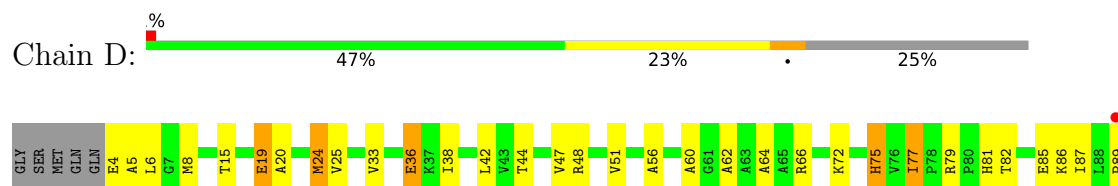
• Molecule 1: Polyhedral bodies



• Molecule 1: Polyhedral bodies



• Molecule 1: Polyhedral bodies



LYS	GLY	ILE	ARG	LEU	VAL	LYS	ASP	PRO	ALA	ALA	ASN	LYS	ALA	ARG	LYS	GLU	ALA	GLU	LEU	ALA	ALA	ALA	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 1: Polyhedral bodies



GLY	SER	MET	GLN	GLN	E4	A5	L6	G7	M8	V9	T15	A16	E19	M24	M31	G41	V45	R48	V51	G52	A53	V64	K55	A56	A57	T58	D59	A64	V68	K72	A73	V74	K86	P89	LYS	GLY	ILE	ARG	LEU	VAL	LYS	ASP	PRO	ALA	ALA	ASN
-----	-----	-----	-----	-----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LYS	ALA	ARG	LYS	GLU	ALA	GLU	LEU	ALA	ALA	ALA	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

● Molecule 1: Polyhedral bodies



GLY	SER	MET	GLN	GLU	A5	L6	G7	K12	G13	L14	T15	A16	A17	I18	E19	A20	M24	M31	L32	V33	G34	G49	D50	V51	A57	T58	D59	A60	G61	H75	V76	I77	P78	H81	T82	I87	L88	PRO	LYS	GLY	ILE	ARG	LEU	VAL	LYS	ASP	PRO	ALA	ALA	ASN
-----	-----	-----	-----	-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LYS	ALA	ARG	LYS	GLU	ALA	GLU	LEU	ALA	ALA	ALA	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.24Å 93.30Å 63.05Å 90.00° 105.03° 90.00°	Depositor
Resolution (Å)	60.89 – 1.72 60.89 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.3 (60.89-1.72) 99.3 (60.89-1.72)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.180 , 0.230 0.178 , 0.228	Depositor DCC
R_{free} test set	2706 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3837	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% 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	1.76	10/604 (1.7%)	1.48	7/819 (0.9%)
1	B	1.66	3/611 (0.5%)	1.58	8/830 (1.0%)
1	C	1.57	3/514 (0.6%)	1.48	3/696 (0.4%)
1	D	1.87	14/611 (2.3%)	1.71	6/830 (0.7%)
1	E	1.91	5/611 (0.8%)	1.56	5/830 (0.6%)
1	F	1.93	10/594 (1.7%)	1.68	6/806 (0.7%)
All	All	1.79	45/3545 (1.3%)	1.59	35/4811 (0.7%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77	ILE	N-CA	8.29	1.52	1.46
1	C	24	MET	SD-CE	-7.34	1.61	1.79
1	F	76	VAL	CA-CB	7.11	1.63	1.54
1	A	20	ALA	N-CA	7.06	1.54	1.46
1	A	23	ALA	N-CA	6.96	1.54	1.46
1	A	47	VAL	CA-C	6.39	1.60	1.52
1	F	34	GLY	N-CA	6.35	1.52	1.45
1	A	44	THR	N-CA	6.30	1.53	1.46
1	F	77	ILE	N-CA	6.26	1.51	1.46
1	D	44	THR	N-CA	6.17	1.53	1.46
1	A	23	ALA	C-O	6.15	1.31	1.24
1	A	14	LEU	CA-C	6.12	1.60	1.52
1	D	36	GLU	CA-C	-6.00	1.45	1.52
1	D	75	HIS	CA-C	-5.99	1.45	1.52
1	E	68	VAL	N-CA	5.92	1.52	1.46
1	E	4	GLU	N-CA	5.89	1.57	1.46
1	E	45	VAL	CA-C	5.86	1.60	1.52
1	D	60	ALA	CA-C	5.81	1.60	1.52
1	D	24	MET	SD-CE	-5.81	1.65	1.79
1	D	15	THR	N-CA	5.79	1.53	1.46
1	E	64	ALA	C-O	5.72	1.30	1.24
1	D	47	VAL	N-CA	5.71	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	61	GLY	N-CA	5.64	1.53	1.45
1	B	10	GLU	CA-C	-5.61	1.46	1.52
1	A	60	ALA	CA-C	5.54	1.59	1.52
1	F	16	ALA	C-O	5.45	1.30	1.24
1	F	7	GLY	CA-C	5.45	1.56	1.51
1	F	76	VAL	N-CA	-5.44	1.39	1.46
1	B	18	ILE	CA-C	5.38	1.59	1.52
1	D	56	ALA	CA-C	5.33	1.59	1.52
1	D	79	ARG	CA-CB	5.30	1.60	1.53
1	E	59	ASP	CA-C	5.27	1.59	1.52
1	A	24	MET	N-CA	5.25	1.52	1.46
1	F	59	ASP	CA-C	5.23	1.59	1.52
1	D	19	GLU	CA-C	5.22	1.59	1.52
1	D	60	ALA	N-CA	5.22	1.52	1.46
1	D	64	ALA	N-CA	5.21	1.52	1.46
1	B	16	ALA	N-CA	5.20	1.52	1.46
1	F	49	GLY	N-CA	5.16	1.50	1.45
1	D	64	ALA	C-O	5.16	1.30	1.24
1	A	81	HIS	CG-CD2	5.13	1.41	1.35
1	A	34	GLY	N-CA	5.12	1.49	1.45
1	C	54	VAL	N-CA	5.11	1.52	1.46
1	F	61	GLY	N-CA	5.10	1.52	1.45
1	F	14	LEU	CA-C	5.06	1.59	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	MET	CG-SD-CE	-16.93	63.66	100.90
1	C	24	MET	CG-SD-CE	-9.72	79.51	100.90
1	A	24	MET	CG-SD-CE	-9.21	80.63	100.90
1	F	31	MET	CG-SD-CE	-9.03	81.03	100.90
1	F	24	MET	CG-SD-CE	-9.03	81.04	100.90
1	B	17	ALA	N-CA-C	8.47	120.52	111.28
1	D	87	ILE	N-CA-C	7.56	119.39	112.29
1	E	6	LEU	CA-C-N	-6.82	117.01	121.65
1	E	6	LEU	C-N-CA	-6.82	117.01	121.65
1	B	33	VAL	N-CA-C	-6.78	104.39	111.58
1	B	24	MET	CG-SD-CE	-6.50	86.59	100.90
1	A	68	VAL	N-CA-C	-6.46	106.50	112.96
1	B	51	VAL	N-CA-C	6.35	117.10	110.62
1	E	19	GLU	N-CA-C	-6.25	104.47	111.28
1	E	15	THR	N-CA-C	-6.17	104.47	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	8	MET	CG-SD-CE	-6.13	87.42	100.90
1	A	79	ARG	CB-CA-C	-5.76	102.21	111.02
1	C	7	GLY	N-CA-C	-5.62	101.63	111.46
1	F	51	VAL	N-CA-C	5.52	116.25	110.62
1	F	78	PRO	CA-C-N	-5.51	115.65	122.42
1	F	78	PRO	C-N-CA	-5.51	115.65	122.42
1	B	68	VAL	CB-CA-C	-5.47	106.04	111.30
1	F	33	VAL	N-CA-C	-5.43	105.83	111.58
1	B	52	GLY	CA-C-N	5.34	127.44	120.28
1	B	52	GLY	C-N-CA	5.34	127.44	120.28
1	D	60	ALA	CA-C-N	5.33	125.86	119.94
1	D	60	ALA	C-N-CA	5.33	125.86	119.94
1	B	87	ILE	N-CA-C	5.28	117.18	112.17
1	C	27	SER	N-CA-C	5.25	119.54	113.18
1	A	15	THR	O-C-N	5.23	127.53	122.09
1	A	68	VAL	CB-CA-C	-5.19	106.49	111.06
1	A	12	LYS	CA-C-N	-5.11	111.39	121.41
1	A	12	LYS	C-N-CA	-5.11	111.39	121.41
1	D	86	LYS	N-CA-C	5.10	117.58	111.71
1	E	53	ALA	N-CA-C	-5.01	105.90	111.36

There are no chirality outliers.

There are no planarity outliers.

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	600	0	620	39	0
1	B	606	0	630	14	0
1	C	512	0	537	23	0
1	D	606	0	630	38	0
1	E	606	0	630	25	0
1	F	590	0	617	19	0
2	A	52	0	0	11	0
2	B	41	0	0	2	0
2	C	35	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	53	0	0	6	0
2	E	76	0	0	8	1
2	F	60	0	0	3	1
All	All	3837	0	3664	138	1

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 19.

All (138) 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:D:6:LEU:HD23	1:D:48:ARG:CD	1.66	1.25
1:E:24:MET:CE	1:E:58:THR:HA	1.70	1.19
1:B:15:THR:HG23	1:C:8:MET:CE	1.74	1.18
1:A:87:ILE:HD12	1:A:87:ILE:O	1.42	1.17
1:E:24:MET:HE2	1:E:58:THR:CA	1.82	1.09
1:B:15:THR:HG23	1:C:8:MET:HE3	1.09	1.07
1:D:6:LEU:CD2	1:D:48:ARG:CD	2.34	1.05
1:D:6:LEU:HD23	1:D:48:ARG:HD2	1.36	1.05
1:D:6:LEU:CD2	1:D:48:ARG:HD3	1.87	1.04
1:A:58:THR:HB	2:A:250:HOH:O	0.85	1.03
1:B:31:MET:HE2	2:B:217:HOH:O	1.61	1.00
1:F:5:ALA:N	2:F:258:HOH:O	1.97	0.96
1:A:48:ARG:CZ	2:A:251:HOH:O	2.15	0.91
1:B:15:THR:CG2	1:C:8:MET:HE3	2.00	0.91
1:A:8:MET:HG2	1:A:46:ILE:HD13	1.56	0.87
1:E:24:MET:HE2	1:E:58:THR:HA	0.88	0.86
1:C:32:LEU:HD11	1:C:45:VAL:HG13	1.59	0.85
1:D:6:LEU:HD21	1:D:48:ARG:HD3	1.57	0.84
1:D:48:ARG:HG3	2:D:241:HOH:O	1.77	0.83
1:A:25:VAL:HG23	2:E:240:HOH:O	1.82	0.79
1:D:36:GLU:HG2	1:D:89:PRO:HG3	1.64	0.79
1:C:8:MET:HG3	2:C:234:HOH:O	1.83	0.79
1:E:9:VAL:HG23	1:E:24:MET:HE1	1.66	0.78
1:E:51:VAL:HG12	1:E:55:LYS:HE3	1.67	0.77
1:E:9:VAL:HG21	1:E:24:MET:HE3	1.65	0.76
1:E:4:GLU:N	2:E:267:HOH:O	2.19	0.75
1:A:6:LEU:HD13	1:A:48:ARG:HH11	1.50	0.75
1:D:81:HIS:CD2	2:E:251:HOH:O	2.39	0.75
1:D:81:HIS:HD2	2:E:251:HOH:O	1.70	0.74
1:A:87:ILE:C	2:A:229:HOH:O	2.32	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:HIS:NE2	1:F:77:ILE:HD11	2.04	0.71
1:A:6:LEU:HB2	1:A:48:ARG:NH1	2.06	0.71
1:A:87:ILE:O	1:A:87:ILE:CD1	2.32	0.71
1:C:8:MET:HE2	2:C:234:HOH:O	1.90	0.70
1:E:9:VAL:CG2	1:E:24:MET:CE	2.70	0.70
1:A:58:THR:HG23	2:A:241:HOH:O	1.93	0.67
1:C:79:ARG:C	2:C:214:HOH:O	2.37	0.67
1:A:58:THR:HG21	1:A:76:VAL:CG2	2.25	0.66
1:F:5:ALA:N	2:F:230:HOH:O	2.27	0.66
1:A:3:GLN:HB3	1:A:50:ASP:HA	1.77	0.66
1:B:15:THR:CG2	1:C:8:MET:CE	2.65	0.66
1:A:79:ARG:NE	2:A:201:HOH:O	2.30	0.65
1:E:9:VAL:CG2	1:E:24:MET:HE1	2.27	0.65
1:A:81:HIS:HE1	2:C:207:HOH:O	1.80	0.65
1:D:33:VAL:CG2	1:D:48:ARG:HG2	2.28	0.64
1:D:6:LEU:HD23	1:D:48:ARG:NE	2.13	0.64
1:E:31:MET:HE3	1:E:48:ARG:HG3	1.79	0.62
1:B:24:MET:HG2	1:B:57:ALA:O	1.98	0.62
1:B:15:THR:HG23	1:C:8:MET:HE1	1.77	0.61
1:A:87:ILE:HD13	1:C:35:TYR:CE2	2.36	0.61
1:E:9:VAL:CG2	1:E:24:MET:HE3	2.31	0.61
1:E:9:VAL:HG23	1:E:24:MET:CE	2.30	0.61
1:D:6:LEU:CD2	1:D:48:ARG:NE	2.63	0.61
1:D:25:VAL:HG12	1:F:81:HIS:CD2	2.36	0.60
1:A:3:GLN:HG2	2:A:208:HOH:O	2.02	0.60
1:A:48:ARG:NE	2:A:251:HOH:O	2.30	0.59
1:E:86:LYS:HD3	2:E:212:HOH:O	2.02	0.59
1:A:81:HIS:HD2	1:A:83:ASP:H	1.51	0.59
1:D:25:VAL:HG11	1:F:81:HIS:ND1	2.19	0.58
1:D:75:HIS:NE2	1:D:77:ILE:HD11	2.19	0.58
2:B:236:HOH:O	1:C:79:ARG:HB3	2.04	0.57
1:E:9:VAL:HG21	1:E:24:MET:CE	2.35	0.57
2:D:231:HOH:O	1:F:77:ILE:HD12	2.04	0.57
1:F:12:LYS:HD3	2:F:254:HOH:O	2.04	0.57
1:A:33:VAL:CG2	1:A:48:ARG:HG2	2.35	0.57
1:F:31:MET:HE1	1:F:33:VAL:HG22	1.86	0.56
1:A:87:ILE:HD12	1:A:87:ILE:C	2.26	0.56
1:A:75:HIS:NE2	1:A:77:ILE:HD11	2.20	0.56
1:D:19:GLU:OE1	1:F:77:ILE:HD11	2.04	0.56
1:B:31:MET:HE3	1:B:48:ARG:HH11	1.72	0.55
1:C:8:MET:HG2	1:C:46:ILE:HG12	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:VAL:HG23	2:D:237:HOH:O	2.07	0.53
1:A:83:ASP:HA	1:A:86:LYS:HE3	1.90	0.53
1:E:24:MET:HG2	1:E:57:ALA:O	2.08	0.53
1:C:8:MET:CG	2:C:234:HOH:O	2.50	0.53
1:D:20:ALA:O	1:D:24:MET:HG3	2.09	0.52
1:D:75:HIS:NE2	1:D:77:ILE:CD1	2.73	0.52
1:D:77:ILE:HD11	1:E:19:GLU:OE1	2.09	0.52
1:D:25:VAL:O	2:D:222:HOH:O	2.19	0.52
1:C:32:LEU:CD1	1:C:45:VAL:HG13	2.37	0.52
1:A:58:THR:HG21	1:A:76:VAL:HG23	1.92	0.51
1:D:38:ILE:HG13	1:E:41:GLY:HA2	1.92	0.51
1:A:75:HIS:CD2	1:A:77:ILE:HD11	2.47	0.50
1:F:75:HIS:NE2	1:F:77:ILE:CD1	2.74	0.50
1:B:18:ILE:HD13	1:B:35:TYR:OH	2.12	0.50
1:B:18:ILE:HD13	1:B:35:TYR:CZ	2.47	0.49
1:E:4:GLU:N	2:E:252:HOH:O	2.45	0.49
1:A:8:MET:HG2	1:A:46:ILE:CD1	2.36	0.48
1:D:25:VAL:CG1	1:F:81:HIS:CE1	2.97	0.48
1:E:24:MET:HE1	1:E:58:THR:HG22	1.94	0.48
1:C:24:MET:HE3	1:C:58:THR:HA	1.94	0.48
1:E:31:MET:HE2	2:E:231:HOH:O	2.14	0.47
1:D:77:ILE:CD1	1:E:19:GLU:OE1	2.62	0.47
1:D:24:MET:HB3	1:D:24:MET:HE2	1.87	0.47
1:D:25:VAL:HG11	1:F:81:HIS:CG	2.50	0.47
1:D:25:VAL:CG1	1:F:81:HIS:CG	2.98	0.47
1:D:48:ARG:NH1	1:D:85:GLU:OE1	2.40	0.46
1:F:31:MET:HB3	1:F:31:MET:HE2	1.49	0.46
1:A:33:VAL:HG21	1:A:48:ARG:HG2	1.97	0.46
1:E:86:LYS:HD3	2:E:209:HOH:O	2.15	0.46
1:A:38:ILE:HG22	1:C:37:LYS:HD3	1.97	0.46
1:A:79:ARG:NH2	2:A:201:HOH:O	2.49	0.46
1:A:77:ILE:HD11	1:C:19:GLU:OE1	2.16	0.46
1:D:62:ALA:O	1:D:66:ARG:HG3	2.15	0.46
1:C:8:MET:HE3	1:C:8:MET:HB2	1.81	0.45
1:D:33:VAL:HG21	1:D:48:ARG:HG2	1.99	0.45
1:C:79:ARG:HD2	1:C:79:ARG:HA	1.48	0.45
1:C:51:VAL:HG23	2:C:215:HOH:O	2.17	0.45
1:A:3:GLN:HB3	1:A:50:ASP:CA	2.44	0.44
1:C:78:PRO:O	1:C:79:ARG:HB3	2.18	0.44
1:C:78:PRO:O	1:C:79:ARG:CB	2.65	0.44
1:A:58:THR:CG2	2:A:241:HOH:O	2.60	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LEU:HD11	1:A:18:ILE:HD11	1.99	0.44
1:D:25:VAL:HG11	1:F:81:HIS:CE1	2.53	0.44
1:D:75:HIS:CD2	1:D:77:ILE:HD11	2.51	0.44
1:A:54:VAL:O	1:A:58:THR:HG22	2.19	0.43
1:A:4:GLU:OE2	1:A:79:ARG:HG2	2.18	0.43
1:B:31:MET:CE	1:B:48:ARG:HH11	2.31	0.43
1:D:82:THR:O	1:D:85:GLU:HG2	2.18	0.43
1:F:20:ALA:O	1:F:24:MET:HG3	2.19	0.43
1:F:24:MET:HG2	1:F:57:ALA:O	2.19	0.42
1:E:16:ALA:HA	1:E:68:VAL:CG2	2.49	0.42
1:A:55:LYS:NZ	2:A:203:HOH:O	2.38	0.42
1:D:89:PRO:C	2:D:215:HOH:O	2.63	0.42
1:E:8:MET:HE2	1:E:8:MET:HB2	1.82	0.42
1:D:4:GLU:HG2	2:D:245:HOH:O	2.20	0.42
1:E:72:LYS:HA	1:E:72:LYS:HD2	1.84	0.42
1:D:5:ALA:HB2	1:D:51:VAL:HG22	2.03	0.41
1:B:87:ILE:HD12	1:F:18:ILE:HD13	2.02	0.41
1:C:21:ALA:HB2	1:C:45:VAL:HG11	2.01	0.41
1:A:77:ILE:HD12	2:C:216:HOH:O	2.20	0.41
1:A:79:ARG:CZ	2:A:201:HOH:O	2.67	0.41
1:A:75:HIS:NE2	1:A:77:ILE:CD1	2.83	0.41
1:B:31:MET:CE	1:B:48:ARG:HD2	2.51	0.41
1:D:42:LEU:CD2	1:D:72:LYS:HG3	2.50	0.41
1:B:54:VAL:O	1:B:58:THR:HG23	2.21	0.40
1:A:62:ALA:O	1:A:66:ARG:HG3	2.21	0.40
1:D:25:VAL:CG1	1:F:81:HIS:CD2	3.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:232:HOH:O	2:F:204:HOH:O[2_756]	2.17	0.03

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	83/115 (72%)	82 (99%)	1 (1%)	0	100	100
1	B	84/115 (73%)	84 (100%)	0	0	100	100
1	C	72/115 (63%)	72 (100%)	0	0	100	100
1	D	84/115 (73%)	84 (100%)	0	0	100	100
1	E	84/115 (73%)	83 (99%)	1 (1%)	0	100	100
1	F	82/115 (71%)	81 (99%)	1 (1%)	0	100	100
All	All	489/690 (71%)	486 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	60/81 (74%)	58 (97%)	2 (3%)	33	10
1	B	61/81 (75%)	60 (98%)	1 (2%)	55	34
1	C	50/81 (62%)	49 (98%)	1 (2%)	48	26
1	D	61/81 (75%)	61 (100%)	0	100	100
1	E	61/81 (75%)	60 (98%)	1 (2%)	55	34
1	F	59/81 (73%)	58 (98%)	1 (2%)	53	31
All	All	352/486 (72%)	346 (98%)	6 (2%)	53	31

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	THR
1	A	87	ILE
1	B	31	MET
1	C	40	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	74	VAL
1	F	82	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	B	81	HIS
1	C	67	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	85/115 (73%)	0.29	2 (2%) 59 67	19, 27, 47, 78	0
1	B	86/115 (74%)	0.34	1 (1%) 76 81	20, 27, 47, 54	0
1	C	74/115 (64%)	0.42	2 (2%) 56 64	21, 31, 45, 59	0
1	D	86/115 (74%)	0.05	1 (1%) 76 81	16, 23, 43, 54	0
1	E	86/115 (74%)	-0.25	0 100 100	16, 22, 32, 39	0
1	F	84/115 (73%)	-0.24	1 (1%) 76 81	15, 21, 36, 50	0
All	All	501/690 (72%)	0.09	7 (1%) 73 79	15, 25, 44, 78	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	ILE	5.9
1	F	87	ILE	2.8
1	A	86	LYS	2.5
1	D	89	PRO	2.5
1	C	33	VAL	2.3
1	B	35	TYR	2.3
1	C	50	ASP	2.2

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.