Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:33 PM GMT

PDB ID	:	4P7T
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
http://wwpdb.org/validation/2016/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:

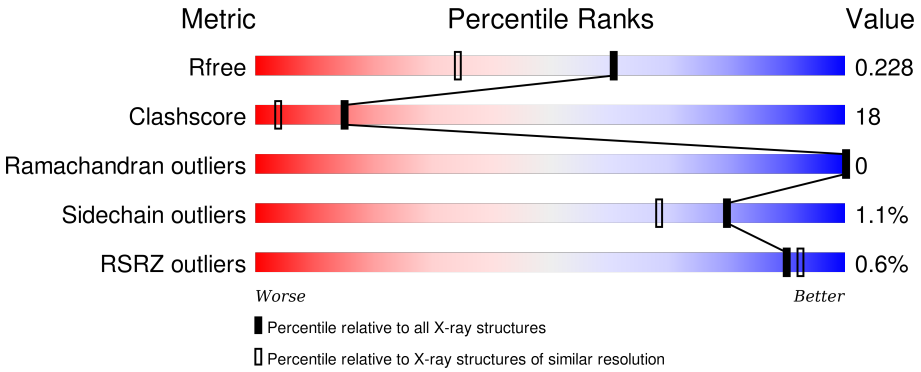
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

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. 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	115	2% 50% 22% • 26%
1	B	115	64% 10% • 25%
1	C	115	53% 11% 36%
1	D	115	% 54% 18% • 25%
1	E	115	58% 15% • 25%

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Mol	Chain	Length	Quality of chain
1	F	115	

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

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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

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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

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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

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

- Molecule 2 is water.

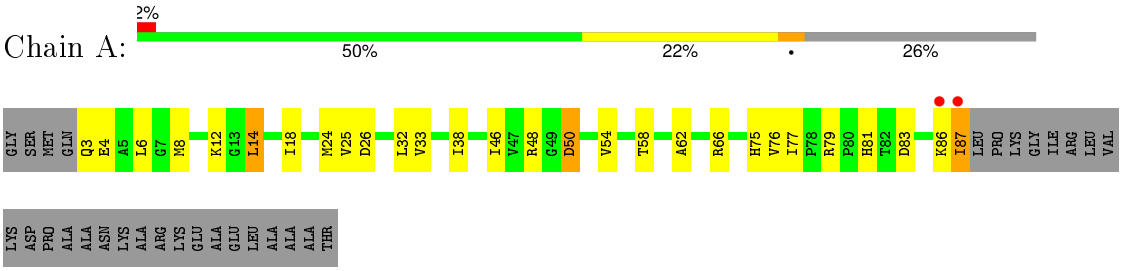
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	52	Total O 52 52	0	0
2	B	41	Total O 41 41	0	0
2	C	35	Total O 35 35	0	0
2	D	53	Total O 53 53	0	0
2	E	76	Total O 76 76	0	0
2	F	60	Total O 60 60	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

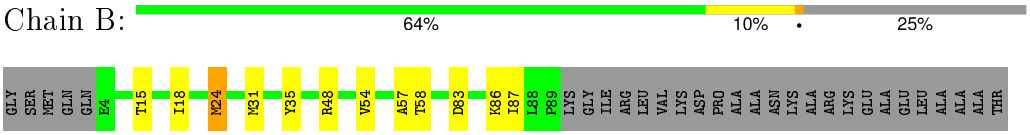
- Molecule 1: Polyhedral bodies

Chain A:



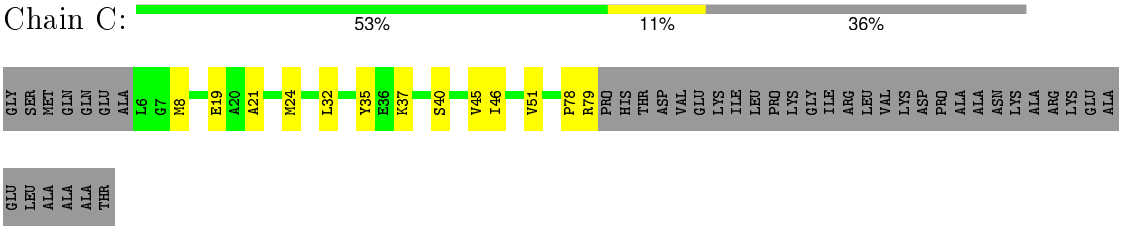
- Molecule 1: Polyhedral bodies

Chain B:



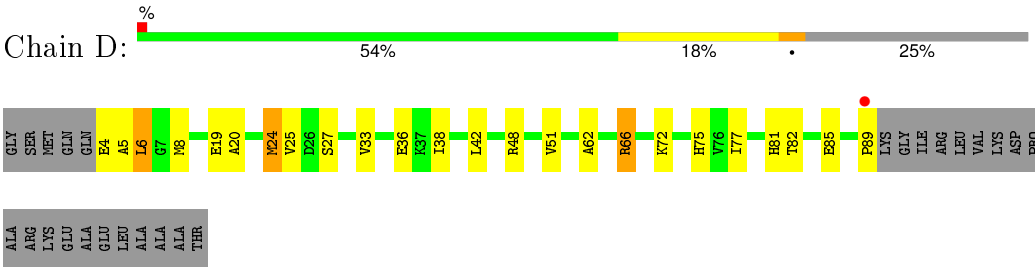
- Molecule 1: Polyhedral bodies

Chain C:



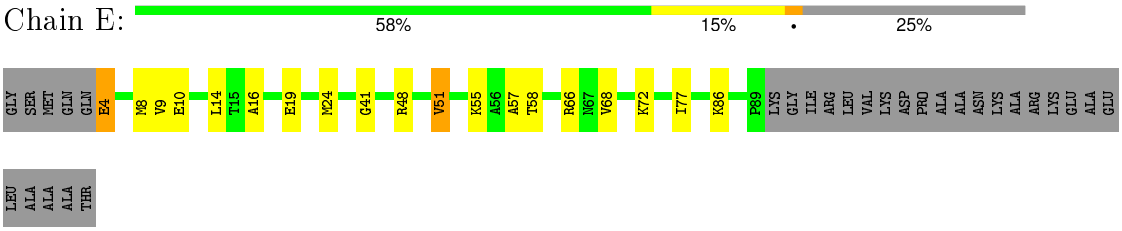
- Molecule 1: Polyhedral bodies

Chain D:



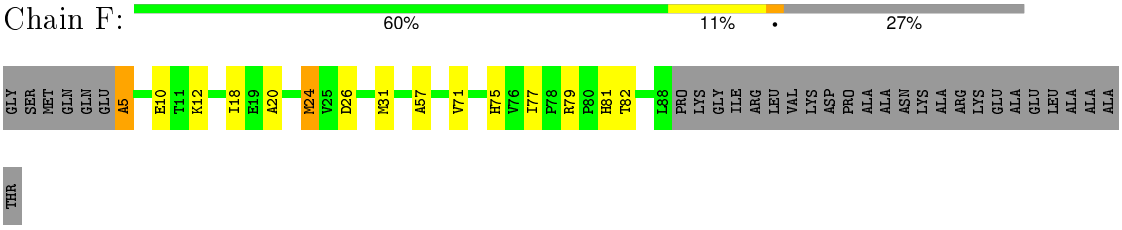
- Molecule 1: Polyhedral bodies

Chain E:



- Molecule 1: Polyhedral bodies

Chain F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.35%)	DCC
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 52.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 53299 reflections (0.002%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.18	0/604	1.25	6/819 (0.7%)
1	B	1.17	0/611	1.19	2/830 (0.2%)
1	C	1.06	0/514	1.22	1/696 (0.1%)
1	D	1.27	1/611 (0.2%)	1.46	4/830 (0.5%)
1	E	1.36	2/611 (0.3%)	1.31	6/830 (0.7%)
1	F	1.36	1/594 (0.2%)	1.50	7/806 (0.9%)
All	All	1.24	4/3545 (0.1%)	1.33	26/4811 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	10	GLU	CG-CD	5.58	1.60	1.51
1	D	27	SER	CB-OG	5.56	1.49	1.42
1	E	4	GLU	N-CA	5.55	1.57	1.46
1	E	10	GLU	CG-CD	5.46	1.60	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	24	MET	CG-SD-CE	-22.84	63.66	100.20
1	C	24	MET	CG-SD-CE	-12.93	79.51	100.20
1	A	24	MET	CG-SD-CE	-12.23	80.63	100.20
1	F	31	MET	CG-SD-CE	-11.98	81.03	100.20
1	F	24	MET	CG-SD-CE	-11.98	81.04	100.20
1	B	24	MET	CG-SD-CE	-8.51	86.59	100.20
1	D	8	MET	CG-SD-CE	-7.99	87.42	100.20
1	D	6	LEU	CB-CG-CD1	-6.98	99.13	111.00
1	A	32	LEU	CB-CG-CD2	-6.48	99.98	111.00
1	F	79	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	E	66	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	E	48	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	E	48	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	26	ASP	CB-CG-OD2	-5.88	113.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	79	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	F	26	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	E	51	VAL	CG1-CB-CG2	-5.70	101.77	110.90
1	B	86	LYS	CD-CE-NZ	-5.66	98.69	111.70
1	A	14	LEU	CB-CG-CD1	5.42	120.22	111.00
1	F	5	ALA	N-CA-CB	5.26	117.47	110.10
1	F	71	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	A	12	LYS	C-N-CA	-5.19	111.39	122.30
1	A	50	ASP	CB-CG-OD1	5.16	122.94	118.30
1	E	66	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	E	14	LEU	CB-CG-CD1	5.05	119.59	111.00
1	D	66	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

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	600	0	620	38	0
1	B	606	0	630	12	0
1	C	512	0	537	20	0
1	D	606	0	630	36	0
1	E	606	0	630	22	0
1	F	590	0	617	17	0
2	A	52	0	0	10	0
2	B	41	0	0	2	0
2	C	35	0	0	7	0
2	D	53	0	0	5	0
2	E	76	0	0	7	1
2	F	60	0	0	3	1
All	All	3837	0	3664	126	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 18.

All (126) 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	1.84	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:B:31:MET:HE2	2:B:217:HOH:O	1.56	1.04
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:15:THR:CG2	1:C:8:MET:HE3	1.91	1.01
1:B:15:THR:HG23	1:C:8:MET:HE3	0.99	0.99
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:E:24:MET:HE2	1:E:58:THR:HA	0.90	0.89
1:A:8:MET:HG2	1:A:46:ILE:HD13	1.56	0.87
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:E:9:VAL:HG21	1:E:24:MET:HE3	1.62	0.80
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:51:VAL:HG12	1:E:55:LYS:HE3	1.67	0.77
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:E:9:VAL:HG23	1:E:24:MET:HE1	1.71	0.73
1:C:8:MET:HE2	2:C:234:HOH:O	1.89	0.72
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:E:9:VAL:CG2	1:E:24:MET:CE	2.70	0.70
1:A:87:ILE:C	2:A:229:HOH:O	2.32	0.68
1:A:58:THR:HG23	2:A:241:HOH:O	1.93	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:E:9:VAL:CG2	1:E:24:MET:HE3	2.26	0.65
1:A:79:ARG:NE	2:A:201:HOH:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:79:ARG:C	2:C:214:HOH:O	2.37	0.63
1:B:24:MET:HG2	1:B:57:ALA:O	1.98	0.62
1:B:15:THR:CG2	1:C:8:MET:CE	2.65	0.61
1:A:87:ILE:HD13	1:C:35:TYR:CE2	2.36	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:E:9:VAL:CG2	1:E:24:MET:HE1	2.31	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
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: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:C:8:MET:HG2	1:C:46:ILE:HG12	1.89	0.54
1:D:51:VAL:HG23	2:D:237:HOH:O	2.07	0.53
1:E:24:MET:HG2	1:E:57:ALA:O	2.08	0.53
1:A:83:ASP:HA	1:A:86:LYS:HE3	1.90	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:E:24:MET:HE1	1:E:58:THR:HG22	1.90	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:87:ILE:HD12	1:A:87:ILE:C	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:77:ILE:CD1	1:E:19:GLU:OE1	2.62	0.47
1:D:25:VAL:CG1	1:F:81:HIS:CG	2.98	0.47
1:D:25:VAL:HG11	1:F:81:HIS:CG	2.50	0.47
1:D:48:ARG:NH1	1:D:85:GLU:OE1	2.40	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:D:33:VAL:HG21	1:D:48:ARG:HG2	1.99	0.45
1:C:79:ARG:HA	1:C:79:ARG:HD2	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
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:D:4:GLU:HG2	2:D:245:HOH:O	2.20	0.42
1:E:72:LYS:HD2	1:E:72:LYS:HA	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:B:31:MET:CE	1:B:48:ARG:HD2	2.51	0.41
1:A:75:HIS:NE2	1:A:77:ILE:CD1	2.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ALA:O	1:A:66:ARG:HG3	2.21	0.40
1:E:8:MET:HE1	1:E:77:ILE:HD12	2.03	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 (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	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 (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	60/81 (74%)	59 (98%)	1 (2%)	68	50
1	B	61/81 (75%)	60 (98%)	1 (2%)	70	53
1	C	50/81 (62%)	49 (98%)	1 (2%)	63	43
1	D	61/81 (75%)	61 (100%)	0	100	100
1	E	61/81 (75%)	61 (100%)	0	100	100
1	F	59/81 (73%)	58 (98%)	1 (2%)	68	50
All	All	352/486 (72%)	348 (99%)	4 (1%)	80	68

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ILE
1	B	83	ASP
1	C	40	SER
1	F	82	THR

Some 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 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	85/115 (73%)	-0.06	2 (2%) 62 67	19, 27, 47, 78	0
1	B	86/115 (74%)	-0.13	0 100 100	20, 27, 47, 54	0
1	C	74/115 (64%)	-0.12	0 100 100	21, 31, 45, 59	0
1	D	86/115 (74%)	-0.10	1 (1%) 81 85	16, 23, 43, 54	0
1	E	86/115 (74%)	-0.32	0 100 100	16, 22, 32, 39	0
1	F	84/115 (73%)	-0.25	0 100 100	15, 21, 36, 50	0
All	All	501/690 (72%)	-0.16	3 (0%) 90 92	15, 25, 44, 78	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	LYS	4.0
1	A	87	ILE	3.4
1	D	89	PRO	2.3

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 (i)

There are no such residues in this entry.