



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:33 AM UTC

PDB ID : 6EUS / pdb_00006eus
Title : Crystal structure of the outer membrane channel DcaP of *Acinetobacter baumannii*
Authors : Zahn, M.; van den Berg, B.
Deposited on : 2017-10-31
Resolution : 2.20 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)
Validation Pipeline (wwPDB-VP)	:	2.49

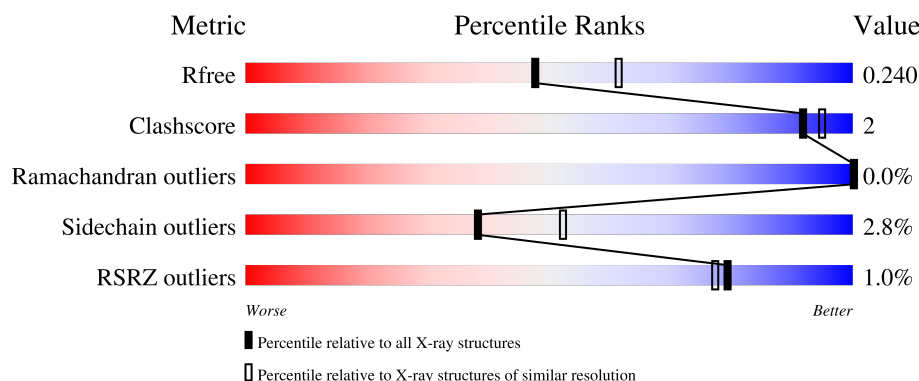
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	380	84% 6% • 9%
1	B	380	86% 5% • 9%
1	C	380	83% 6% • 9%
1	D	380	84% 7% • 9%
1	E	380	85% 5% • 9%

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Mol	Chain	Length	Quality of chain
1	F	380	2% 82% 7% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16600 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 DcaP-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	Se	0	0	0
			2651	1664	450	533	4			
1	B	346	Total	C	N	O	Se	0	0	0
			2651	1664	450	533	4			
1	C	346	Total	C	N	O	Se	0	0	0
			2651	1664	450	533	4			
1	D	346	Total	C	N	O	Se	0	0	0
			2651	1664	450	533	4			
1	E	346	Total	C	N	O	Se	0	0	0
			2651	1664	450	533	4			
1	F	346	Total	C	N	O	Se	0	0	0
			2651	1664	450	533	4			

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ALA	-	expression tag	UNP A0A0B9X9I7
A	27	ASN	-	expression tag	UNP A0A0B9X9I7
A	28	VAL	-	expression tag	UNP A0A0B9X9I7
A	29	ARG	-	expression tag	UNP A0A0B9X9I7
A	30	LEU	-	expression tag	UNP A0A0B9X9I7
A	31	GLN	-	expression tag	UNP A0A0B9X9I7
A	32	HIS	-	expression tag	UNP A0A0B9X9I7
A	33	HIS	-	expression tag	UNP A0A0B9X9I7
A	34	HIS	-	expression tag	UNP A0A0B9X9I7
A	35	HIS	-	expression tag	UNP A0A0B9X9I7
A	36	HIS	-	expression tag	UNP A0A0B9X9I7
A	37	HIS	-	expression tag	UNP A0A0B9X9I7
A	38	HIS	-	expression tag	UNP A0A0B9X9I7
A	39	LEU	-	expression tag	UNP A0A0B9X9I7
A	40	GLU	-	expression tag	UNP A0A0B9X9I7
A	41	VAL	-	expression tag	UNP A0A0B9X9I7
A	42	GLN	-	expression tag	UNP A0A0B9X9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	280	MSE	LEU	conflict	UNP A0A0B9X9I7
A	282	MSE	LEU	conflict	UNP A0A0B9X9I7
B	26	ALA	-	expression tag	UNP A0A0B9X9I7
B	27	ASN	-	expression tag	UNP A0A0B9X9I7
B	28	VAL	-	expression tag	UNP A0A0B9X9I7
B	29	ARG	-	expression tag	UNP A0A0B9X9I7
B	30	LEU	-	expression tag	UNP A0A0B9X9I7
B	31	GLN	-	expression tag	UNP A0A0B9X9I7
B	32	HIS	-	expression tag	UNP A0A0B9X9I7
B	33	HIS	-	expression tag	UNP A0A0B9X9I7
B	34	HIS	-	expression tag	UNP A0A0B9X9I7
B	35	HIS	-	expression tag	UNP A0A0B9X9I7
B	36	HIS	-	expression tag	UNP A0A0B9X9I7
B	37	HIS	-	expression tag	UNP A0A0B9X9I7
B	38	HIS	-	expression tag	UNP A0A0B9X9I7
B	39	LEU	-	expression tag	UNP A0A0B9X9I7
B	40	GLU	-	expression tag	UNP A0A0B9X9I7
B	41	VAL	-	expression tag	UNP A0A0B9X9I7
B	42	GLN	-	expression tag	UNP A0A0B9X9I7
B	280	MSE	LEU	conflict	UNP A0A0B9X9I7
B	282	MSE	LEU	conflict	UNP A0A0B9X9I7
C	26	ALA	-	expression tag	UNP A0A0B9X9I7
C	27	ASN	-	expression tag	UNP A0A0B9X9I7
C	28	VAL	-	expression tag	UNP A0A0B9X9I7
C	29	ARG	-	expression tag	UNP A0A0B9X9I7
C	30	LEU	-	expression tag	UNP A0A0B9X9I7
C	31	GLN	-	expression tag	UNP A0A0B9X9I7
C	32	HIS	-	expression tag	UNP A0A0B9X9I7
C	33	HIS	-	expression tag	UNP A0A0B9X9I7
C	34	HIS	-	expression tag	UNP A0A0B9X9I7
C	35	HIS	-	expression tag	UNP A0A0B9X9I7
C	36	HIS	-	expression tag	UNP A0A0B9X9I7
C	37	HIS	-	expression tag	UNP A0A0B9X9I7
C	38	HIS	-	expression tag	UNP A0A0B9X9I7
C	39	LEU	-	expression tag	UNP A0A0B9X9I7
C	40	GLU	-	expression tag	UNP A0A0B9X9I7
C	41	VAL	-	expression tag	UNP A0A0B9X9I7
C	42	GLN	-	expression tag	UNP A0A0B9X9I7
C	280	MSE	LEU	conflict	UNP A0A0B9X9I7
C	282	MSE	LEU	conflict	UNP A0A0B9X9I7
D	26	ALA	-	expression tag	UNP A0A0B9X9I7
D	27	ASN	-	expression tag	UNP A0A0B9X9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	28	VAL	-	expression tag	UNP A0A0B9X9I7
D	29	ARG	-	expression tag	UNP A0A0B9X9I7
D	30	LEU	-	expression tag	UNP A0A0B9X9I7
D	31	GLN	-	expression tag	UNP A0A0B9X9I7
D	32	HIS	-	expression tag	UNP A0A0B9X9I7
D	33	HIS	-	expression tag	UNP A0A0B9X9I7
D	34	HIS	-	expression tag	UNP A0A0B9X9I7
D	35	HIS	-	expression tag	UNP A0A0B9X9I7
D	36	HIS	-	expression tag	UNP A0A0B9X9I7
D	37	HIS	-	expression tag	UNP A0A0B9X9I7
D	38	HIS	-	expression tag	UNP A0A0B9X9I7
D	39	LEU	-	expression tag	UNP A0A0B9X9I7
D	40	GLU	-	expression tag	UNP A0A0B9X9I7
D	41	VAL	-	expression tag	UNP A0A0B9X9I7
D	42	GLN	-	expression tag	UNP A0A0B9X9I7
D	280	MSE	LEU	conflict	UNP A0A0B9X9I7
D	282	MSE	LEU	conflict	UNP A0A0B9X9I7
E	26	ALA	-	expression tag	UNP A0A0B9X9I7
E	27	ASN	-	expression tag	UNP A0A0B9X9I7
E	28	VAL	-	expression tag	UNP A0A0B9X9I7
E	29	ARG	-	expression tag	UNP A0A0B9X9I7
E	30	LEU	-	expression tag	UNP A0A0B9X9I7
E	31	GLN	-	expression tag	UNP A0A0B9X9I7
E	32	HIS	-	expression tag	UNP A0A0B9X9I7
E	33	HIS	-	expression tag	UNP A0A0B9X9I7
E	34	HIS	-	expression tag	UNP A0A0B9X9I7
E	35	HIS	-	expression tag	UNP A0A0B9X9I7
E	36	HIS	-	expression tag	UNP A0A0B9X9I7
E	37	HIS	-	expression tag	UNP A0A0B9X9I7
E	38	HIS	-	expression tag	UNP A0A0B9X9I7
E	39	LEU	-	expression tag	UNP A0A0B9X9I7
E	40	GLU	-	expression tag	UNP A0A0B9X9I7
E	41	VAL	-	expression tag	UNP A0A0B9X9I7
E	42	GLN	-	expression tag	UNP A0A0B9X9I7
E	280	MSE	LEU	conflict	UNP A0A0B9X9I7
E	282	MSE	LEU	conflict	UNP A0A0B9X9I7
F	26	ALA	-	expression tag	UNP A0A0B9X9I7
F	27	ASN	-	expression tag	UNP A0A0B9X9I7
F	28	VAL	-	expression tag	UNP A0A0B9X9I7
F	29	ARG	-	expression tag	UNP A0A0B9X9I7
F	30	LEU	-	expression tag	UNP A0A0B9X9I7
F	31	GLN	-	expression tag	UNP A0A0B9X9I7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	32	HIS	-	expression tag	UNP A0A0B9X9I7
F	33	HIS	-	expression tag	UNP A0A0B9X9I7
F	34	HIS	-	expression tag	UNP A0A0B9X9I7
F	35	HIS	-	expression tag	UNP A0A0B9X9I7
F	36	HIS	-	expression tag	UNP A0A0B9X9I7
F	37	HIS	-	expression tag	UNP A0A0B9X9I7
F	38	HIS	-	expression tag	UNP A0A0B9X9I7
F	39	LEU	-	expression tag	UNP A0A0B9X9I7
F	40	GLU	-	expression tag	UNP A0A0B9X9I7
F	41	VAL	-	expression tag	UNP A0A0B9X9I7
F	42	GLN	-	expression tag	UNP A0A0B9X9I7
F	280	MSE	LEU	conflict	UNP A0A0B9X9I7
F	282	MSE	LEU	conflict	UNP A0A0B9X9I7

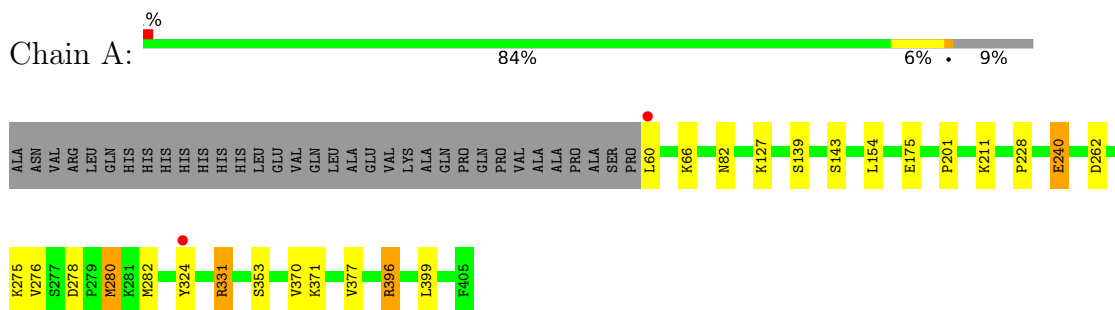
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	106	Total	O	0	0
			106	106		
2	B	131	Total	O	0	0
			131	131		
2	C	100	Total	O	0	0
			100	100		
2	D	111	Total	O	0	0
			111	111		
2	E	132	Total	O	0	0
			132	132		
2	F	114	Total	O	0	0
			114	114		

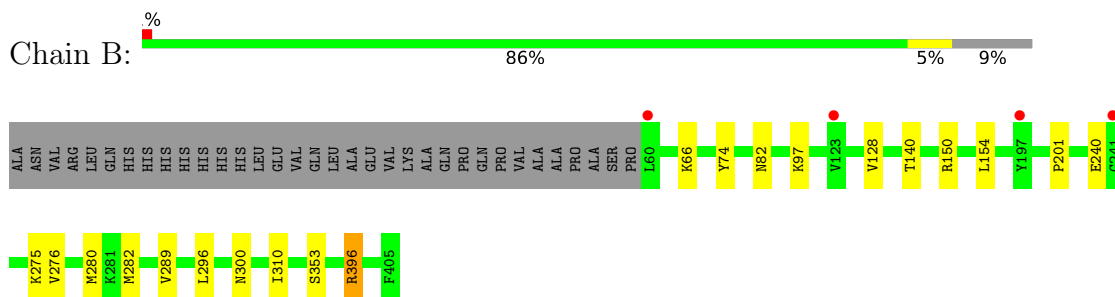
3 Residue-property plots

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.

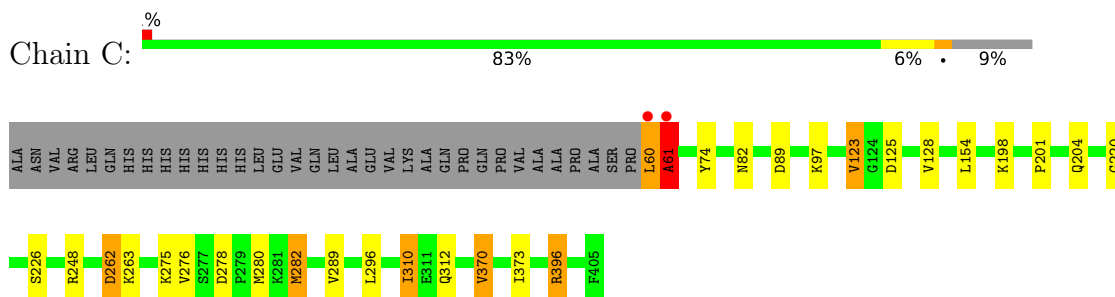
- Molecule 1: DcaP-like protein



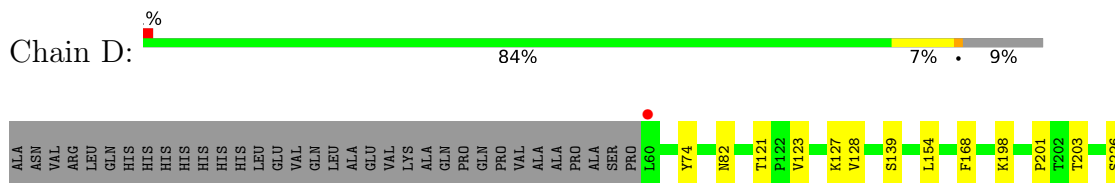
- Molecule 1: DcaP-like protein

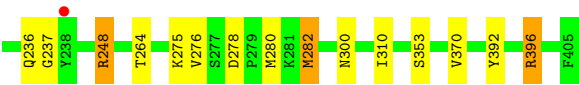


- Molecule 1: DcaP-like protein

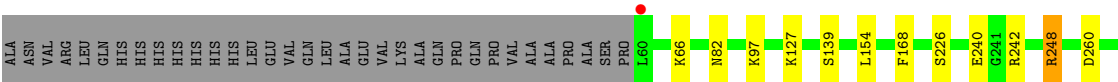
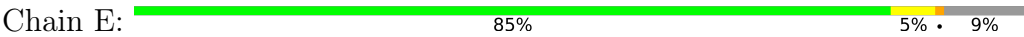


- Molecule 1: DcaP-like protein

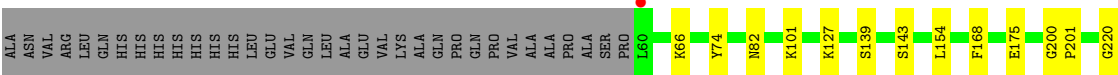
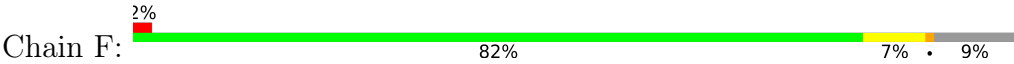




• Molecule 1: DcaP-like protein



• Molecule 1: DcaP-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.85Å 108.38Å 216.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.10 – 2.20 108.10 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (108.10-2.20) 97.1 (108.10-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.200 , 0.234 0.208 , 0.240	Depositor DCC
R_{free} test set	2362 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.049 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16600	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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	1.22	6/2701 (0.2%)	1.10	8/3650 (0.2%)
1	B	1.24	6/2701 (0.2%)	1.18	11/3650 (0.3%)
1	C	1.22	7/2701 (0.3%)	1.17	16/3650 (0.4%)
1	D	1.23	5/2701 (0.2%)	1.13	16/3650 (0.4%)
1	E	1.23	2/2701 (0.1%)	1.14	13/3650 (0.4%)
1	F	1.22	7/2701 (0.3%)	1.14	13/3650 (0.4%)
All	All	1.23	33/16206 (0.2%)	1.14	77/21900 (0.4%)

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	C	0	1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	123	VAL	C-O	-8.37	1.14	1.24
1	E	248	ARG	CD-NE	-7.03	1.36	1.46
1	B	201	PRO	C-O	-6.70	1.15	1.24
1	D	139	SER	CB-OG	-6.33	1.29	1.42
1	A	228	PRO	C-O	-5.89	1.16	1.23
1	D	201	PRO	C-O	-5.80	1.17	1.24
1	F	264	THR	C-O	-5.66	1.17	1.24
1	C	61	ALA	C-O	-5.64	1.16	1.24
1	F	101	LYS	C-O	-5.63	1.16	1.24
1	E	278	ASP	CA-C	5.63	1.59	1.52
1	F	143	SER	C-O	-5.57	1.17	1.24
1	C	125	ASP	N-CA	5.55	1.53	1.46
1	A	211	LYS	C-O	-5.47	1.17	1.24
1	D	264	THR	C-O	-5.40	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	ASN	CA-C	5.39	1.60	1.53
1	A	143	SER	CB-OG	-5.38	1.31	1.42
1	F	278	ASP	CA-C	5.37	1.58	1.52
1	B	140	THR	C-O	-5.33	1.17	1.23
1	A	262	ASP	N-CA	-5.27	1.39	1.45
1	B	276	VAL	C-O	-5.24	1.18	1.24
1	F	248	ARG	CD-NE	-5.22	1.39	1.46
1	B	150	ARG	N-CA	-5.19	1.40	1.47
1	D	300	ASN	CA-C	5.18	1.60	1.53
1	C	262	ASP	CB-CG	-5.18	1.39	1.52
1	C	89	ASP	C-O	-5.18	1.18	1.23
1	B	150	ARG	CA-C	5.11	1.57	1.53
1	C	220	GLY	C-O	-5.10	1.17	1.24
1	D	237	GLY	C-O	-5.09	1.17	1.23
1	A	201	PRO	C-O	-5.07	1.18	1.24
1	A	278	ASP	CA-C	5.05	1.58	1.52
1	C	278	ASP	CA-C	5.01	1.58	1.52
1	F	261	ASP	CG-OD2	5.01	1.34	1.25
1	F	220	GLY	C-O	-5.00	1.17	1.24

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	GLU	CA-C-N	14.64	148.06	121.70
1	B	240	GLU	C-N-CA	14.64	148.06	121.70
1	C	248	ARG	NE-CZ-NH1	-12.12	109.38	121.50
1	C	248	ARG	NE-CZ-NH2	11.93	129.94	119.20
1	B	240	GLU	O-C-N	-11.11	104.34	122.23
1	E	396	ARG	NE-CZ-NH1	-10.88	110.62	121.50
1	C	396	ARG	NE-CZ-NH1	-10.84	110.66	121.50
1	E	396	ARG	NE-CZ-NH2	10.13	128.32	119.20
1	B	282	MSE	CG-SE-CE	-10.03	76.86	98.92
1	B	396	ARG	NE-CZ-NH1	-9.81	111.69	121.50
1	B	396	ARG	NE-CZ-NH2	9.78	128.00	119.20
1	E	282	MSE	CG-SE-CE	-9.66	77.67	98.92
1	C	396	ARG	NE-CZ-NH2	9.37	127.63	119.20
1	D	248	ARG	NE-CZ-NH2	-8.84	111.25	119.20
1	E	280	MSE	CG-SE-CE	8.51	117.64	98.92
1	E	248	ARG	NE-CZ-NH2	-8.41	111.63	119.20
1	F	248	ARG	NE-CZ-NH2	-8.16	111.85	119.20
1	F	396	ARG	NE-CZ-NH2	-8.05	111.95	119.20
1	D	396	ARG	NE-CZ-NH2	-7.88	112.11	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	ARG	NE-CZ-NH2	-7.68	112.28	119.20
1	C	280	MSE	CG-SE-CE	7.58	115.59	98.92
1	D	248	ARG	NE-CZ-NH1	7.18	128.68	121.50
1	F	331	ARG	NE-CZ-NH1	-7.16	114.34	121.50
1	F	240	GLU	CA-CB-CG	7.09	128.28	114.10
1	F	248	ARG	NE-CZ-NH1	6.97	128.47	121.50
1	F	396	ARG	NE-CZ-NH1	6.96	128.46	121.50
1	A	331	ARG	NE-CZ-NH1	-6.95	114.55	121.50
1	D	280	MSE	CG-SE-CE	-6.77	84.03	98.92
1	D	282	MSE	CA-CB-CG	-6.75	100.60	114.10
1	F	331	ARG	NE-CZ-NH2	6.47	125.03	119.20
1	B	240	GLU	CA-C-O	-6.42	113.05	121.08
1	E	248	ARG	NE-CZ-NH1	6.40	127.90	121.50
1	C	310	ILE	CB-CA-C	6.30	119.41	110.84
1	B	282	MSE	CA-CB-CG	-6.29	101.53	114.10
1	E	282	MSE	CA-CB-CG	-6.29	101.53	114.10
1	D	282	MSE	CG-SE-CE	6.22	112.61	98.92
1	C	282	MSE	CA-CB-CG	-6.17	101.75	114.10
1	D	396	ARG	NE-CZ-NH1	6.13	127.63	121.50
1	E	127	LYS	CB-CG-CD	-6.13	97.19	111.30
1	B	280	MSE	CG-SE-CE	-6.10	85.50	98.92
1	F	310	ILE	N-CA-CB	-6.00	103.80	110.99
1	F	201	PRO	N-CA-C	-5.94	101.83	110.80
1	E	310	ILE	CB-CA-C	5.91	118.88	110.84
1	C	123	VAL	CA-C-O	-5.89	113.42	120.78
1	A	143	SER	CB-CA-C	-5.84	99.14	110.46
1	C	123	VAL	CB-CA-C	5.74	120.71	111.29
1	B	240	GLU	N-CA-C	5.71	119.44	111.90
1	E	396	ARG	CD-NE-CZ	5.70	132.38	124.40
1	C	262	ASP	N-CA-CB	-5.68	101.77	110.85
1	C	201	PRO	N-CA-C	-5.60	102.41	111.03
1	B	353	SER	CA-CB-OG	-5.54	100.02	111.10
1	D	278	ASP	CA-C-N	-5.53	114.07	120.04
1	D	278	ASP	C-N-CA	-5.53	114.07	120.04
1	A	240	GLU	CA-CB-CG	5.53	125.16	114.10
1	D	396	ARG	CD-NE-CZ	5.47	132.06	124.40
1	A	331	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	C	396	ARG	CD-NE-CZ	5.41	131.97	124.40
1	C	278	ASP	CA-C-N	-5.40	114.20	120.04
1	C	278	ASP	C-N-CA	-5.40	114.20	120.04
1	D	310	ILE	CB-CA-C	-5.40	103.49	110.84
1	A	396	ARG	NE-CZ-NH1	5.37	126.87	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	248	ARG	CB-CG-CD	-5.35	98.99	111.30
1	D	139	SER	CA-CB-OG	-5.34	100.41	111.10
1	C	123	VAL	CA-CB-CG1	5.32	119.45	110.40
1	C	97	LYS	CD-CE-NZ	-5.31	94.91	111.90
1	D	226	SER	CA-CB-OG	-5.26	100.57	111.10
1	E	97	LYS	CG-CD-CE	5.22	123.31	111.30
1	F	200	GLY	CA-C-N	-5.19	114.45	119.90
1	F	200	GLY	C-N-CA	-5.19	114.45	119.90
1	E	248	ARG	CD-NE-CZ	5.16	131.63	124.40
1	D	310	ILE	N-CA-CB	-5.15	104.81	110.99
1	E	242	ARG	CB-CG-CD	5.14	123.13	111.30
1	D	248	ARG	CB-CG-CD	-5.12	99.51	111.30
1	A	353	SER	CA-CB-OG	-5.12	100.87	111.10
1	D	353	SER	CA-CB-OG	-5.11	100.87	111.10
1	F	349	ARG	CG-CD-NE	-5.11	100.75	112.00
1	A	280	MSE	CG-SE-CE	5.10	110.15	98.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	61	ALA	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2651	0	2550	12	0
1	B	2651	0	2550	6	0
1	C	2651	0	2550	10	0
1	D	2651	0	2550	9	1
1	E	2651	0	2550	9	1
1	F	2651	0	2550	16	0
2	A	106	0	0	0	0
2	B	131	0	0	0	0
2	C	100	0	0	0	0
2	D	111	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	132	0	0	2	0
2	F	114	0	0	2	0
All	All	16600	0	15300	51	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 2.

All (51) 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:E:168:PHE:O	1:E:248:ARG:HD2	1.87	0.73
1:A:276:VAL:HG13	1:F:340:PHE:HE1	1.55	0.71
1:D:168:PHE:O	1:D:248:ARG:HD2	1.91	0.71
1:F:280:MSE:HE2	1:F:282:MSE:HG3	1.76	0.66
1:F:168:PHE:O	1:F:248:ARG:HD2	1.95	0.66
1:D:276:VAL:CG2	1:D:282:MSE:HE2	2.26	0.65
1:C:276:VAL:CG2	1:C:282:MSE:HE2	2.27	0.65
1:F:240:GLU:O	1:F:240:GLU:HG3	1.97	0.64
1:A:276:VAL:HG13	1:F:340:PHE:CE1	2.33	0.64
1:A:276:VAL:CG2	1:A:282:MSE:HE2	2.29	0.62
1:D:276:VAL:HG21	1:D:282:MSE:HE2	1.82	0.62
1:E:289:VAL:HG21	1:E:296:LEU:HD13	1.82	0.61
1:D:74:TYR:HB3	1:F:66:LYS:HD3	1.83	0.61
1:A:280:MSE:HE3	1:A:282:MSE:HG2	1.83	0.60
1:A:280:MSE:SE	1:A:324:TYR:CD2	3.06	0.59
1:A:280:MSE:SE	1:A:324:TYR:CE2	3.06	0.58
1:A:175:GLU:OE2	1:A:331:ARG:NH1	2.36	0.58
1:F:175:GLU:OE2	1:F:331:ARG:NH1	2.37	0.58
1:B:66:LYS:HD3	1:C:74:TYR:HB3	1.86	0.57
1:C:60:LEU:O	1:C:61:ALA:HB2	2.05	0.55
1:B:289:VAL:HG21	1:B:296:LEU:HD13	1.89	0.55
1:C:289:VAL:HG21	1:C:296:LEU:HD13	1.89	0.55
1:C:276:VAL:HG21	1:C:282:MSE:HE2	1.90	0.54
1:A:175:GLU:CD	1:A:331:ARG:HH12	2.17	0.53
1:D:168:PHE:O	1:D:248:ARG:CD	2.57	0.52
1:F:289:VAL:HG21	1:F:296:LEU:HD13	1.91	0.51
1:D:128:VAL:HG13	1:E:373:ILE:HD11	1.93	0.50
1:F:346:ASP:OD1	1:F:349:ARG:NH1	2.45	0.50
1:F:168:PHE:O	1:F:248:ARG:CD	2.58	0.50
1:E:275:LYS:NZ	2:E:506:HOH:O	2.45	0.49
1:E:168:PHE:O	1:E:248:ARG:CD	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:GLU:O	1:F:240:GLU:CG	2.60	0.48
1:D:128:VAL:HG21	1:E:370:VAL:HG21	1.93	0.48
1:D:203:THR:HB	1:D:236:GLN:OE1	2.13	0.48
1:F:402:LYS:NZ	2:F:512:HOH:O	2.49	0.46
1:B:310:ILE:HD13	1:B:310:ILE:HG21	1.80	0.45
1:A:276:VAL:HG23	1:A:282:MSE:HE2	1.99	0.44
1:A:66:LYS:HD3	1:B:74:TYR:HB3	1.99	0.44
1:F:175:GLU:CD	1:F:331:ARG:HH12	2.26	0.43
1:A:370:VAL:HG21	1:C:128:VAL:HG21	1.99	0.43
1:E:402:LYS:NZ	2:E:513:HOH:O	2.51	0.42
1:F:392:TYR:OH	2:F:501:HOH:O	2.17	0.42
1:B:128:VAL:HG21	1:C:370:VAL:HG21	2.01	0.42
1:D:121:THR:O	1:D:123:VAL:HG23	2.19	0.42
1:F:377:VAL:HG13	1:F:399:LEU:HD23	2.01	0.42
1:B:128:VAL:HG13	1:C:373:ILE:HD11	2.02	0.42
1:C:263:LYS:HD3	1:C:312:GLN:CD	2.45	0.41
1:C:198:LYS:HA	1:C:204:GLN:HE22	1.86	0.41
1:E:66:LYS:HD3	1:F:74:TYR:HB3	2.02	0.41
1:E:263:LYS:NZ	1:E:310:ILE:O	2.54	0.40
1:A:377:VAL:HG13	1:A:399:LEU:HD23	2.03	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)
1:D:392:TYR:OH	1:E:260:ASP:OD2[4_466]	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	344/380 (90%)	335 (97%)	9 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	344/380 (90%)	334 (97%)	10 (3%)	0	100	100
1	C	344/380 (90%)	333 (97%)	10 (3%)	1 (0%)	36	42
1	D	344/380 (90%)	335 (97%)	9 (3%)	0	100	100
1	E	344/380 (90%)	337 (98%)	7 (2%)	0	100	100
1	F	344/380 (90%)	333 (97%)	11 (3%)	0	100	100
All	All	2064/2280 (90%)	2007 (97%)	56 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	61	ALA

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	280/304 (92%)	271 (97%)	9 (3%)	34	47
1	B	280/304 (92%)	275 (98%)	5 (2%)	51	68
1	C	280/304 (92%)	270 (96%)	10 (4%)	31	42
1	D	280/304 (92%)	273 (98%)	7 (2%)	42	56
1	E	280/304 (92%)	272 (97%)	8 (3%)	37	51
1	F	280/304 (92%)	272 (97%)	8 (3%)	37	51
All	All	1680/1824 (92%)	1633 (97%)	47 (3%)	38	52

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	82	ASN
1	A	127	LYS
1	A	139	SER
1	A	154	LEU

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Mol	Chain	Res	Type
1	A	240	GLU
1	A	275	LYS
1	A	371	LYS
1	A	396	ARG
1	B	82	ASN
1	B	97	LYS
1	B	154	LEU
1	B	275	LYS
1	B	396	ARG
1	C	60	LEU
1	C	82	ASN
1	C	123	VAL
1	C	154	LEU
1	C	226	SER
1	C	262	ASP
1	C	275	LYS
1	C	310	ILE
1	C	370	VAL
1	C	396	ARG
1	D	82	ASN
1	D	127	LYS
1	D	154	LEU
1	D	198	LYS
1	D	275	LYS
1	D	370	VAL
1	D	396	ARG
1	E	82	ASN
1	E	139	SER
1	E	154	LEU
1	E	226	SER
1	E	240	GLU
1	E	263	LYS
1	E	275	LYS
1	E	396	ARG
1	F	82	ASN
1	F	127	LYS
1	F	139	SER
1	F	154	LEU
1	F	240	GLU
1	F	275	LYS
1	F	296	LEU
1	F	396	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	163	GLN
1	A	236	GLN
1	A	253	ASN
1	A	257	GLN
1	B	103	HIS
1	B	196	ASN
1	B	253	ASN
1	B	359	GLN
1	C	103	HIS
1	C	163	GLN
1	C	204	GLN
1	C	253	ASN
1	C	313	ASN
1	C	359	GLN
1	D	72	ASN
1	D	103	HIS
1	D	196	ASN
1	D	253	ASN
1	D	359	GLN
1	D	381	ASN
1	E	103	HIS
1	E	158	ASN
1	E	163	GLN
1	E	236	GLN
1	E	253	ASN
1	E	359	GLN
1	F	72	ASN
1	F	253	ASN
1	F	381	ASN

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 [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	342/380 (90%)	-0.06	2 (0%) 85 83	28, 39, 62, 80	0
1	B	342/380 (90%)	-0.21	4 (1%) 76 74	27, 35, 56, 87	0
1	C	342/380 (90%)	-0.15	2 (0%) 85 83	28, 38, 61, 81	0
1	D	342/380 (90%)	-0.11	2 (0%) 85 83	27, 37, 58, 81	0
1	E	342/380 (90%)	-0.31	1 (0%) 90 88	26, 34, 49, 78	0
1	F	342/380 (90%)	0.04	9 (2%) 57 54	27, 39, 64, 109	0
All	All	2052/2280 (90%)	-0.13	20 (0%) 79 77	26, 37, 60, 109	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	239	ALA	5.4
1	A	324	TYR	4.2
1	F	238	TYR	4.1
1	C	60	LEU	3.5
1	B	60	LEU	3.3
1	C	61	ALA	3.1
1	F	242	ARG	3.0
1	A	60	LEU	2.9
1	D	238	TYR	2.8
1	F	243	GLY	2.7
1	F	241	GLY	2.7
1	F	245	ALA	2.5
1	F	60	LEU	2.5
1	B	197	TYR	2.5
1	D	60	LEU	2.5
1	F	261	ASP	2.3
1	B	241	GLY	2.3
1	E	60	LEU	2.1
1	F	237	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	123	VAL	2.0

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.