



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 11:29 AM EDT

PDB ID : 6EUS  
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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>.

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The following versions of software and data (see [references ⓘ](#)) 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	:	2.37.1
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)	:	2.37.1



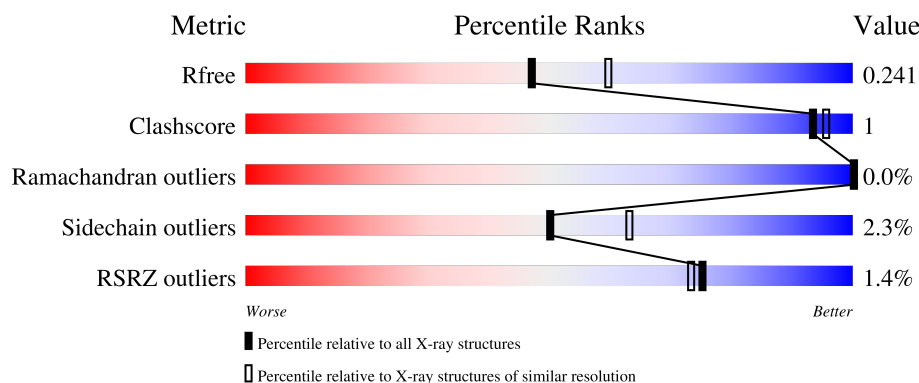
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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  $\geq 3$ , 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 83%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>6% • 9%</span> </div> </div>
1	B	380	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 83%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>7% • 9%</span> </div> </div>
1	C	380	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 82%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>82%</span> <span>7% • 9%</span> </div> </div>
1	D	380	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 83%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>8% • 9%</span> </div> </div>
1	E	380	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 85%, yellow 1%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span></span> <span>85%</span> <span>6% • 9%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	380	<div><div></div><div>3%</div><div>83%</div><div>6%</div><div>9%</div></div>



## 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 2651	C 1664	N 450	O 533	Se 4	0	0	0
1	B	346	Total 2651	C 1664	N 450	O 533	Se 4	0	0	0
1	C	346	Total 2651	C 1664	N 450	O 533	Se 4	0	0	0
1	D	346	Total 2651	C 1664	N 450	O 533	Se 4	0	0	0
1	E	346	Total 2651	C 1664	N 450	O 533	Se 4	0	0	0
1	F	346	Total 2651	C 1664	N 450	O 533	Se 4	0	0	0

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.

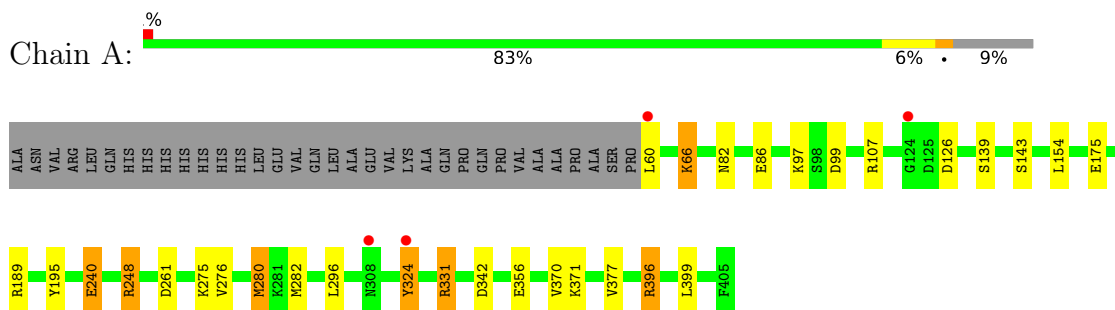
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	106	Total O 106 106	0	0
2	B	131	Total O 131 131	0	0
2	C	100	Total O 100 100	0	0
2	D	111	Total O 111 111	0	0
2	E	132	Total O 132 132	0	0
2	F	114	Total O 114 114	0	0



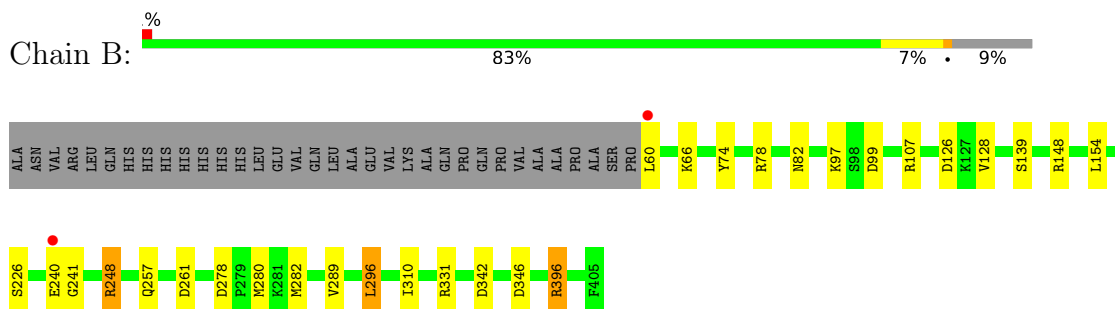
### 3 Residue-property plots [i](#)

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.

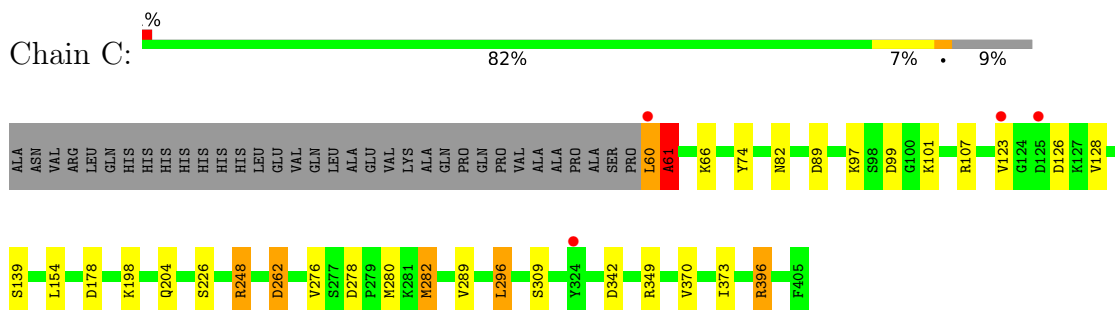
- Molecule 1: DcaP-like protein



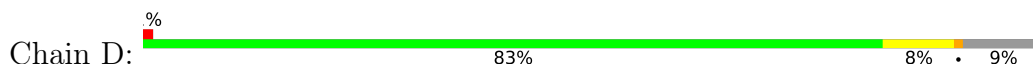
- Molecule 1: DcaP-like protein



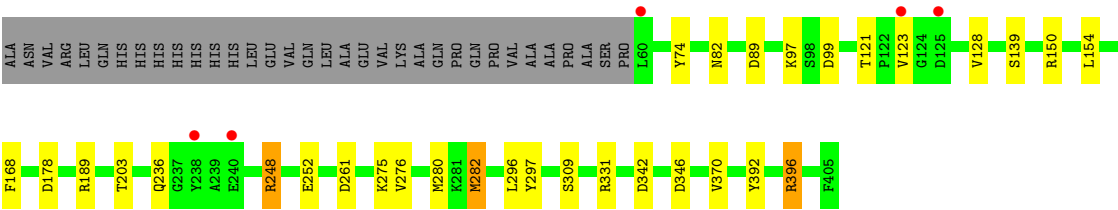
- Molecule 1: DcaP-like protein



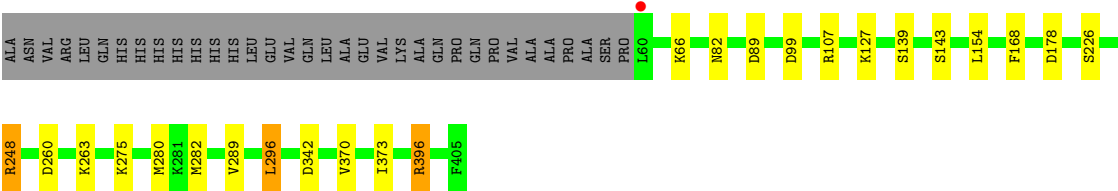
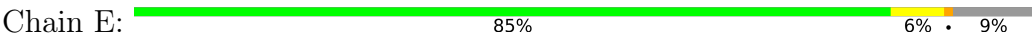
- Molecule 1: DcaP-like protein



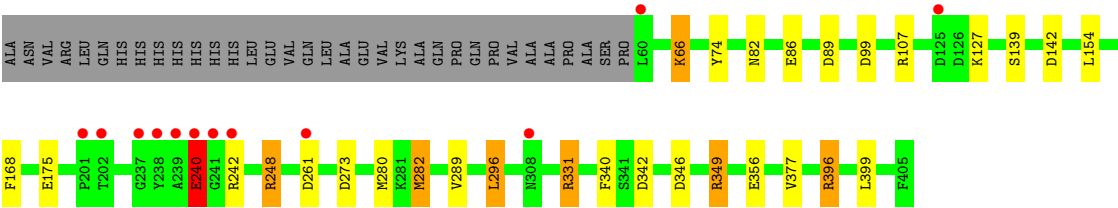
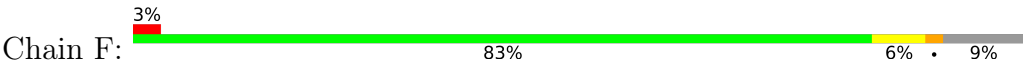




● Molecule 1: DcaP-like protein



● 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, $\alpha$ , $\beta$ , $\gamma$	107.85Å 108.38Å 216.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.10 – 2.20 48.44 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (108.10-2.20) 97.1 (48.44-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.200 , 0.234 0.208 , 0.241	Depositor DCC
$R_{free}$ test set	2362 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	1.00	4/2701 (0.1%)	1.13	20/3650 (0.5%)
1	B	1.00	4/2701 (0.1%)	1.20	24/3650 (0.7%)
1	C	0.98	3/2701 (0.1%)	1.25	24/3650 (0.7%)
1	D	1.03	3/2701 (0.1%)	1.20	23/3650 (0.6%)
1	E	0.99	2/2701 (0.1%)	1.19	18/3650 (0.5%)
1	F	0.98	2/2701 (0.1%)	1.23	23/3650 (0.6%)
All	All	1.00	18/16206 (0.1%)	1.20	132/21900 (0.6%)

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

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	139	SER	CB-OG	-9.81	1.29	1.42
1	A	143	SER	CB-OG	-8.36	1.31	1.42
1	F	86	GLU	CD-OE1	7.64	1.34	1.25
1	C	139	SER	CB-OG	-6.91	1.33	1.42
1	B	139	SER	CB-OG	-6.25	1.34	1.42

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	248	ARG	NE-CZ-NH1	-21.85	109.38	120.30
1	E	396	ARG	NE-CZ-NH1	-19.36	110.62	120.30
1	C	396	ARG	NE-CZ-NH1	-19.29	110.66	120.30
1	C	248	ARG	NE-CZ-NH2	19.27	129.94	120.30
1	D	248	ARG	NE-CZ-NH2	-18.11	111.25	120.30



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 ⓘ

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	2549	6	0
1	C	2651	0	2550	9	0
1	D	2651	0	2550	9	1
1	E	2651	0	2550	7	1
1	F	2651	0	2550	13	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
2	E	132	0	0	1	0
2	F	114	0	0	0	0
All	All	16600	0	15299	45	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 1.

The worst 5 of 45 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

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
1	B	344/380 (90%)	334 (97%)	10 (3%)	0	100	100
1	C	344/380 (90%)	333 (97%)	10 (3%)	1 (0%)	41	46
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 [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	280/304 (92%)	270 (96%)	10 (4%)	35	45
1	B	280/304 (92%)	275 (98%)	5 (2%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	280/304 (92%)	273 (98%)	7 (2%)	47	60
1	D	280/304 (92%)	275 (98%)	5 (2%)	59	72
1	E	280/304 (92%)	274 (98%)	6 (2%)	53	67
1	F	280/304 (92%)	274 (98%)	6 (2%)	53	67
All	All	1680/1824 (92%)	1641 (98%)	39 (2%)	50	63

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	139	SER
1	F	139	SER
1	E	154	LEU
1	E	396	ARG
1	F	240	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	C	204	GLN
1	D	381	ASN
1	F	381	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 monosaccharides 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	342/380 (90%)	-0.20	4 (1%) 79 77	28, 39, 62, 80	0
1	B	342/380 (90%)	-0.31	2 (0%) 89 88	27, 35, 56, 87	0
1	C	342/380 (90%)	-0.30	4 (1%) 79 77	28, 38, 61, 81	0
1	D	342/380 (90%)	-0.25	5 (1%) 73 72	27, 37, 58, 81	0
1	E	342/380 (90%)	-0.35	1 (0%) 94 93	26, 34, 49, 78	0
1	F	342/380 (90%)	-0.10	12 (3%) 44 42	27, 39, 64, 109	0
All	All	2052/2280 (90%)	-0.25	28 (1%) 75 73	26, 37, 60, 109	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	239	ALA	7.1
1	F	238	TYR	5.2
1	D	60	LEU	4.8
1	B	60	LEU	4.6
1	F	242	ARG	4.4

### 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 monosaccharides 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.