



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 08:43 pm BST

PDB ID : 1RQC  
Title : Crystals of peptide deformylase from Plasmodium falciparum with ten subunits per asymmetric unit reveal critical characteristics of the active site for drug design  
Authors : Robien, M.A.; Nguyen, K.T.; Kumar, A.; Hirsh, I.; Turley, S.; Pei, D.; Hol, W.G.  
Deposited on : 2003-12-04  
Resolution : 2.80 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)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

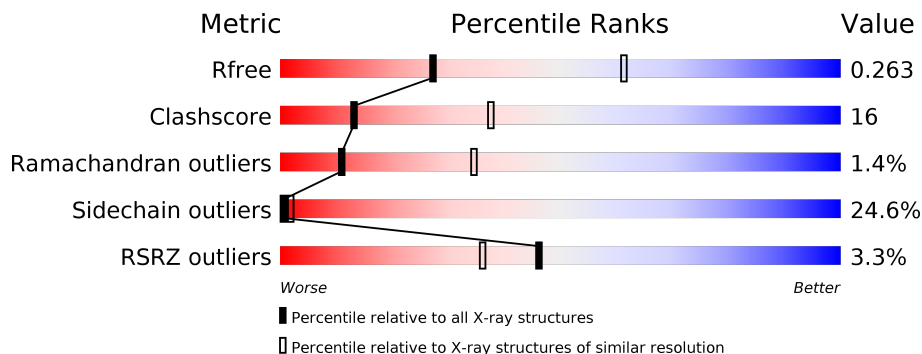
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	185	
1	B	185	
1	C	185	
1	D	185	
1	E	185	
1	F	185	

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Mol	Chain	Length	Quality of chain
1	G	185	<p>52% 30% 9% 8%</p>
1	H	185	<p>55% 28% 9% 6%</p>
1	I	185	<p>47% 33% 11% 8%</p>
1	J	185	<p>46% 36% 10% 8%</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14498 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 formylmethionine deformylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	178	1478	948	262	264	1	3	3	0	0
1	B	178	1478	948	262	264	1	3	3	0	0
1	C	168	1393	897	246	246	1	3	3	0	0
1	D	173	1434	920	253	257	1	3	3	0	0
1	E	175	1449	931	255	259	1	3	3	0	0
1	F	172	1425	915	252	254	1	3	3	0	0
1	G	171	1416	910	251	251	1	3	3	0	0
1	H	173	1434	920	253	257	1	3	3	0	0
1	I	171	1416	910	251	251	1	3	3	0	0
1	J	171	1416	910	251	251	1	3	3	0	0

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
A	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
A	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
A	240	LEU	-	EXPRESSION TAG	UNP Q8I372
A	241	GLU	-	EXPRESSION TAG	UNP Q8I372
A	242	HIS	-	EXPRESSION TAG	UNP Q8I372
A	243	HIS	-	EXPRESSION TAG	UNP Q8I372
A	244	HIS	-	EXPRESSION TAG	UNP Q8I372
A	245	HIS	-	EXPRESSION TAG	UNP Q8I372

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Chain	Residue	Modelled	Actual	Comment	Reference
A	246	HIS	-	EXPRESSION TAG	UNP Q8I372
A	247	HIS	-	EXPRESSION TAG	UNP Q8I372
B	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
B	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
B	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
B	240	LEU	-	EXPRESSION TAG	UNP Q8I372
B	241	GLU	-	EXPRESSION TAG	UNP Q8I372
B	242	HIS	-	EXPRESSION TAG	UNP Q8I372
B	243	HIS	-	EXPRESSION TAG	UNP Q8I372
B	244	HIS	-	EXPRESSION TAG	UNP Q8I372
B	245	HIS	-	EXPRESSION TAG	UNP Q8I372
B	246	HIS	-	EXPRESSION TAG	UNP Q8I372
B	247	HIS	-	EXPRESSION TAG	UNP Q8I372
C	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
C	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
C	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
C	240	LEU	-	EXPRESSION TAG	UNP Q8I372
C	241	GLU	-	EXPRESSION TAG	UNP Q8I372
C	242	HIS	-	EXPRESSION TAG	UNP Q8I372
C	243	HIS	-	EXPRESSION TAG	UNP Q8I372
C	244	HIS	-	EXPRESSION TAG	UNP Q8I372
C	245	HIS	-	EXPRESSION TAG	UNP Q8I372
C	246	HIS	-	EXPRESSION TAG	UNP Q8I372
C	247	HIS	-	EXPRESSION TAG	UNP Q8I372
D	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
D	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
D	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
D	240	LEU	-	EXPRESSION TAG	UNP Q8I372
D	241	GLU	-	EXPRESSION TAG	UNP Q8I372
D	242	HIS	-	EXPRESSION TAG	UNP Q8I372
D	243	HIS	-	EXPRESSION TAG	UNP Q8I372
D	244	HIS	-	EXPRESSION TAG	UNP Q8I372
D	245	HIS	-	EXPRESSION TAG	UNP Q8I372
D	246	HIS	-	EXPRESSION TAG	UNP Q8I372
D	247	HIS	-	EXPRESSION TAG	UNP Q8I372
E	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
E	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
E	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
E	240	LEU	-	EXPRESSION TAG	UNP Q8I372
E	241	GLU	-	EXPRESSION TAG	UNP Q8I372
E	242	HIS	-	EXPRESSION TAG	UNP Q8I372
E	243	HIS	-	EXPRESSION TAG	UNP Q8I372

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Chain	Residue	Modelled	Actual	Comment	Reference
E	244	HIS	-	EXPRESSION TAG	UNP Q8I372
E	245	HIS	-	EXPRESSION TAG	UNP Q8I372
E	246	HIS	-	EXPRESSION TAG	UNP Q8I372
E	247	HIS	-	EXPRESSION TAG	UNP Q8I372
F	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
F	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
F	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
F	240	LEU	-	EXPRESSION TAG	UNP Q8I372
F	241	GLU	-	EXPRESSION TAG	UNP Q8I372
F	242	HIS	-	EXPRESSION TAG	UNP Q8I372
F	243	HIS	-	EXPRESSION TAG	UNP Q8I372
F	244	HIS	-	EXPRESSION TAG	UNP Q8I372
F	245	HIS	-	EXPRESSION TAG	UNP Q8I372
F	246	HIS	-	EXPRESSION TAG	UNP Q8I372
F	247	HIS	-	EXPRESSION TAG	UNP Q8I372
G	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
G	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
G	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
G	240	LEU	-	EXPRESSION TAG	UNP Q8I372
G	241	GLU	-	EXPRESSION TAG	UNP Q8I372
G	242	HIS	-	EXPRESSION TAG	UNP Q8I372
G	243	HIS	-	EXPRESSION TAG	UNP Q8I372
G	244	HIS	-	EXPRESSION TAG	UNP Q8I372
G	245	HIS	-	EXPRESSION TAG	UNP Q8I372
G	246	HIS	-	EXPRESSION TAG	UNP Q8I372
G	247	HIS	-	EXPRESSION TAG	UNP Q8I372
H	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
H	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
H	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
H	240	LEU	-	EXPRESSION TAG	UNP Q8I372
H	241	GLU	-	EXPRESSION TAG	UNP Q8I372
H	242	HIS	-	EXPRESSION TAG	UNP Q8I372
H	243	HIS	-	EXPRESSION TAG	UNP Q8I372
H	244	HIS	-	EXPRESSION TAG	UNP Q8I372
H	245	HIS	-	EXPRESSION TAG	UNP Q8I372
H	246	HIS	-	EXPRESSION TAG	UNP Q8I372
H	247	HIS	-	EXPRESSION TAG	UNP Q8I372
I	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
I	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
I	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
I	240	LEU	-	EXPRESSION TAG	UNP Q8I372
I	241	GLU	-	EXPRESSION TAG	UNP Q8I372

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Chain	Residue	Modelled	Actual	Comment	Reference
I	242	HIS	-	EXPRESSION TAG	UNP Q8I372
I	243	HIS	-	EXPRESSION TAG	UNP Q8I372
I	244	HIS	-	EXPRESSION TAG	UNP Q8I372
I	245	HIS	-	EXPRESSION TAG	UNP Q8I372
I	246	HIS	-	EXPRESSION TAG	UNP Q8I372
I	247	HIS	-	EXPRESSION TAG	UNP Q8I372
J	96	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
J	100	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
J	212	MSE	MET	MODIFIED RESIDUE	UNP Q8I372
J	240	LEU	-	EXPRESSION TAG	UNP Q8I372
J	241	GLU	-	EXPRESSION TAG	UNP Q8I372
J	242	HIS	-	EXPRESSION TAG	UNP Q8I372
J	243	HIS	-	EXPRESSION TAG	UNP Q8I372
J	244	HIS	-	EXPRESSION TAG	UNP Q8I372
J	245	HIS	-	EXPRESSION TAG	UNP Q8I372
J	246	HIS	-	EXPRESSION TAG	UNP Q8I372
J	247	HIS	-	EXPRESSION TAG	UNP Q8I372

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Co 1 1	0	0
2	J	1	Total Co 1 1	0	0
2	D	1	Total Co 1 1	0	0
2	E	1	Total Co 1 1	0	0
2	H	1	Total Co 1 1	0	0
2	B	1	Total Co 1 1	0	0
2	I	1	Total Co 1 1	0	0
2	C	1	Total Co 1 1	0	0
2	A	1	Total Co 1 1	0	0
2	F	1	Total Co 1 1	0	0

- Molecule 3 is water.

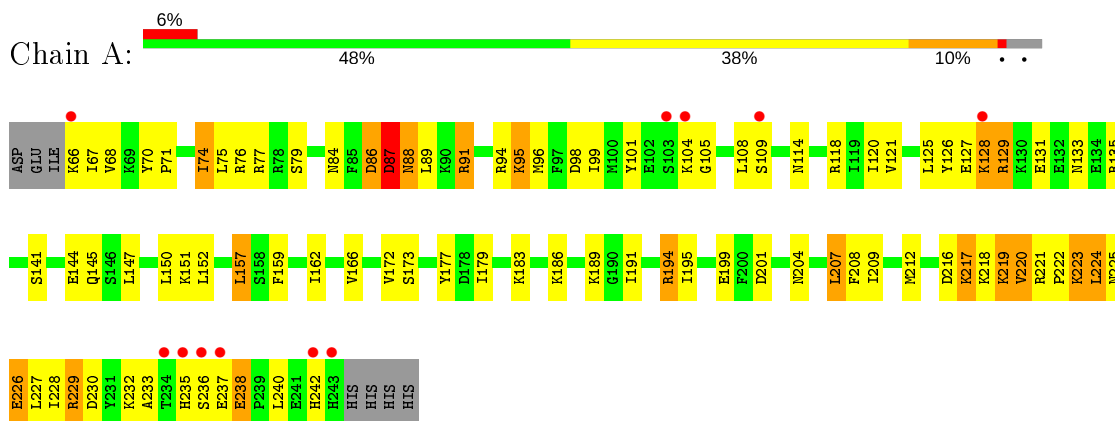
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	20	Total 20	O 20	0	0
3	B	18	Total 18	O 18	0	0
3	C	12	Total 12	O 12	0	0
3	D	14	Total 14	O 14	0	0
3	E	12	Total 12	O 12	0	0
3	F	27	Total 27	O 27	0	0
3	G	9	Total 9	O 9	0	0
3	H	9	Total 9	O 9	0	0
3	I	14	Total 14	O 14	0	0
3	J	14	Total 14	O 14	0	0



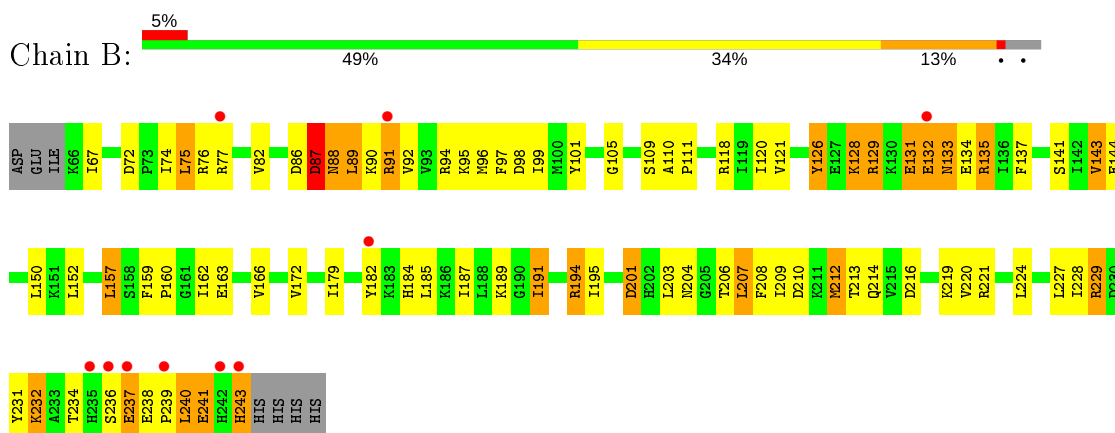
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

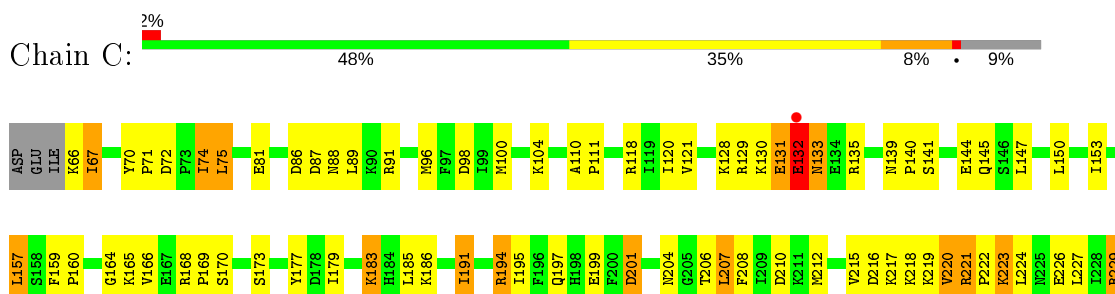
- Molecule 1: formylmethionine deformylase

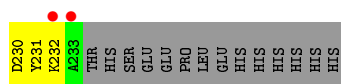


- Molecule 1: formylmethionine deformylase

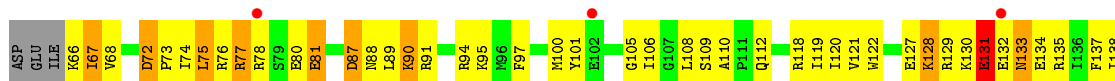


- Molecule 1: formylmethionine deformylase

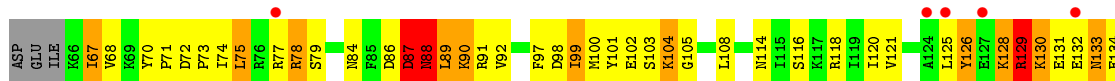




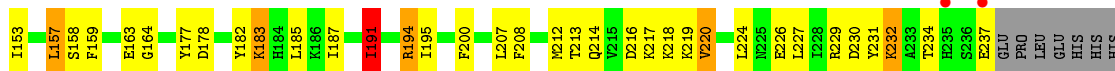
• Molecule 1: formylmethionine deformylase



• Molecule 1: formylmethionine deformylase

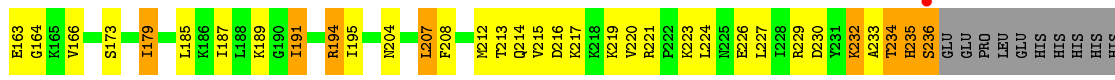


• Molecule 1: formylmethionine deformylase



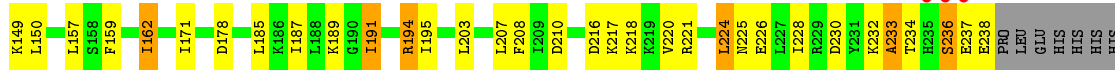
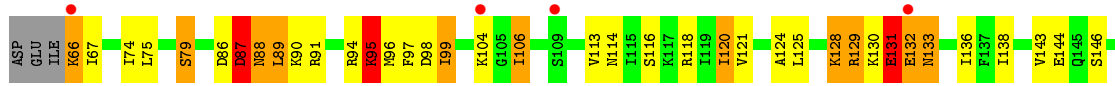
• Molecule 1: formylmethionine deformylase





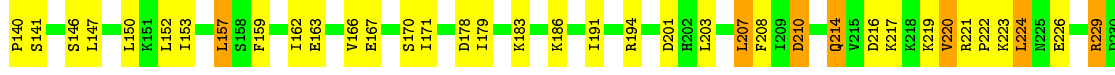
HIS

• Molecule 1: formylmethionine deformylase



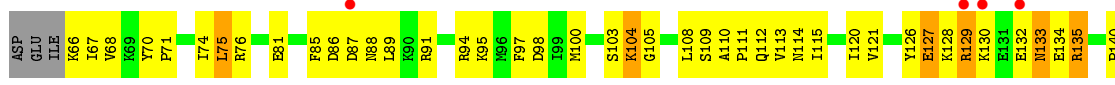
HIS  
HIS

• Molecule 1: formylmethionine deformylase



Y231, K232, A233, T234, R235, S236, GLU, PRO, LEU, LEU, HIS, HIS, HIS, HIS, HIS, HIS, HIS

• Molecule 1: formylmethionine deformylase



T234, R235, S236, GLU, PRO, PRO, LEU, LEU, HIS, HIS, HIS, HIS, HIS, HIS, HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.26Å 121.26Å 177.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.5 (20.00-2.80) 82.5 (19.98-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.79Å)	Xtrriage
Refinement program	REFMAC 5.1.24, CNS	Depositor
R, $R_{free}$	0.225 , 0.277 0.214 , 0.263	Depositor DCC
$R_{free}$ test set	5187 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtrriage
Anisotropy	0.295	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.042 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	14498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CO

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	0.74	1/1505 (0.1%)	0.91	7/2016 (0.3%)
1	B	0.66	1/1505 (0.1%)	0.88	7/2016 (0.3%)
1	C	0.68	0/1416	0.87	5/1894 (0.3%)
1	D	0.64	1/1458 (0.1%)	0.98	8/1951 (0.4%)
1	E	0.64	0/1474	0.85	6/1974 (0.3%)
1	F	0.70	0/1449	0.85	2/1939 (0.1%)
1	G	1.01	1/1440 (0.1%)	0.88	5/1927 (0.3%)
1	H	0.68	0/1458	0.91	9/1951 (0.5%)
1	I	0.62	0/1440	0.89	6/1927 (0.3%)
1	J	0.66	0/1440	0.87	3/1927 (0.2%)
All	All	0.71	4/14585 (0.0%)	0.89	58/19522 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	95	LYS	CG-CD	29.21	2.51	1.52
1	A	95	LYS	CG-CD	-16.42	0.96	1.52
1	B	95	LYS	CG-CD	8.23	1.80	1.52
1	D	95	LYS	CG-CD	5.42	1.70	1.52

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	95	LYS	CG-CD-CE	-18.45	56.55	111.90
1	B	95	LYS	CG-CD-CE	-14.63	68.02	111.90
1	A	95	LYS	CB-CG-CD	14.04	148.11	111.60
1	A	95	LYS	CG-CD-CE	-12.87	73.30	111.90
1	G	95	LYS	CG-CD-CE	-12.82	73.45	111.90

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	1478	0	1525	57	0
1	B	1478	0	1525	50	1
1	C	1393	0	1456	40	0
1	D	1434	0	1487	60	0
1	E	1449	0	1505	51	1
1	F	1425	0	1481	47	0
1	G	1416	0	1475	32	0
1	H	1434	0	1487	40	0
1	I	1416	0	1475	64	0
1	J	1416	0	1475	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	20	0	0	1	0
3	B	18	0	0	0	0
3	C	12	0	0	1	0
3	D	14	0	0	4	0
3	E	12	0	0	1	0
3	F	27	0	0	1	0
3	G	9	0	0	1	0
3	H	9	0	0	1	0
3	I	14	0	0	1	0
3	J	14	0	0	0	0
All	All	14498	0	14891	475	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 16.

The worst 5 of 475 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:C:100:MSE:SE	1:C:100:MSE:CE	2.14	1.43
1:G:164:GLY:HA3	1:G:212:MSE:HE2	1.22	1.14
1:F:164:GLY:HA3	1:F:212:MSE:HE2	1.27	1.09
1:I:131:GLU:O	1:I:133:ASN:N	1.88	1.06
1:I:229:ARG:HG3	1:I:229:ARG:HH11	1.18	1.06

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:B:163:GLU:OE1	1:E:221:ARG:NH1[4_564]	2.11	0.09

## 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	176/185 (95%)	152 (86%)	23 (13%)	1 (1%)	25	56
1	B	176/185 (95%)	160 (91%)	13 (7%)	3 (2%)	9	29
1	C	166/185 (90%)	148 (89%)	14 (8%)	4 (2%)	6	20
1	D	171/185 (92%)	155 (91%)	14 (8%)	2 (1%)	13	39
1	E	173/185 (94%)	152 (88%)	17 (10%)	4 (2%)	6	21
1	F	170/185 (92%)	157 (92%)	11 (6%)	2 (1%)	13	39
1	G	169/185 (91%)	148 (88%)	19 (11%)	2 (1%)	13	39
1	H	171/185 (92%)	154 (90%)	15 (9%)	2 (1%)	13	39
1	I	169/185 (91%)	154 (91%)	12 (7%)	3 (2%)	8	28
1	J	169/185 (91%)	158 (94%)	10 (6%)	1 (1%)	25	56
All	All	1710/1850 (92%)	1538 (90%)	148 (9%)	24 (1%)	11	34

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	132	GLU
1	C	131	GLU
1	D	132	GLU
1	E	129	ARG
1	E	132	GLU

### 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	167/171 (98%)	126 (75%)	41 (25%)	0	2
1	B	167/171 (98%)	126 (75%)	41 (25%)	0	2
1	C	157/171 (92%)	122 (78%)	35 (22%)	1	2
1	D	162/171 (95%)	121 (75%)	41 (25%)	0	1
1	E	164/171 (96%)	116 (71%)	48 (29%)	0	1
1	F	161/171 (94%)	128 (80%)	33 (20%)	1	3
1	G	160/171 (94%)	115 (72%)	45 (28%)	0	1
1	H	162/171 (95%)	126 (78%)	36 (22%)	1	2
1	I	160/171 (94%)	119 (74%)	41 (26%)	0	1
1	J	160/171 (94%)	122 (76%)	38 (24%)	0	2
All	All	1620/1710 (95%)	1221 (75%)	399 (25%)	0	2

5 of 399 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	135	ARG
1	F	158	SER
1	J	91	ARG
1	E	172	VAL
1	E	229	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such



sidechains are listed below:

Mol	Chain	Res	Type
1	E	184	HIS
1	F	180	ASN
1	J	114	ASN
1	F	114	ASN
1	F	133	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 [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	175/185 (94%)	0.09	11 (6%) 20 12	23, 41, 86, 97	1 (0%)
1	B	175/185 (94%)	-0.03	10 (5%) 23 15	15, 36, 83, 101	1 (0%)
1	C	165/185 (89%)	-0.17	3 (1%) 68 61	12, 32, 65, 76	1 (0%)
1	D	170/185 (91%)	-0.22	3 (1%) 68 61	19, 38, 78, 91	1 (0%)
1	E	172/185 (92%)	0.01	8 (4%) 31 22	17, 36, 88, 97	1 (0%)
1	F	169/185 (91%)	-0.26	3 (1%) 68 61	8, 28, 71, 96	1 (0%)
1	G	168/185 (90%)	-0.19	2 (1%) 79 73	17, 35, 70, 89	1 (0%)
1	H	170/185 (91%)	-0.15	7 (4%) 37 27	12, 32, 78, 98	1 (0%)
1	I	168/185 (90%)	-0.15	3 (1%) 68 61	15, 35, 76, 88	1 (0%)
1	J	168/185 (90%)	-0.09	6 (3%) 42 32	18, 35, 74, 87	1 (0%)
All	All	1700/1850 (91%)	-0.11	56 (3%) 46 36	8, 35, 78, 101	10 (0%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	233	ALA	8.0
1	E	237	GLU	6.3
1	A	243	HIS	5.7
1	G	236	SER	5.3
1	F	235	HIS	4.8

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	CO	D	331	1/1	0.98	0.07	28,28,28,28	0
2	CO	C	321	1/1	0.98	0.11	27,27,27,27	0
2	CO	A	301	1/1	0.99	0.07	34,34,34,34	0
2	CO	G	361	1/1	0.99	0.09	26,26,26,26	0
2	CO	B	311	1/1	0.99	0.13	27,27,27,27	0
2	CO	H	371	1/1	0.99	0.11	27,27,27,27	0
2	CO	I	381	1/1	0.99	0.13	37,37,37,37	0
2	CO	F	351	1/1	0.99	0.13	18,18,18,18	0
2	CO	E	341	1/1	1.00	0.07	29,29,29,29	0
2	CO	J	391	1/1	1.00	0.12	34,34,34,34	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.