



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2017 – 10:04 AM EDT

PDB ID : 5UE6  
Title : Structure of nitrite reductase AniA from *Neisseria gonorrhoeae*, space group I4122  
Authors : Hamza, A.; Williamson, Z.A.; Reed, R.W.; Sikora, A.E.; Korotkov, K.V.  
Deposited on : unknown  
Resolution : 2.35 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

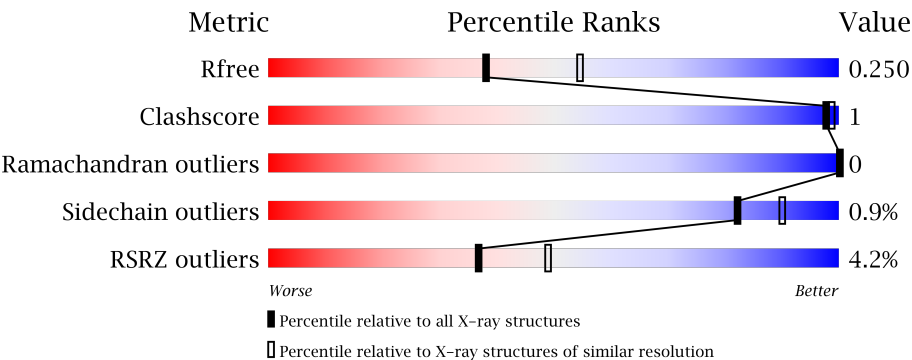
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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.



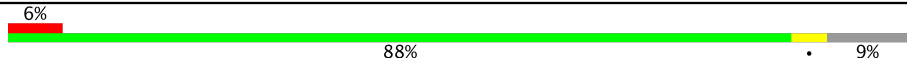

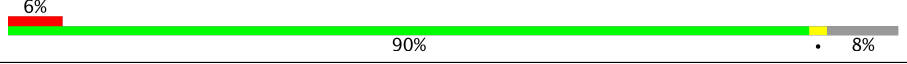

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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. 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	337	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>90%7%</div></div>
1	B	337	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>90%8%</div></div>
1	C	337	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>4%89%8%</div></div>
1	D	337	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>2%87%5%8%</div></div>
1	E	337	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>5%88%8%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	337	
1	G	337	
1	H	337	
1	I	337	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CU	A	501	-	-	-	X
2	CU	A	504	-	-	-	X
3	NA	A	503	-	-	-	X
3	NA	E	503	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 43082 atoms, of which 20829 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 Nitrite reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	314	Total	C	H	N	O	S	0	0	0
			4713	1514	2333	400	456	10			
1	B	310	Total	C	H	N	O	S	0	0	0
			4668	1500	2311	396	451	10			
1	C	310	Total	C	H	N	O	S	0	0	0
			4668	1500	2311	396	451	10			
1	D	309	Total	C	H	N	O	S	0	0	0
			4654	1495	2306	395	448	10			
1	E	310	Total	C	H	N	O	S	0	0	0
			4668	1500	2311	396	451	10			
1	F	307	Total	C	H	N	O	S	0	0	0
			4632	1489	2295	393	445	10			
1	G	314	Total	C	H	N	O	S	0	0	0
			4713	1514	2333	400	456	10			
1	H	310	Total	C	H	N	O	S	0	0	0
			4667	1500	2310	396	451	10			
1	I	311	Total	C	H	N	O	S	0	0	0
			4688	1509	2319	397	453	10			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	-	initiating methionine	UNP Q5F7A4
A	365	VAL	-	expression tag	UNP Q5F7A4
A	366	PRO	-	expression tag	UNP Q5F7A4
A	367	ARG	-	expression tag	UNP Q5F7A4
A	368	GLY	-	expression tag	UNP Q5F7A4
A	369	SER	-	expression tag	UNP Q5F7A4
A	370	LEU	-	expression tag	UNP Q5F7A4
A	371	GLU	-	expression tag	UNP Q5F7A4
A	372	HIS	-	expression tag	UNP Q5F7A4
A	373	HIS	-	expression tag	UNP Q5F7A4
A	374	HIS	-	expression tag	UNP Q5F7A4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	375	HIS	-	expression tag	UNP Q5F7A4
A	376	HIS	-	expression tag	UNP Q5F7A4
A	377	HIS	-	expression tag	UNP Q5F7A4
B	41	MET	-	initiating methionine	UNP Q5F7A4
B	365	VAL	-	expression tag	UNP Q5F7A4
B	366	PRO	-	expression tag	UNP Q5F7A4
B	367	ARG	-	expression tag	UNP Q5F7A4
B	368	GLY	-	expression tag	UNP Q5F7A4
B	369	SER	-	expression tag	UNP Q5F7A4
B	370	LEU	-	expression tag	UNP Q5F7A4
B	371	GLU	-	expression tag	UNP Q5F7A4
B	372	HIS	-	expression tag	UNP Q5F7A4
B	373	HIS	-	expression tag	UNP Q5F7A4
B	374	HIS	-	expression tag	UNP Q5F7A4
B	375	HIS	-	expression tag	UNP Q5F7A4
B	376	HIS	-	expression tag	UNP Q5F7A4
B	377	HIS	-	expression tag	UNP Q5F7A4
C	41	MET	-	initiating methionine	UNP Q5F7A4
C	365	VAL	-	expression tag	UNP Q5F7A4
C	366	PRO	-	expression tag	UNP Q5F7A4
C	367	ARG	-	expression tag	UNP Q5F7A4
C	368	GLY	-	expression tag	UNP Q5F7A4
C	369	SER	-	expression tag	UNP Q5F7A4
C	370	LEU	-	expression tag	UNP Q5F7A4
C	371	GLU	-	expression tag	UNP Q5F7A4
C	372	HIS	-	expression tag	UNP Q5F7A4
C	373	HIS	-	expression tag	UNP Q5F7A4
C	374	HIS	-	expression tag	UNP Q5F7A4
C	375	HIS	-	expression tag	UNP Q5F7A4
C	376	HIS	-	expression tag	UNP Q5F7A4
C	377	HIS	-	expression tag	UNP Q5F7A4
D	41	MET	-	initiating methionine	UNP Q5F7A4
D	365	VAL	-	expression tag	UNP Q5F7A4
D	366	PRO	-	expression tag	UNP Q5F7A4
D	367	ARG	-	expression tag	UNP Q5F7A4
D	368	GLY	-	expression tag	UNP Q5F7A4
D	369	SER	-	expression tag	UNP Q5F7A4
D	370	LEU	-	expression tag	UNP Q5F7A4
D	371	GLU	-	expression tag	UNP Q5F7A4
D	372	HIS	-	expression tag	UNP Q5F7A4
D	373	HIS	-	expression tag	UNP Q5F7A4
D	374	HIS	-	expression tag	UNP Q5F7A4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	375	HIS	-	expression tag	UNP Q5F7A4
D	376	HIS	-	expression tag	UNP Q5F7A4
D	377	HIS	-	expression tag	UNP Q5F7A4
E	41	MET	-	initiating methionine	UNP Q5F7A4
E	365	VAL	-	expression tag	UNP Q5F7A4
E	366	PRO	-	expression tag	UNP Q5F7A4
E	367	ARG	-	expression tag	UNP Q5F7A4
E	368	GLY	-	expression tag	UNP Q5F7A4
E	369	SER	-	expression tag	UNP Q5F7A4
E	370	LEU	-	expression tag	UNP Q5F7A4
E	371	GLU	-	expression tag	UNP Q5F7A4
E	372	HIS	-	expression tag	UNP Q5F7A4
E	373	HIS	-	expression tag	UNP Q5F7A4
E	374	HIS	-	expression tag	UNP Q5F7A4
E	375	HIS	-	expression tag	UNP Q5F7A4
E	376	HIS	-	expression tag	UNP Q5F7A4
E	377	HIS	-	expression tag	UNP Q5F7A4
F	41	MET	-	initiating methionine	UNP Q5F7A4
F	365	VAL	-	expression tag	UNP Q5F7A4
F	366	PRO	-	expression tag	UNP Q5F7A4
F	367	ARG	-	expression tag	UNP Q5F7A4
F	368	GLY	-	expression tag	UNP Q5F7A4
F	369	SER	-	expression tag	UNP Q5F7A4
F	370	LEU	-	expression tag	UNP Q5F7A4
F	371	GLU	-	expression tag	UNP Q5F7A4
F	372	HIS	-	expression tag	UNP Q5F7A4
F	373	HIS	-	expression tag	UNP Q5F7A4
F	374	HIS	-	expression tag	UNP Q5F7A4
F	375	HIS	-	expression tag	UNP Q5F7A4
F	376	HIS	-	expression tag	UNP Q5F7A4
F	377	HIS	-	expression tag	UNP Q5F7A4
G	41	MET	-	initiating methionine	UNP Q5F7A4
G	365	VAL	-	expression tag	UNP Q5F7A4
G	366	PRO	-	expression tag	UNP Q5F7A4
G	367	ARG	-	expression tag	UNP Q5F7A4
G	368	GLY	-	expression tag	UNP Q5F7A4
G	369	SER	-	expression tag	UNP Q5F7A4
G	370	LEU	-	expression tag	UNP Q5F7A4
G	371	GLU	-	expression tag	UNP Q5F7A4
G	372	HIS	-	expression tag	UNP Q5F7A4
G	373	HIS	-	expression tag	UNP Q5F7A4
G	374	HIS	-	expression tag	UNP Q5F7A4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	375	HIS	-	expression tag	UNP Q5F7A4
G	376	HIS	-	expression tag	UNP Q5F7A4
G	377	HIS	-	expression tag	UNP Q5F7A4
H	41	MET	-	initiating methionine	UNP Q5F7A4
H	365	VAL	-	expression tag	UNP Q5F7A4
H	366	PRO	-	expression tag	UNP Q5F7A4
H	367	ARG	-	expression tag	UNP Q5F7A4
H	368	GLY	-	expression tag	UNP Q5F7A4
H	369	SER	-	expression tag	UNP Q5F7A4
H	370	LEU	-	expression tag	UNP Q5F7A4
H	371	GLU	-	expression tag	UNP Q5F7A4
H	372	HIS	-	expression tag	UNP Q5F7A4
H	373	HIS	-	expression tag	UNP Q5F7A4
H	374	HIS	-	expression tag	UNP Q5F7A4
H	375	HIS	-	expression tag	UNP Q5F7A4
H	376	HIS	-	expression tag	UNP Q5F7A4
H	377	HIS	-	expression tag	UNP Q5F7A4
I	41	MET	-	initiating methionine	UNP Q5F7A4
I	365	VAL	-	expression tag	UNP Q5F7A4
I	366	PRO	-	expression tag	UNP Q5F7A4
I	367	ARG	-	expression tag	UNP Q5F7A4
I	368	GLY	-	expression tag	UNP Q5F7A4
I	369	SER	-	expression tag	UNP Q5F7A4
I	370	LEU	-	expression tag	UNP Q5F7A4
I	371	GLU	-	expression tag	UNP Q5F7A4
I	372	HIS	-	expression tag	UNP Q5F7A4
I	373	HIS	-	expression tag	UNP Q5F7A4
I	374	HIS	-	expression tag	UNP Q5F7A4
I	375	HIS	-	expression tag	UNP Q5F7A4
I	376	HIS	-	expression tag	UNP Q5F7A4
I	377	HIS	-	expression tag	UNP Q5F7A4

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	3	Total Cu 3 3	0	0
2	D	3	Total Cu 3 3	0	0
2	E	2	Total Cu 2 2	0	0
2	H	2	Total Cu 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Cu 2	0	0
2	I	1	Total 1	Cu 1	0	0
2	C	1	Total 1	Cu 1	0	0
2	A	3	Total 3	Cu 3	0	0
2	F	1	Total 1	Cu 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0
3	E	1	Total 1	Na 1	0	0
3	H	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0
3	I	1	Total 1	Na 1	0	0
3	C	1	Total 1	Na 1	0	0
3	A	1	Total 1	Na 1	0	0
3	F	1	Total 1	Na 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total 187	O 187	0	0
4	B	160	Total 160	O 160	0	0
4	C	135	Total 135	O 135	0	0

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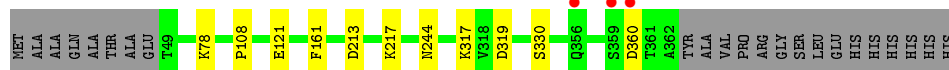
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	93	Total 93	O 93	0	0
4	E	85	Total 85	O 85	0	0
4	F	68	Total 68	O 68	0	0
4	G	101	Total 101	O 101	0	0
4	H	84	Total 84	O 84	0	0
4	I	71	Total 71	O 71	0	0

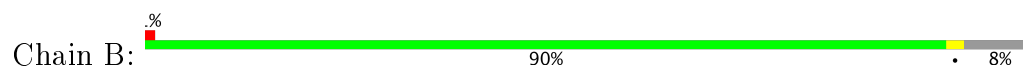
### 3 Residue-property plots [i](#)

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.

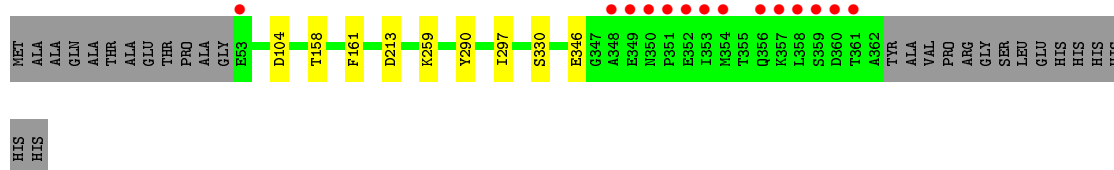
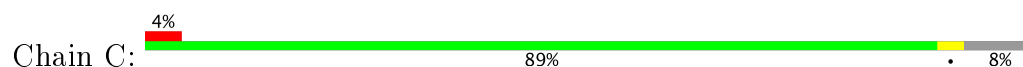
#### • Molecule 1: Nitrite reductase



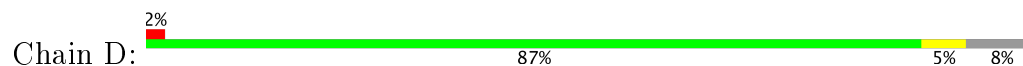
#### • Molecule 1: Nitrite reductase



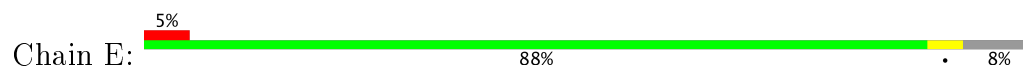
#### • Molecule 1: Nitrite reductase

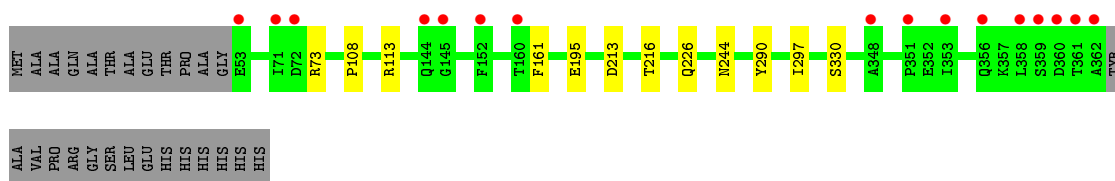


#### • Molecule 1: Nitrite reductase

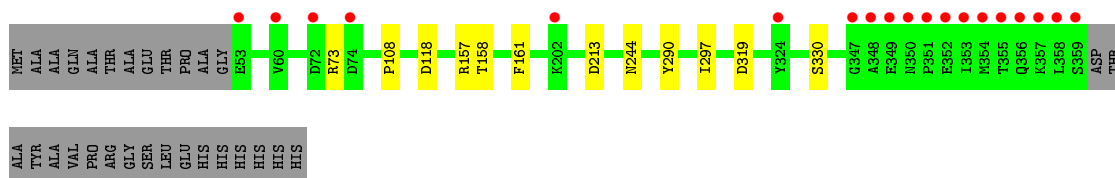
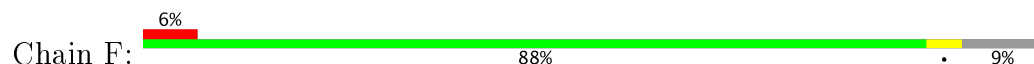


#### • Molecule 1: Nitrite reductase

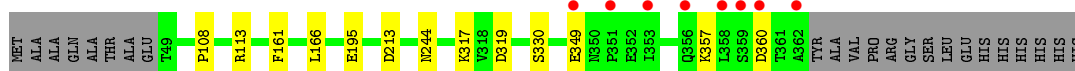
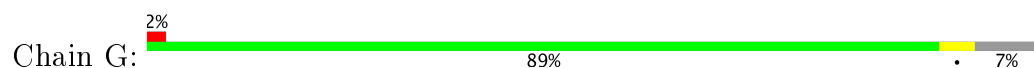




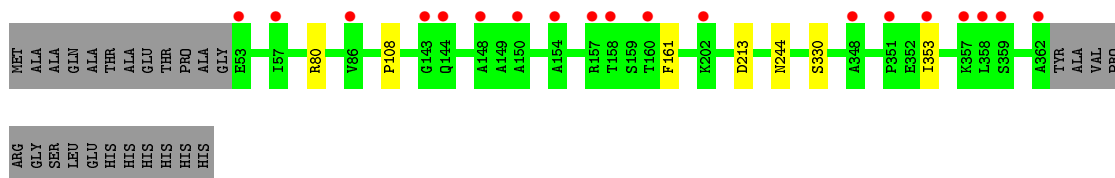
• Molecule 1: Nitrite reductase



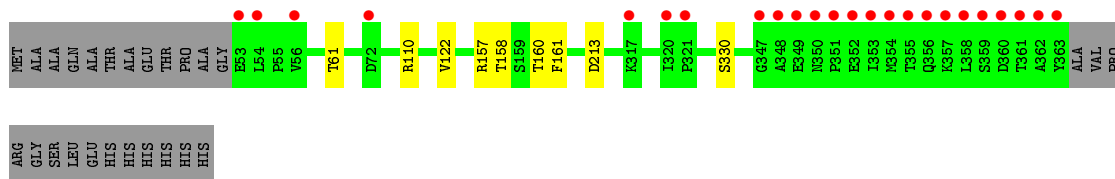
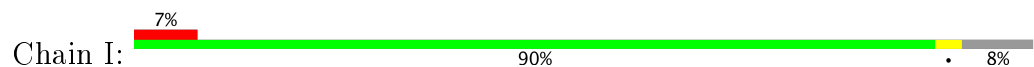
• Molecule 1: Nitrite reductase



• Molecule 1: Nitrite reductase



• Molecule 1: Nitrite reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.34Å 177.34Å 449.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.68 – 2.35 88.67 – 2.35	Depositor EDS
% Data completeness (in resolution range)	82.5 (83.68-2.35) 85.0 (88.67-2.35)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.34Å)	Xtriage
Refinement program	PHENIX (dev_2481)	Depositor
R, $R_{free}$	0.236 , 0.259 0.223 , 0.250	Depositor DCC
$R_{free}$ test set	6322 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.9	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	43082	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.46 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5159e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

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

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	0.28	0/2436	0.50	0/3307
1	B	0.27	0/2412	0.50	0/3273
1	C	0.27	0/2412	0.48	0/3273
1	D	0.27	0/2403	0.48	0/3261
1	E	0.26	0/2412	0.48	0/3273
1	F	0.26	0/2392	0.47	0/3245
1	G	0.27	0/2436	0.49	0/3307
1	H	0.27	0/2412	0.48	0/3273
1	I	0.26	0/2425	0.48	0/3291
All	All	0.27	0/21740	0.49	0/29503

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	330	SER	Peptide
1	B	330	SER	Peptide
1	C	330	SER	Peptide
1	D	330	SER	Peptide
1	E	330	SER	Peptide
1	F	330	SER	Peptide
1	G	330	SER	Peptide
1	H	330	SER	Peptide
1	I	330	SER	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	2380	2333	2332	5	0
1	B	2357	2311	2310	2	0
1	C	2357	2311	2310	4	0
1	D	2348	2306	2304	9	0
1	E	2357	2311	2310	4	0
1	F	2337	2295	2294	6	0
1	G	2380	2333	2332	8	0
1	H	2357	2310	2310	3	0
1	I	2369	2319	2319	4	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	G	3	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
4	A	187	0	0	1	0
4	B	160	0	0	0	0
4	C	135	0	0	1	0
4	D	93	0	0	1	0
4	E	85	0	0	0	0
4	F	68	0	0	1	0
4	G	101	0	0	0	0
4	H	84	0	0	1	0
4	I	71	0	0	0	0
All	All	22253	20829	20821	38	0

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.

All (38) 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:61:THR:O	1:D:110:ARG:NH2	2.17	0.77
1:I:61:THR:O	1:I:110:ARG:NH2	2.24	0.71
1:D:356:GLN:OE1	4:D:601:HOH:O	2.11	0.67
1:G:360:ASP:HA	1:I:158:THR:O	1.95	0.67
1:D:349:GLU:OE2	1:I:157:ARG:NH2	2.29	0.66
1:A:360:ASP:HA	1:C:158:THR:O	2.01	0.61
1:D:356:GLN:HG3	1:G:360:ASP:O	2.01	0.60
1:A:317:LYS:NZ	1:A:319:ASP:OD1	2.29	0.60
1:F:157:ARG:NH2	1:G:349:GLU:OE2	2.35	0.59
1:F:73:ARG:NH2	1:F:118:ASP:OD2	2.39	0.55
1:D:360:ASP:HA	1:F:158:THR:O	2.08	0.54
1:G:166:LEU:HD21	1:H:353:ILE:HD12	1.91	0.52
1:H:80:ARG:NH1	4:H:603:HOH:O	2.43	0.50
1:D:74:ASP:OD1	1:D:75:TYR:HD1	1.96	0.49
1:A:217:LYS:NZ	4:A:604:HOH:O	2.40	0.48
1:B:108:PRO:HD3	1:B:244:ASN:HA	1.95	0.48
1:E:113:ARG:NE	1:E:195:GLU:OE2	2.47	0.47
1:G:357:LYS:HD3	1:G:360:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:PRO:HD3	1:H:244:ASN:HA	1.98	0.46
1:A:108:PRO:HD3	1:A:244:ASN:HA	1.98	0.46
1:G:113:ARG:NE	1:G:195:GLU:OE2	2.48	0.45
1:F:319:ASP:N	4:F:607:HOH:O	2.49	0.44
1:D:73:ARG:NH1	1:D:118:ASP:OD2	2.46	0.44
1:D:78:LYS:HE2	1:D:121:GLU:OE1	2.17	0.44
1:C:104:ASP:OD2	4:C:601:HOH:O	2.21	0.43
1:A:78:LYS:HE2	1:A:121:GLU:OE1	2.18	0.43
1:E:216:THR:HB	1:E:226:GLN:HB3	2.01	0.43
1:G:317:LYS:HE3	1:G:319:ASP:OD1	2.18	0.43
1:E:108:PRO:HD3	1:E:244:ASN:HA	2.00	0.43
1:F:290:TYR:CE2	1:F:297:ILE:HD11	2.54	0.43
1:D:108:PRO:HD3	1:D:244:ASN:HA	2.01	0.42
1:G:108:PRO:HD3	1:G:244:ASN:HA	2.01	0.42
1:B:216:THR:HB	1:B:226:GLN:HB3	2.01	0.42
1:C:259:LYS:HE2	1:C:346:GLU:OE2	2.20	0.41
1:C:290:TYR:CE2	1:C:297:ILE:HD11	2.56	0.41
1:I:122:VAL:O	1:I:160:THR:HA	2.21	0.41
1:F:108:PRO:HD3	1:F:244:ASN:HA	2.03	0.40
1:E:290:TYR:CE2	1:E:297:ILE:HD11	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/337 (93%)	308 (99%)	4 (1%)	0	100	100
1	B	308/337 (91%)	303 (98%)	5 (2%)	0	100	100
1	C	308/337 (91%)	303 (98%)	5 (2%)	0	100	100
1	D	307/337 (91%)	303 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	308/337 (91%)	304 (99%)	4 (1%)	0	100	100
1	F	305/337 (90%)	300 (98%)	5 (2%)	0	100	100
1	G	312/337 (93%)	308 (99%)	4 (1%)	0	100	100
1	H	308/337 (91%)	304 (99%)	4 (1%)	0	100	100
1	I	309/337 (92%)	304 (98%)	5 (2%)	0	100	100
All	All	2777/3033 (92%)	2737 (99%)	40 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	250/267 (94%)	248 (99%)	2 (1%)	85	91
1	B	248/267 (93%)	246 (99%)	2 (1%)	85	91
1	C	248/267 (93%)	246 (99%)	2 (1%)	85	91
1	D	247/267 (92%)	245 (99%)	2 (1%)	85	91
1	E	248/267 (93%)	245 (99%)	3 (1%)	75	86
1	F	246/267 (92%)	244 (99%)	2 (1%)	85	91
1	G	250/267 (94%)	248 (99%)	2 (1%)	85	91
1	H	248/267 (93%)	246 (99%)	2 (1%)	85	91
1	I	249/267 (93%)	247 (99%)	2 (1%)	85	91
All	All	2234/2403 (93%)	2215 (99%)	19 (1%)	82	90

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	PHE
1	A	213	ASP
1	B	161	PHE
1	B	213	ASP

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Mol	Chain	Res	Type
1	C	161	PHE
1	C	213	ASP
1	D	161	PHE
1	D	213	ASP
1	E	73	ARG
1	E	161	PHE
1	E	213	ASP
1	F	161	PHE
1	F	213	ASP
1	G	161	PHE
1	G	213	ASP
1	H	161	PHE
1	H	213	ASP
1	I	161	PHE
1	I	213	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 27 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

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<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	314/337 (93%)	0.39	3 (0%)	82 90	20, 28, 54, 104	0
1	B	310/337 (91%)	0.17	5 (1%)	72 81	18, 27, 53, 75	0
1	C	310/337 (91%)	0.35	14 (4%)	34 46	20, 29, 55, 118	0
1	D	309/337 (91%)	0.26	8 (2%)	56 66	29, 38, 62, 109	0
1	E	310/337 (91%)	0.38	16 (5%)	28 40	27, 36, 63, 80	0
1	F	307/337 (91%)	0.40	19 (6%)	21 30	27, 38, 61, 117	0
1	G	314/337 (93%)	0.12	8 (2%)	58 68	26, 32, 55, 116	0
1	H	310/337 (91%)	0.40	19 (6%)	22 31	28, 38, 60, 79	0
1	I	311/337 (92%)	0.48	24 (7%)	14 21	29, 38, 64, 120	0
All	All	2795/3033 (92%)	0.33	116 (4%)	37 49	18, 35, 60, 120	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	348	ALA	8.5
1	I	363	TYR	6.1
1	F	351	PRO	5.3
1	E	358	LEU	5.2
1	I	357	LYS	5.0
1	F	353	ILE	5.0
1	D	362	ALA	5.0
1	I	53	GLU	4.9
1	C	360	ASP	4.9
1	I	353	ILE	4.9
1	G	356	GLN	4.8
1	I	361	THR	4.8
1	F	348	ALA	4.8
1	I	358	LEU	4.7
1	F	358	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	357	LYS	4.7
1	I	360	ASP	4.6
1	I	356	GLN	4.5
1	I	354	MET	4.5
1	I	352	GLU	4.5
1	F	53	GLU	4.4
1	C	348	ALA	4.3
1	F	356	GLN	4.3
1	C	361	THR	4.3
1	E	356	GLN	4.3
1	I	359	SER	4.2
1	I	351	PRO	4.2
1	D	356	GLN	4.1
1	H	150	ALA	4.1
1	G	360	ASP	4.0
1	I	362	ALA	3.9
1	F	359	SER	3.7
1	F	60	VAL	3.7
1	C	351	PRO	3.7
1	H	53	GLU	3.7
1	C	358	LEU	3.7
1	H	362	ALA	3.6
1	E	72	ASP	3.6
1	D	360	ASP	3.5
1	C	349	GLU	3.5
1	F	350	ASN	3.4
1	I	355	THR	3.4
1	H	353	ILE	3.4
1	I	320	ILE	3.2
1	A	356	GLN	3.2
1	E	360	ASP	3.2
1	E	353	ILE	3.2
1	C	357	LYS	3.2
1	H	359	SER	3.1
1	C	359	SER	3.0
1	F	355	THR	3.0
1	H	358	LEU	3.0
1	F	349	GLU	3.0
1	B	362	ALA	3.0
1	F	352	GLU	2.9
1	C	352	GLU	2.9
1	D	348	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	53	GLU	2.9
1	G	353	ILE	2.9
1	C	350	ASN	2.8
1	F	72	ASP	2.8
1	I	349	GLU	2.8
1	G	349	GLU	2.8
1	C	53	GLU	2.8
1	H	148	ALA	2.7
1	C	356	GLN	2.7
1	F	354	MET	2.7
1	H	143	GLY	2.7
1	E	160	THR	2.7
1	E	351	PRO	2.7
1	I	321	PRO	2.6
1	F	74	ASP	2.6
1	G	362	ALA	2.6
1	H	351	PRO	2.6
1	H	348	ALA	2.6
1	E	348	ALA	2.5
1	I	350	ASN	2.5
1	H	158	THR	2.5
1	D	361	THR	2.5
1	I	54	LEU	2.5
1	E	152	PHE	2.5
1	H	86	VAL	2.4
1	I	72	ASP	2.4
1	G	359	SER	2.4
1	C	353	ILE	2.4
1	F	324	TYR	2.4
1	D	353	ILE	2.3
1	E	144	GLN	2.3
1	B	358	LEU	2.3
1	E	359	SER	2.3
1	H	202	LYS	2.3
1	G	351	PRO	2.2
1	E	362	ALA	2.2
1	E	145	GLY	2.2
1	I	347	GLY	2.2
1	H	357	LYS	2.2
1	B	158	THR	2.2
1	H	57	ILE	2.2
1	A	360	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	160	THR	2.2
1	C	354	MET	2.2
1	H	144	GLN	2.2
1	D	355	THR	2.1
1	B	53	GLU	2.1
1	E	71	ILE	2.1
1	G	358	LEU	2.1
1	E	361	THR	2.1
1	I	317	LYS	2.1
1	B	143	GLY	2.1
1	F	347	GLY	2.1
1	I	56	VAL	2.1
1	A	359	SER	2.1
1	D	347	GLY	2.1
1	H	157	ARG	2.0
1	H	154	ALA	2.0
1	F	202	LYS	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CU	A	501	1/1	1.00	0.21	4.59	30,30,30,30	0
3	NA	E	503	1/1	0.96	0.23	3.64	42,42,42,42	0
2	CU	A	504	1/1	0.99	0.18	2.52	33,33,33,33	0
3	NA	A	503	1/1	0.94	0.23	2.47	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	G	503	1/1	0.96	0.20	1.61	37,37,37,37	0
3	NA	B	503	1/1	0.98	0.18	1.48	32,32,32,32	0
3	NA	D	503	1/1	0.82	0.22	1.44	45,45,45,45	0
2	CU	G	504	1/1	0.99	0.17	1.35	43,43,43,43	0
2	CU	G	501	1/1	0.99	0.14	0.19	31,31,31,31	0
3	NA	C	502	1/1	0.97	0.17	-0.04	30,30,30,30	0
2	CU	D	504	1/1	0.99	0.12	-0.45	43,43,43,43	0
2	CU	I	501	1/1	0.97	0.12	-0.67	37,37,37,37	0
2	CU	B	501	1/1	1.00	0.12	-0.75	28,28,28,28	0
3	NA	H	503	1/1	0.94	0.13	-0.75	34,34,34,34	0
2	CU	E	501	1/1	0.99	0.12	-0.96	39,39,39,39	0
2	CU	C	501	1/1	1.00	0.15	-1.28	27,27,27,27	0
2	CU	D	501	1/1	0.99	0.13	-1.33	34,34,34,34	0
2	CU	A	502	1/1	1.00	0.12	-1.44	28,28,28,28	0
2	CU	G	502	1/1	0.97	0.12	-1.56	39,39,39,39	0
2	CU	B	502	1/1	0.98	0.12	-1.80	29,29,29,29	0
3	NA	I	502	1/1	0.96	0.10	-2.06	40,40,40,40	0
2	CU	H	501	1/1	0.98	0.09	-2.09	41,41,41,41	0
2	CU	D	502	1/1	0.99	0.12	-2.29	45,45,45,45	0
3	NA	F	502	1/1	0.96	0.11	-2.76	39,39,39,39	0
2	CU	F	501	1/1	0.98	0.11	-3.41	40,40,40,40	0
2	CU	E	502	1/1	0.98	0.10	-3.78	39,39,39,39	0
2	CU	H	502	1/1	0.99	0.08	-4.05	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.