



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:58 PM UTC

PDB ID : 5UE6 / pdb_00005ue6
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 : 2016-12-29
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

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
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

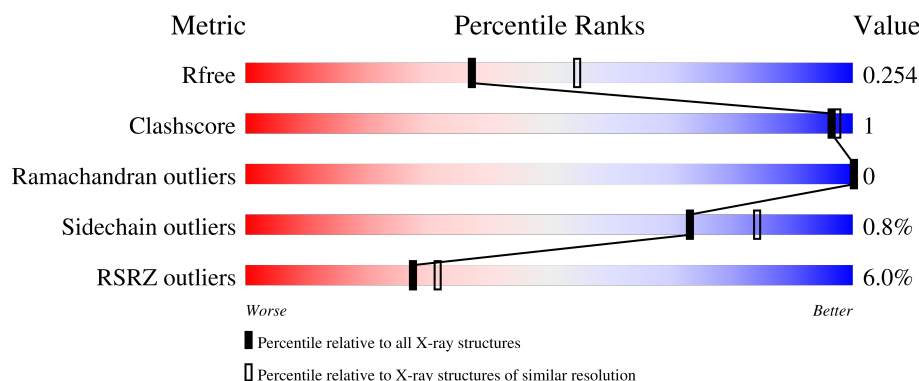
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	337	4% 90% 7%
1	B	337	3% 89% 8%
1	C	337	4% 89% 8%
1	D	337	8% 87% 8%
1	E	337	5% 88% 8%

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Mol	Chain	Length	Quality of chain
1	F	337	7% 88% 9%
1	G	337	6% 90% 7%
1	H	337	6% 90% 8%
1	I	337	7% 89% 8%

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 (CCD ID: CU) (formula: Cu).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total 2	Cu 2	0	0
2	F	1	Total 1	Cu 1	0	0
2	G	3	Total 3	Cu 3	0	0
2	H	2	Total 2	Cu 2	0	0
2	I	1	Total 1	Cu 1	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Na 1	0	0
3	B	1	Total 1	Na 1	0	0
3	C	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	F	1	Total 1	Na 1	0	0
3	G	1	Total 1	Na 1	0	0
3	H	1	Total 1	Na 1	0	0
3	I	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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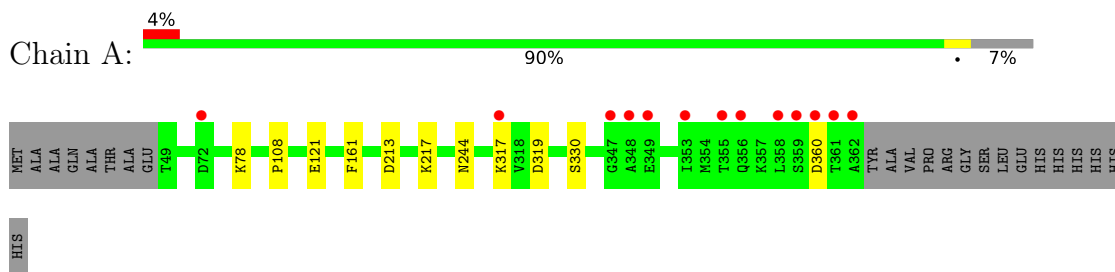
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	93	Total 93	O 93	0	0
4	E	85	Total 85	O 85	0	0
4	F	68	Total 68	O 68	0	0
4	G	101	Total 101	O 101	0	0
4	H	84	Total 84	O 84	0	0
4	I	71	Total 71	O 71	0	0

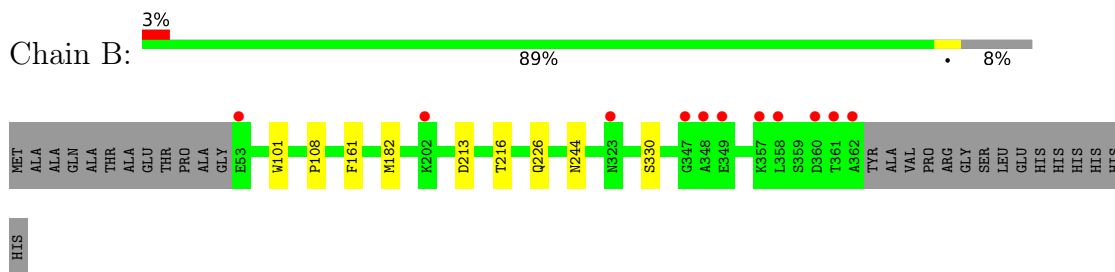
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

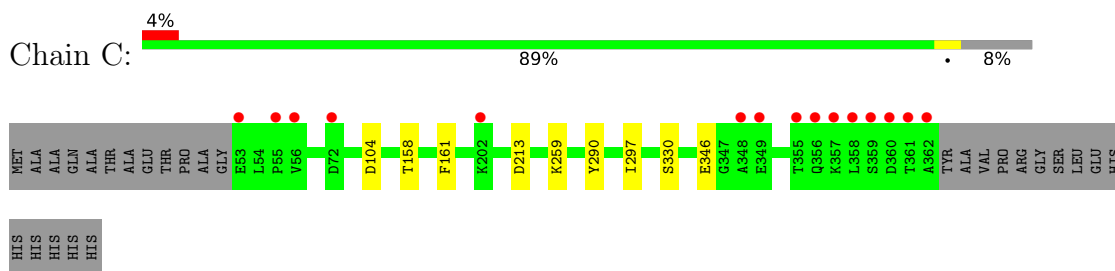
- Molecule 1: Nitrite reductase



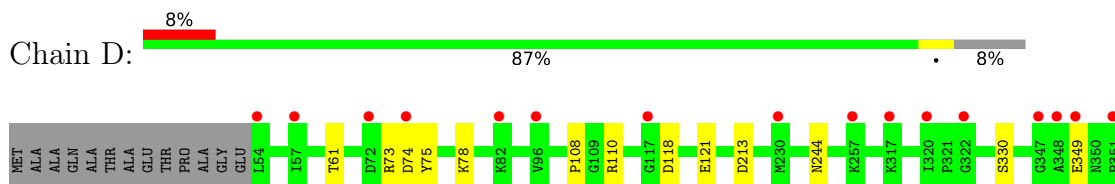
- Molecule 1: Nitrite reductase

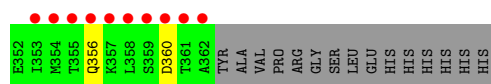


- Molecule 1: Nitrite reductase

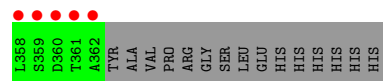
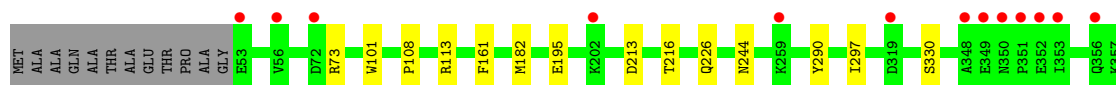
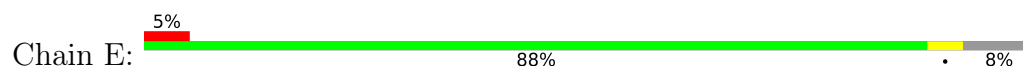


- Molecule 1: Nitrite reductase

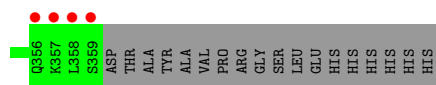
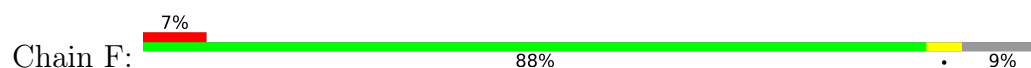




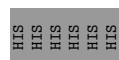
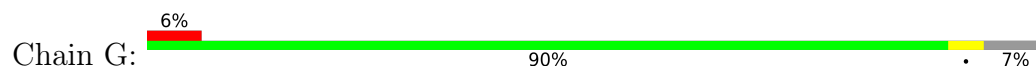
• Molecule 1: Nitrite reductase



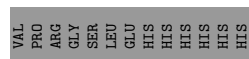
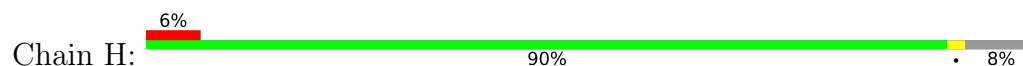
• Molecule 1: Nitrite reductase



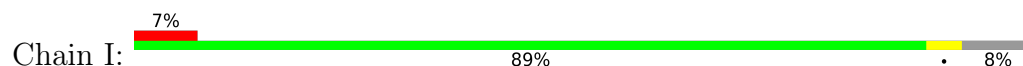
• Molecule 1: Nitrite reductase

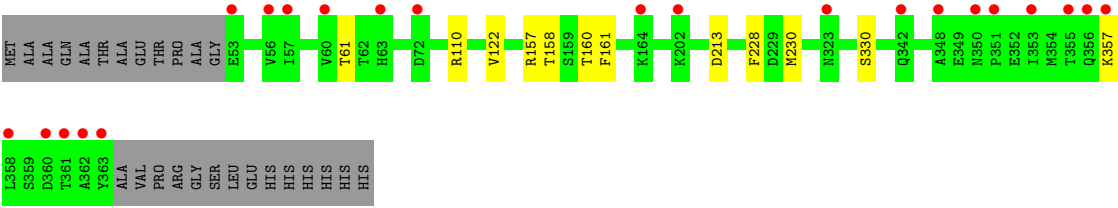


• Molecule 1: Nitrite reductase



• Molecule 1: Nitrite reductase





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	177.34Å 177.34Å 449.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.68 – 2.35 83.68 – 2.35	Depositor EDS
% Data completeness (in resolution range)	82.5 (83.68-2.35) 85.0 (83.68-2.35)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (dev_2481)	Depositor
R, R_{free}	0.236 , 0.259 0.229 , 0.254	Depositor DCC
R_{free} test set	6337 reflections (3.52%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	43082	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage'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.*

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

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	0.15	0/2436	0.37	0/3307
1	B	0.14	0/2412	0.36	0/3273
1	C	0.14	0/2412	0.34	0/3273
1	D	0.14	0/2403	0.34	0/3261
1	E	0.13	0/2412	0.34	0/3273
1	F	0.13	0/2392	0.33	0/3245
1	G	0.15	0/2436	0.36	0/3307
1	H	0.13	0/2412	0.34	0/3273
1	I	0.13	0/2425	0.33	0/3291
All	All	0.14	0/21740	0.35	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	3	0
1	C	2357	2311	2310	4	0
1	D	2348	2306	2304	9	0
1	E	2357	2311	2310	5	0
1	F	2337	2295	2294	6	0
1	G	2380	2333	2332	8	0
1	H	2357	2310	2310	4	0
1	I	2369	2319	2319	6	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	42	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 (42) 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:F:157:ARG:NH2	1:G:349:GLU:OE2	2.35	0.59
1:A:317:LYS:NZ	1:A:319:ASP:OD1	2.29	0.58
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:H:152:PHE:O	1:I:357:LYS:NZ	2.44	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:357:LYS:HD3	1:G:360:ASP:HB2	1.96	0.47
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:I:228:PHE:HE2	1:I:230:MET:HE2	1.80	0.46
1:G:113:ARG:NE	1:G:195:GLU:OE2	2.48	0.45
1:B:101:TRP:CH2	1:B:182:MET:HE3	2.52	0.44
1:E:101:TRP:CH2	1:E:182:MET:HE3	2.53	0.44
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 [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	312/337 (93%)	308 (99%)	4 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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 [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	250/267 (94%)	248 (99%)	2 (1%)	73	84
1	B	248/267 (93%)	246 (99%)	2 (1%)	73	84
1	C	248/267 (93%)	246 (99%)	2 (1%)	73	84
1	D	247/267 (92%)	246 (100%)	1 (0%)	84	91
1	E	248/267 (93%)	245 (99%)	3 (1%)	63	77
1	F	246/267 (92%)	244 (99%)	2 (1%)	73	84
1	G	250/267 (94%)	249 (100%)	1 (0%)	84	91
1	H	248/267 (93%)	246 (99%)	2 (1%)	73	84
1	I	249/267 (93%)	247 (99%)	2 (1%)	73	84
All	All	2234/2403 (93%)	2217 (99%)	17 (1%)	73	84

All (17) 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
1	C	161	PHE
1	C	213	ASP
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	213	ASP
1	H	161	PHE
1	H	213	ASP
1	I	161	PHE
1	I	213	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	336	ASN
1	E	336	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 ⓘ

There are no oligosaccharides 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 [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	314/337 (93%)	0.22	13 (4%)	41	47	21, 30, 58, 119	0
1	B	310/337 (91%)	0.12	11 (3%)	47	53	20, 30, 58, 85	0
1	C	310/337 (91%)	0.18	15 (4%)	35	41	22, 32, 62, 137	0
1	D	309/337 (91%)	0.78	26 (8%)	17	19	32, 42, 68, 122	0
1	E	310/337 (91%)	0.57	18 (5%)	29	33	28, 39, 68, 89	0
1	F	307/337 (91%)	0.63	22 (7%)	21	24	30, 42, 66, 134	0
1	G	314/337 (93%)	0.46	20 (6%)	25	28	28, 36, 64, 137	0
1	H	310/337 (91%)	0.64	20 (6%)	25	28	31, 42, 66, 87	0
1	I	311/337 (92%)	0.65	22 (7%)	22	25	33, 42, 72, 137	0
All	All	2795/3033 (92%)	0.47	167 (5%)	27	31	20, 38, 66, 137	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	362	ALA	7.6
1	I	363	TYR	5.7
1	C	362	ALA	5.4
1	G	362	ALA	5.4
1	A	362	ALA	5.3
1	E	362	ALA	5.3
1	I	356	GLN	5.1
1	C	356	GLN	4.9
1	H	362	ALA	4.9
1	D	355	THR	4.8
1	F	356	GLN	4.7
1	I	362	ALA	4.7
1	B	362	ALA	4.5
1	G	360	ASP	4.4
1	A	356	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	356	GLN	4.3
1	D	360	ASP	4.3
1	I	358	LEU	4.2
1	D	74	ASP	4.1
1	D	347	GLY	4.1
1	E	358	LEU	4.1
1	C	360	ASP	4.0
1	F	72	ASP	3.9
1	I	53	GLU	3.9
1	F	357	LYS	3.9
1	A	348	ALA	3.9
1	G	49	THR	3.9
1	E	72	ASP	3.8
1	A	359	SER	3.8
1	H	353	ILE	3.7
1	I	348	ALA	3.7
1	F	348	ALA	3.6
1	G	349	GLU	3.5
1	D	351	PRO	3.5
1	F	353	ILE	3.5
1	D	358	LEU	3.5
1	I	63	HIS	3.4
1	A	353	ILE	3.4
1	E	356	GLN	3.4
1	G	356	GLN	3.4
1	D	354	MET	3.4
1	D	361	THR	3.4
1	H	323	ASN	3.4
1	C	361	THR	3.4
1	I	56	VAL	3.4
1	G	348	ALA	3.4
1	G	353	ILE	3.4
1	B	348	ALA	3.3
1	A	361	THR	3.3
1	A	358	LEU	3.3
1	C	53	GLU	3.2
1	F	53	GLU	3.2
1	A	360	ASP	3.2
1	F	60	VAL	3.2
1	F	358	LEU	3.2
1	D	359	SER	3.1
1	H	358	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	355	THR	3.1
1	I	360	ASP	3.1
1	H	190	GLY	3.0
1	A	349	GLU	3.0
1	G	361	THR	3.0
1	F	74	ASP	3.0
1	D	353	ILE	2.9
1	B	360	ASP	2.9
1	I	353	ILE	2.9
1	H	53	GLU	2.9
1	A	72	ASP	2.9
1	E	319	ASP	2.9
1	I	357	LYS	2.8
1	C	56	VAL	2.8
1	D	72	ASP	2.8
1	H	348	ALA	2.8
1	A	355	THR	2.8
1	H	356	GLN	2.8
1	C	358	LEU	2.8
1	E	361	THR	2.7
1	B	361	THR	2.7
1	D	82	LYS	2.7
1	H	73	ARG	2.7
1	E	348	ALA	2.7
1	E	360	ASP	2.7
1	I	72	ASP	2.7
1	F	351	PRO	2.7
1	E	53	GLU	2.7
1	F	352	GLU	2.7
1	G	358	LEU	2.7
1	C	72	ASP	2.6
1	G	359	SER	2.6
1	H	359	SER	2.6
1	D	349	GLU	2.6
1	F	160	THR	2.6
1	E	353	ILE	2.6
1	F	164	LYS	2.6
1	D	54	LEU	2.6
1	B	202	LYS	2.6
1	E	349	GLU	2.5
1	G	352	GLU	2.5
1	G	347	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	63	HIS	2.5
1	F	359	SER	2.5
1	C	348	ALA	2.5
1	D	320	ILE	2.5
1	E	202	LYS	2.5
1	G	308	ALA	2.5
1	D	322	GLY	2.5
1	G	322	GLY	2.5
1	H	202	LYS	2.4
1	B	358	LEU	2.4
1	D	357	LYS	2.4
1	B	323	ASN	2.4
1	E	352	GLU	2.4
1	G	72	ASP	2.4
1	H	357	LYS	2.4
1	E	56	VAL	2.4
1	I	60	VAL	2.4
1	C	202	LYS	2.3
1	D	230	MET	2.3
1	F	350	ASN	2.3
1	C	357	LYS	2.3
1	G	351	PRO	2.3
1	A	347	GLY	2.3
1	I	361	THR	2.3
1	H	72	ASP	2.3
1	H	94	ASP	2.3
1	E	351	PRO	2.3
1	H	349	GLU	2.3
1	D	117	GLY	2.2
1	B	53	GLU	2.2
1	A	317	LYS	2.2
1	D	348	ALA	2.2
1	H	154	ALA	2.2
1	F	75	TYR	2.2
1	D	96	VAL	2.2
1	E	350	ASN	2.2
1	C	349	GLU	2.2
1	B	349	GLU	2.2
1	G	355	THR	2.2
1	C	359	SER	2.1
1	E	359	SER	2.1
1	F	54	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	164	LYS	2.1
1	F	66	GLU	2.1
1	H	127	ASN	2.1
1	H	361	THR	2.1
1	B	357	LYS	2.1
1	D	317	LYS	2.1
1	G	357	LYS	2.1
1	G	71	ILE	2.1
1	F	161	PHE	2.1
1	F	202	LYS	2.1
1	G	350	ASN	2.1
1	I	57	ILE	2.1
1	F	56	VAL	2.1
1	B	347	GLY	2.1
1	D	257	LYS	2.0
1	H	162	SER	2.0
1	H	319	ASP	2.0
1	I	323	ASN	2.0
1	I	350	ASN	2.0
1	C	55	PRO	2.0
1	E	259	LYS	2.0
1	C	355	THR	2.0
1	I	342	GLN	2.0
1	D	57	ILE	2.0
1	I	351	PRO	2.0
1	I	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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
3	NA	E	503	1/1	0.93	0.31	42,42,42,42	0
3	NA	H	503	1/1	0.93	0.15	34,34,34,34	0
3	NA	F	502	1/1	0.94	0.18	39,39,39,39	0
3	NA	G	503	1/1	0.95	0.17	37,37,37,37	0
3	NA	D	503	1/1	0.95	0.23	45,45,45,45	0
3	NA	I	502	1/1	0.95	0.17	40,40,40,40	0
3	NA	A	503	1/1	0.96	0.17	27,27,27,27	0
3	NA	B	503	1/1	0.97	0.19	32,32,32,32	0
2	CU	E	502	1/1	0.98	0.04	39,39,39,39	0
2	CU	G	502	1/1	0.98	0.03	39,39,39,39	0
2	CU	A	504	1/1	0.99	0.05	33,33,33,33	0
2	CU	G	504	1/1	0.99	0.05	43,43,43,43	0
2	CU	H	501	1/1	0.99	0.03	41,41,41,41	0
2	CU	H	502	1/1	0.99	0.05	39,39,39,39	0
2	CU	I	501	1/1	0.99	0.03	37,37,37,37	0
2	CU	B	502	1/1	0.99	0.03	29,29,29,29	0
2	CU	D	501	1/1	0.99	0.02	34,34,34,34	0
3	NA	C	502	1/1	0.99	0.21	30,30,30,30	0
2	CU	D	502	1/1	0.99	0.03	45,45,45,45	0
2	CU	D	504	1/1	0.99	0.04	43,43,43,43	0
2	CU	E	501	1/1	0.99	0.04	39,39,39,39	0
2	CU	A	502	1/1	0.99	0.03	28,28,28,28	0
2	CU	F	501	1/1	0.99	0.03	40,40,40,40	0
2	CU	G	501	1/1	0.99	0.02	31,31,31,31	0
2	CU	B	501	1/1	1.00	0.02	28,28,28,28	0
2	CU	A	501	1/1	1.00	0.07	30,30,30,30	0
2	CU	C	501	1/1	1.00	0.01	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.