

# wwPDB X-ray Structure Validation Summary Report (i)

### Sep 10, 2024 – 04:21 PM JST

PDB ID	:	9JDT
Title	:	Crystal structure of reductase NaAD
Authors	:	Tang, J.; Liuqing, C.
Deposited on	:	2024-09-01
Resolution	:	3.26  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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.26 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$	
$R_{free}$	164625	1482 (3.30-3.22)	
Clashscore	180529	1546 (3.30-3.22)	
Ramachandran outliers	177936	1536 (3.30-3.22)	
Sidechain outliers	177891	1535 (3.30-3.22)	
RSRZ outliers	164620	1483 (3.30-3.22)	

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 <=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	А	266	3%	51%	6% •		
1	В	266	3%	46%	6% • •		
1	С	266	6%	42%	5% 5%		
1	D	266	5%	45%	•••		
1	Е	266	34%	55%	6% • •		
1	F	266	38%	49%	8% •		



Mol	Chain	Length	Quality of chain				
1	G	266	45%	43%	7% • •		
1	Н	266	3% 50%	41%	5% •		
1	Ι	266	2% <b>4</b> 4%	47%	5%••		
1	J	266	45%	44%	6% • •		
1	K	266	36%	52%	8% •		
1	L	266	46%	46%	•••		
1	М	266	6% 39%	48%	6% • •		
1	Ν	266	37%	51%	8% •		
1	О	266	3% 45%	44%	5%••		
1	Р	266	39%	50%	6% • •		



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 29767 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.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
1	Δ	256	Total	С	Ν	0	S	0	0	0
1	Л	230	1852	1161	325	352	14	0	0	0
1	В	257	Total	С	Ν	0	$\mathbf{S}$	0	0	0
1	D	201	1860	1167	326	353	14	0	0	0
1	C	254	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
-	0	204	1839	1152	323	350	14	0	0	0
1	О	256	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
		200	1852	1161	325	352	14			
1	E	255	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
	-		1847	1158	324	351	14	Ŭ		
1	F	255	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
-	-		1847	1158	324	351	14	Ŭ		
1	G	255	Total	С	Ν	Ο	S	0	0	0
			1847	1158	324	351	14			
1	н	256	Total	$\mathbf{C}$	Ν	Ο	$\mathbf{S}$	0	0	0
		200	1852	1161	325	352	14			
1	Ι	257	Total	C	N	0	S	0	0	0
			1860	1167	326	353	14			
1	J	256	Total	С	N	0	S	0	0	0
			1852	1161	325	352	14	_	_	
1	K	256	Total	С	N	0	S	0	0	0
			1852	1161	325	352	14			
1	L	256	Total	C	N	0	S	0	0	0
			1852	1161	325	352	14			
1	М	255	Total	C	N	0	S	0	0	0
			1847	1158	324	351	14			
1	Ν	256	Total	C	N	0	S	0	0	0
			1852	1161	325	352	14			
1	Ο	255	Total	U	N 20.4	0	S	0	0	0
			1847	1158	324	351	14			
1	Р	255	Total	U	N 20.4	0	S	0	0	0
			1847	1158	324	351	14			

• Molecule 1 is a protein called Short-chain dehydrogenase/reductase SDR.



9	J	D	Т
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A4XEP2
A	2	HIS	_	expression tag	UNP A4XEP2
A	3	HIS	_	expression tag	UNP A4XEP2
A	4	HIS	_	expression tag	UNP A4XEP2
A	5	HIS	_	expression tag	UNP A4XEP2
A	6	HIS	_	expression tag	UNP A4XEP2
A	7	HIS	-	expression tag	UNP A4XEP2
A	148	ALA	GLY	conflict	UNP A4XEP2
A	202	LEU	ILE	conflict	UNP A4XEP2
В	1	MET	-	initiating methionine	UNP A4XEP2
В	2	HIS	-	expression tag	UNP A4XEP2
В	3	HIS	-	expression tag	UNP A4XEP2
В	4	HIS	-	expression tag	UNP A4XEP2
В	5	HIS	-	expression tag	UNP A4XEP2
В	6	HIS	-	expression tag	UNP A4XEP2
В	7	HIS	-	expression tag	UNP A4XEP2
В	148	ALA	GLY	conflict	UNP A4XEP2
В	202	LEU	ILE	conflict	UNP A4XEP2
С	1	MET	-	initiating methionine	UNP A4XEP2
С	2	HIS	-	expression tag	UNP A4XEP2
С	3	HIS	-	expression tag	UNP A4XEP2
С	4	HIS	-	expression tag	UNP A4XEP2
С	5	HIS	-	expression tag	UNP A4XEP2
С	6	HIS	-	expression tag	UNP A4XEP2
С	7	HIS	-	expression tag	UNP A4XEP2
С	148	ALA	GLY	conflict	UNP A4XEP2
C	202	LEU	ILE	conflict	UNP A4XEP2
D	1	MET	-	initiating methionine	UNP A4XEP2
D	2	HIS	-	expression tag	UNP A4XEP2
D	3	HIS	-	expression tag	UNP A4XEP2
D	4	HIS	-	expression tag	UNP A4XEP2
D	5	HIS	-	expression tag	UNP A4XEP2
D	6	HIS	-	expression tag	UNP A4XEP2
D	7	HIS	-	expression tag	UNP A4XEP2
D	148	ALA	GLY	conflict	UNP A4XEP2
D	202	LEU	ILE	conflict	UNP A4XEP2
E	1	MET	-	initiating methionine	UNP A4XEP2
E	2	HIS	-	expression tag	UNP A4XEP2
E	3	HIS	-	expression tag	UNP A4XEP2
E	4	HIS	-	expression tag	UNP A4XEP2
E	5	HIS	-	expression tag	UNP A4XEP2
E	6	HIS	-	expression tag	UNP A4XEP2

There are 144 discrepancies between the modelled and reference sequences:



QI	DT
55	

Chain	Residue	Modelled	Actual	Comment	Reference
Е	7	HIS	-	expression tag	UNP A4XEP2
Е	148	ALA	GLY	conflict	UNP A4XEP2
Е	202	LEU	ILE	conflict	UNP A4XEP2
F	1	MET	_	initiating methionine	UNP A4XEP2
F	2	HIS	-	expression tag	UNP A4XEP2
F	3	HIS	-	expression tag	UNP A4XEP2
F	4	HIS	-	expression tag	UNP A4XEP2
F	5	HIS	-	expression tag	UNP A4XEP2
F	6	HIS	-	expression tag	UNP A4XEP2
F	7	HIS	-	expression tag	UNP A4XEP2
F	148	ALA	GLY	conflict	UNP A4XEP2
F	202	LEU	ILE	conflict	UNP A4XEP2
G	1	MET	-	initiating methionine	UNP A4XEP2
G	2	HIS	-	expression tag	UNP A4XEP2
G	3	HIS	-	expression tag	UNP A4XEP2
G	4	HIS	-	expression tag	UNP A4XEP2
G	5	HIS	-	expression tag	UNP A4XEP2
G	6	HIS	-	expression tag	UNP A4XEP2
G	7	HIS	-	expression tag	UNP A4XEP2
G	148	ALA	GLY	conflict	UNP A4XEP2
G	202	LEU	ILE	conflict	UNP A4XEP2
Н	1	MET	-	initiating methionine	UNP A4XEP2
H	2	HIS	-	expression tag	UNP A4XEP2
H	3	HIS	-	expression tag	UNP A4XEP2
H	4	HIS	-	expression tag	UNP A4XEP2
H	5	HIS	-	expression tag	UNP A4XEP2
H	6	HIS	-	expression tag	UNP A4XEP2
H	7	HIS	-	expression tag	UNP A4XEP2
H	148	ALA	GLY	conflict	UNP A4XEP2
H	202	LEU	ILE	conflict	UNP A4XEP2
I	1	MET	-	initiating methionine	UNP A4XEP2
I	2	HIS	-	expression tag	UNP A4XEP2
I	3	HIS	-	expression tag	UNP A4XEP2
I	4	HIS	-	expression tag	UNP A4XEP2
I	5	HIS	-	expression tag	UNP A4XEP2
I	6	HIS	-	expression tag	UNP A4XEP2
	7	HIS	-	expression tag	UNP A4XEP2
I	148	ALA	GLY	conflict	UNP A4XEP2
I	202	LEU	ILE	conflict	UNP A4XEP2
J	1	MET	-	initiating methionine	UNP A4XEP2
J	2	HIS	-	expression tag	UNP A4XEP2
J	3	HIS	-	expression tag	UNP A4XEP2



Chain	Residue	Modelled	Actual	Comment	Reference
J	4	HIS	-	expression tag	UNP A4XEP2
J	5	HIS	-	expression tag	UNP A4XEP2
J	6	HIS	-	expression tag	UNP A4XEP2
J	7	HIS	-	expression tag	UNP A4XEP2
J	148	ALA	GLY	conflict	UNP A4XEP2
J	202	LEU	ILE	conflict	UNP A4XEP2
K	1	MET	-	initiating methionine	UNP A4XEP2
K	2	HIS	-	expression tag	UNP A4XEP2
K	3	HIS	-	expression tag	UNP A4XEP2
K	4	HIS	-	expression tag	UNP A4XEP2
K	5	HIS	-	expression tag	UNP A4XEP2
K	6	HIS	-	expression tag	UNP A4XEP2
K	7	HIS	-	expression tag	UNP A4XEP2
K	148	ALA	GLY	conflict	UNP A4XEP2
K	202	LEU	ILE	conflict	UNP A4XEP2
L	1	MET	-	initiating methionine	UNP A4XEP2
L	2	HIS	-	expression tag	UNP A4XEP2
L	3	HIS	-	expression tag	UNP A4XEP2
L	4	HIS	-	expression tag	UNP A4XEP2
L	5	HIS	-	expression tag	UNP A4XEP2
L	6	HIS	-	expression tag	UNP A4XEP2
L	7	HIS	-	expression tag	UNP A4XEP2
L	148	ALA	GLY	conflict	UNP A4XEP2
L	202	LEU	ILE	conflict	UNP A4XEP2
M	1	MET	-	initiating methionine	UNP A4XEP2
M	2	HIS	-	expression tag	UNP A4XEP2
M	3	HIS	-	expression tag	UNP A4XEP2
M	4	HIS	-	expression tag	UNP A4XEP2
M	5	HIS	-	expression tag	UNP A4XEP2
M	6	HIS	-	expression tag	UNP A4XEP2
M	7	HIS	-	expression tag	UNP A4XEP2
M	148	ALA	GLY	conflict	UNP A4XEP2
M	202	LEU	ILE	conflict	UNP A4XEP2
N	1	MET	-	initiating methionine	UNP A4XEP2
N	2	HIS	-	expression tag	UNP A4XEP2
N N	3	HIS	-	expression tag	UNP A4XEP2
N N	4	HIS	-	expression tag	UNP A4XEP2
N	5	HIS	-	expression tag	UNP A4XEP2
N	6	HIS	-	expression tag	UNP A4XEP2
N N	7	HIS	-	expression tag	UNP A4XEP2
N	148	ALA	GLY	conflict	UNP A4XEP2
N	202	LEU	ILE	conflict	UNP A4XEP2



Chain	Residue	Modelled	Actual	Comment	Reference
0	1	MET	-	initiating methionine	UNP A4XEP2
0	2	HIS	-	expression tag	UNP A4XEP2
0	3	HIS	-	expression tag	UNP A4XEP2
0	4	HIS	-	expression tag	UNP A4XEP2
0	5	HIS	-	expression tag	UNP A4XEP2
0	6	HIS	-	expression tag	UNP A4XEP2
0	7	HIS	-	expression tag	UNP A4XEP2
0	148	ALA	GLY	conflict	UNP A4XEP2
0	202	LEU	ILE	conflict	UNP A4XEP2
Р	1	MET	-	initiating methionine	UNP A4XEP2
Р	2	HIS	-	expression tag	UNP A4XEP2
Р	3	HIS	-	expression tag	UNP A4XEP2
Р	4	HIS	-	expression tag	UNP A4XEP2
Р	5	HIS	-	expression tag	UNP A4XEP2
Р	6	HIS	-	expression tag	UNP A4XEP2
Р	7	HIS	-	expression tag	UNP A4XEP2
Р	148	ALA	GLY	conflict	UNP A4XEP2
Р	202	LEU	ILE	conflict	UNP A4XEP2

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	13	Total         O           13         13	0	0
2	В	11	Total         O           11         11	0	0
2	С	7	Total O 7 7	0	0
2	D	8	Total O 8 8	0	0
2	Е	13	Total         O           13         13	0	0
2	F	4	Total O 4 4	0	0
2	G	9	Total O 9 9	0	0
2	Н	7	Total O 7 7	0	0
2	Ι	11	Total         O           11         11	0	0
2	J	12	TotalO1212	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	10	Total         O           10         10	0	0
2	L	7	Total O 7 7	0	0
2	М	9	Total O 9 9	0	0
2	Ν	12	Total         O           12         12	0	0
2	Ο	14	Total O 14 14	0	0
2	Р	15	$\begin{array}{cc} \text{Total} & \text{O} \\ 15 & 15 \end{array}$	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: Short-chain dehydrogenase/reductase SDR

• Molecule 1: Short-chain dehydrogenase/reductase SDR









<sup>•</sup> Molecule 1: Short-chain dehydrogenase/reductase SDR









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 $\bullet$  Molecule 1: Short-chain dehydrogenase/reduct ase SDR



#### M231 M232 M233 M235 M235 M235 M235 M235 M241 M242 M245 M249 M249 M249 M249 M249 M265 M256 M256

 $\bullet$  Molecule 1: Short-chain dehydrogenase/reduct ase SDR









51%

8%

 $\bullet$  Molecule 1: Short-chain dehydrogenase/reduct ase SDR

37%

Chain N:







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	65.32Å 121.77Å 276.15Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $93.40^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	20.00 - 3.26	Depositor
	20.00 - 3.27	EDS
% Data completeness	99.0 (20.00-3.26)	Depositor
(in resolution range)	81.0 (20.00-3.27)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.83 (at 3.26 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R R.	0.260 , $0.300$	Depositor
$\Lambda, \Lambda_{free}$	0.273 , $0.317$	DCC
$R_{free}$ test set	751 reflections $(1.38\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	44.8	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35 , $70.4$	EDS
L-test for $twinning^2$	$ < L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	29767	wwPDB-VP
Average B, all atoms $(Å^2)$	35.0	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 59.28 % 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 1.8062e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

# 5.1 Standard geometry (i)

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		
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.99	4/1881~(0.2%)	1.30	21/2548~(0.8%)	
1	В	0.93	2/1889~(0.1%)	1.24	11/2559~(0.4%)	
1	С	0.83	0/1868	1.23	16/2530~(0.6%)	
1	D	0.91	2/1881~(0.1%)	1.25	18/2548~(0.7%)	
1	Е	1.01	5/1876~(0.3%)	1.31	19/2541~(0.7%)	
1	F	1.03	8/1876~(0.4%)	1.24	14/2541~(0.6%)	
1	G	1.03	8/1876~(0.4%)	1.35	19/2541~(0.7%)	
1	Н	0.97	8/1881~(0.4%)	1.18	10/2548~(0.4%)	
1	Ι	0.91	6/1889~(0.3%)	1.16	9/2559~(0.4%)	
1	J	1.00	7/1881~(0.4%)	1.35	20/2548~(0.8%)	
1	K	0.95	5/1881~(0.3%)	1.31	24/2548~(0.9%)	
1	L	0.93	4/1881~(0.2%)	1.22	13/2548~(0.5%)	
1	М	0.91	5/1876~(0.3%)	1.21	12/2541~(0.5%)	
1	N	1.00	7/1881~(0.4%)	1.26	19/2548~(0.7%)	
1	0	0.96	5/1876~(0.3%)	1.22	14/2541~(0.6%)	
1	Р	1.00	8/1876~(0.4%)	1.27	20/2541~(0.8%)	
All	All	0.96	84/30069~(0.3%)	1.26	259/40730~(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	А	0	1
1	В	0	4
1	С	0	2
1	D	0	1
1	Е	0	3
1	F	0	3
1	G	0	4
1	Н	0	2
1	Ι	0	4



	0	1 10	
Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	4
1	Κ	0	1
1	L	0	3
1	М	0	8
1	0	0	2
1	Р	0	2
All	All	0	44

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	Ε	176	GLU	CD-OE2	14.86	1.42	1.25
1	Р	157	ALA	C-O	12.16	1.46	1.23
1	Н	99	GLU	CD-OE2	10.82	1.37	1.25
1	Ν	29	GLU	CD-OE2	10.41	1.37	1.25
1	G	99	GLU	CD-OE2	10.08	1.36	1.25

The worst 5 of 259 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	G	230	ARG	NE-CZ-NH1	14.93	127.77	120.30
1	G	233	ARG	NE-CZ-NH1	-13.65	113.48	120.30
1	J	151	ARG	NE-CZ-NH1	12.23	126.42	120.30
1	С	151	ARG	NE-CZ-NH1	-11.33	114.63	120.30
1	J	233	ARG	NE-CZ-NH2	-10.75	114.93	120.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	225	ARG	Sidechain
1	В	108	ARG	Sidechain
1	В	11	ALA	Peptide
1	В	230	ARG	Sidechain
1	В	233	ARG	Sidechain

# 5.2 Too-close contacts (i)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1852	0	1857	145	0
1	В	1860	0	1868	120	1
1	С	1839	0	1841	118	1
1	D	1852	0	1857	133	0
1	Е	1847	0	1852	164	0
1	F	1847	0	1852	156	0
1	G	1847	0	1852	149	0
1	Н	1852	0	1857	125	0
1	Ι	1860	0	1868	159	0
1	J	1852	0	1857	97	0
1	K	1852	0	1857	166	0
1	L	1852	0	1857	127	0
1	М	1847	0	1852	144	0
1	N	1852	0	1857	160	0
1	0	1847	0	1852	139	0
1	Р	1847	0	1852	158	0
2	А	13	0	0	3	0
2	В	11	0	0	1	0
2	С	7	0	0	6	0
2	D	8	0	0	2	0
2	Е	13	0	0	1	0
2	F	4	0	0	2	0
2	G	9	0	0	0	0
2	Н	7	0	0	0	0
2	Ι	11	0	0	2	0
2	J	12	0	0	0	0
2	K	10	0	0	2	0
2	L	7	0	0	6	0
2	М	9	0	0	3	0
2	N	12	0	0	1	0
2	Ο	14	0	0	0	0
2	Р	15	0	0	0	0
All	All	29767	0	29688	2005	1

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 34.

The worst 5 of 2005 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:P:157:ALA:O	1:P:160:CYS:N	1.75	1.19
1:A:54:GLY:HA2	2:A:311:HOH:O	1.46	1.13
1:N:165:ALA:HB1	1:P:161:THR:HG23	1.32	1.10
1:A:12:LEU:HB3	1:A:39:ALA:HB2	1.37	1.06
1:P:158:ALA:HA	1:P:161:THR:HB	1.31	1.05

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:130:GLU:OE1	$1:C:136:ALA:CB[1_455]$	1.92	0.28

# 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	Perc	entiles
1	А	254/266~(96%)	203 (80%)	45 (18%)	6 (2%)	5	23
1	В	255/266~(96%)	213 (84%)	39~(15%)	3 (1%)	11	37
1	С	252/266~(95%)	214 (85%)	33~(13%)	5 (2%)	6	27
1	D	254/266~(96%)	213 (84%)	35~(14%)	6 (2%)	5	23
1	Ε	253/266~(95%)	215 (85%)	31~(12%)	7 (3%)	4	21
1	F	253/266~(95%)	207 (82%)	36 (14%)	10 (4%)	2	14
1	G	253/266~(95%)	224 (88%)	22 (9%)	7 (3%)	4	21
1	Н	254/266~(96%)	216 (85%)	33~(13%)	5 (2%)	6	27
1	Ι	255/266~(96%)	223 (88%)	27~(11%)	5 (2%)	6	27
1	J	254/266~(96%)	225 (89%)	20~(8%)	9 (4%)	3	17
1	Κ	254/266~(96%)	212 (84%)	35~(14%)	7(3%)	4	21
1	L	254/266~(96%)	214 (84%)	37 (15%)	3 (1%)	11	37
1	М	253/266~(95%)	206 (81%)	40 (16%)	7 (3%)	4	21



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Pe	erc	entiles
1	Ν	254/266~(96%)	214 (84%)	34 (13%)	6 (2%)		5	23
1	Ο	253/266~(95%)	214 (85%)	33 (13%)	6 (2%)		5	23
1	Р	253/266~(95%)	207~(82%)	38 (15%)	8 (3%)		3	19
All	All	4058/4256~(95%)	3420 (84%)	538 (13%)	100 (2%)		4	23

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5 of 100 Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	Е	63	VAL
1	F	38	ASN
1	F	45	ASP
1	F	157	ALA
1	G	195	ASP

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	entiles
1	А	188/198~(95%)	177 (94%)	11 (6%)	16	42
1	В	189/198~(96%)	175 (93%)	14 (7%)	11	33
1	С	187/198~(94%)	181 (97%)	6 (3%)	34	59
1	D	188/198~(95%)	182 (97%)	6 (3%)	34	59
1	Е	188/198~(95%)	181 (96%)	7 (4%)	29	55
1	F	188/198~(95%)	179 (95%)	9~(5%)	21	48
1	G	188/198~(95%)	180 (96%)	8 (4%)	25	51
1	Н	188/198~(95%)	180 (96%)	8 (4%)	25	51
1	Ι	189/198~(96%)	185 (98%)	4 (2%)	48	69
1	J	188/198~(95%)	181 (96%)	7 (4%)	29	55
1	Κ	188/198~(95%)	178 (95%)	10 (5%)	19	45
1	L	188/198~(95%)	179 (95%)	9 (5%)	21	48
1	М	188/198~(95%)	177 (94%)	11 (6%)	16	42



Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	Ν	188/198~(95%)	178~(95%)	10~(5%)	19	45
1	Ο	188/198~(95%)	181 (96%)	7~(4%)	29	55
1	Р	188/198~(95%)	177~(94%)	11 (6%)	16	42
All	All	3009/3168~(95%)	2871 (95%)	138 (5%)	23	50

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5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	Ν	224	MET
1	Ν	264	SER
1	Р	93	SER
1	F	180	LEU
1	F	144	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	L	88	HIS
1	М	265	GLN
1	L	143	ASN
1	М	61	HIS
1	Ν	77	GLN

#### 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 oligosaccharides in this entry.



# 5.6 Ligand geometry (i)

There are no ligands in this entry.

# 5.7 Other polymers (i)

There are no such residues in this entry.

# 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 6 Fit of model and data (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,  $95^{th}$  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	$OWAB(A^2)$	Q<0.9
1	А	256/266~(96%)	0.36	8 (3%) 51 38	4, 25, 62, 107	0
1	В	257/266~(96%)	0.32	9 (3%) 47 35	0, 25, 63, 128	0
1	С	254/266~(95%)	0.47	17 (6%) 25 20	4, 36, 90, 163	0
1	D	256/266~(96%)	0.53	12 (4%) 37 28	9, 37, 84, 130	0
1	Ε	255/266~(95%)	0.55	18 (7%) 23 19	1, 33, 94, 150	0
1	F	255/266~(95%)	0.54	14 (5%) 32 25	8, 32, 66, 89	0
1	G	255/266~(95%)	0.32	8 (3%) 51 38	0, 33, 76, 106	0
1	Н	256/266~(96%)	0.43	8 (3%) 51 38	6, 33, 73, 119	0
1	Ι	257/266~(96%)	0.28	4 (1%) 70 57	5, 31, 61, 96	0
1	J	256/266~(96%)	0.27	4 (1%) 70 57	5, 26, 56, 95	0
1	Κ	256/266~(96%)	0.46	14 (5%) 32 25	4, 31, 71, 126	0
1	L	256/266~(96%)	0.37	8 (3%) 51 38	8, 33, 66, 123	0
1	М	255/266~(95%)	0.54	16 (6%) 27 22	10, 39, 82, 138	0
1	Ν	256/266~(96%)	0.53	18 (7%) 24 19	6, 36, 87, 159	0
1	Ο	255/266~(95%)	0.29	8 (3%) 51 38	7, 26, 57, 85	0
1	Р	$25\overline{5}/266~(95\%)$	0.49	16 (6%) 27 22	9, 31, 79, 117	0
All	All	4090/4256~(96%)	0.42	182 (4%) 39 30	0, 31, 74, 163	0

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	140	SER	5.4
1	А	120	GLY	5.2
1	М	13	ASN	4.5
1	Ν	213	PRO	4.3
1	Е	51	ASP	4.2



# 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.

