



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 10:14 pm BST

PDB ID : 5AYY  
Title : CRYSTAL STRUCTURE OF HUMAN QUINOLINATE PHOSPHORIBOSYLTRANSFERASE IN COMPLEX WITH THE REACTANT QUINOLINATE  
Authors : Youn, H.S.; Kim, T.G.; Kim, M.K.; Kang, G.B.; Kang, J.Y.; Seo, Y.J.; Lee, J.G.; An, J.Y.; Park, K.R.; Lee, Y.; Im, Y.J.; Lee, J.H.; Fukuoka, S.I.; Eom, S.H.  
Deposited on : 2015-09-14  
Resolution : 3.09 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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

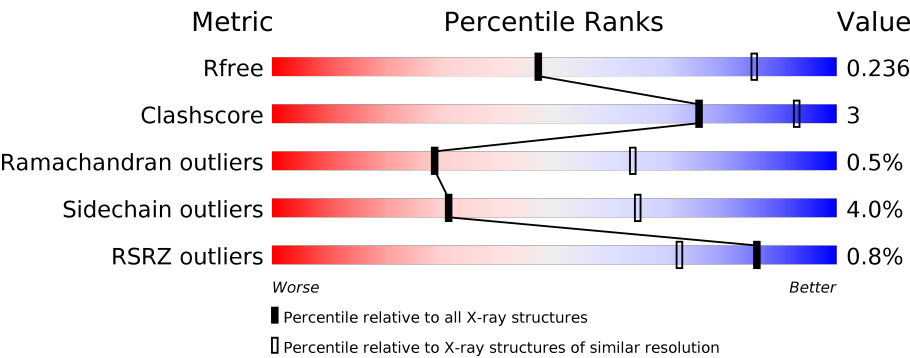
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.09 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	305	<div><div></div><div>86%7% • 5%</div></div>
1	B	305	<div>2%<div><div></div><div>83%10% • 5%</div></div></div>
1	C	305	<div>%<div><div></div><div>87%7% • 5%</div></div></div>
1	D	305	<div>%<div><div></div><div>85%9% 5%</div></div></div>
1	E	305	<div>%<div><div></div><div>85%9% 5%</div></div></div>
1	F	305	<div>%<div><div></div><div>86%8% • 5%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	305	<div><div></div><div>83%</div><div>10% • 5%</div></div>
1	H	305	<div><div></div><div>83%</div><div>10% • 5%</div></div>
1	I	305	<div><div></div><div>87%</div><div>7% • 5%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19117 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 Nicotinate-nucleotide pyrophosphorylase [carboxylating].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	B	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	C	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	D	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	E	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	F	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	G	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	H	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	I	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	LEU	-	expression tag	UNP V9HWJ5
A	299	GLU	-	expression tag	UNP V9HWJ5
A	300	HIS	-	expression tag	UNP V9HWJ5
A	301	HIS	-	expression tag	UNP V9HWJ5
A	302	HIS	-	expression tag	UNP V9HWJ5
A	303	HIS	-	expression tag	UNP V9HWJ5
A	304	HIS	-	expression tag	UNP V9HWJ5
A	305	HIS	-	expression tag	UNP V9HWJ5
B	298	LEU	-	expression tag	UNP V9HWJ5
B	299	GLU	-	expression tag	UNP V9HWJ5
B	300	HIS	-	expression tag	UNP V9HWJ5

*Continued on next page...*

*Continued from previous page...*

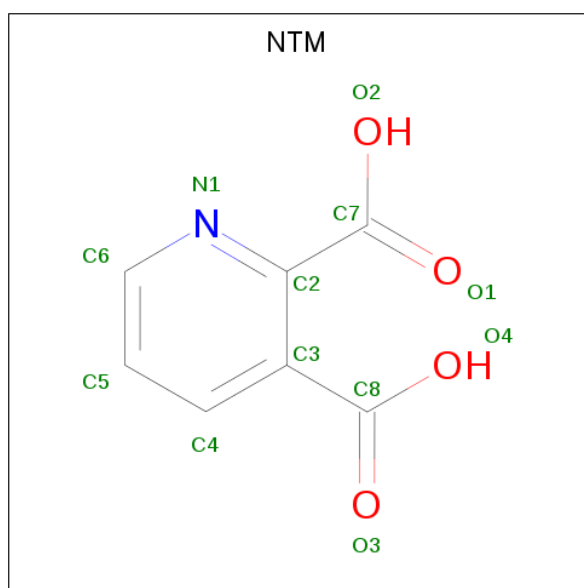
Chain	Residue	Modelled	Actual	Comment	Reference
B	301	HIS	-	expression tag	UNP V9HWJ5
B	302	HIS	-	expression tag	UNP V9HWJ5
B	303	HIS	-	expression tag	UNP V9HWJ5
B	304	HIS	-	expression tag	UNP V9HWJ5
B	305	HIS	-	expression tag	UNP V9HWJ5
C	298	LEU	-	expression tag	UNP V9HWJ5
C	299	GLU	-	expression tag	UNP V9HWJ5
C	300	HIS	-	expression tag	UNP V9HWJ5
C	301	HIS	-	expression tag	UNP V9HWJ5
C	302	HIS	-	expression tag	UNP V9HWJ5
C	303	HIS	-	expression tag	UNP V9HWJ5
C	304	HIS	-	expression tag	UNP V9HWJ5
C	305	HIS	-	expression tag	UNP V9HWJ5
D	298	LEU	-	expression tag	UNP V9HWJ5
D	299	GLU	-	expression tag	UNP V9HWJ5
D	300	HIS	-	expression tag	UNP V9HWJ5
D	301	HIS	-	expression tag	UNP V9HWJ5
D	302	HIS	-	expression tag	UNP V9HWJ5
D	303	HIS	-	expression tag	UNP V9HWJ5
D	304	HIS	-	expression tag	UNP V9HWJ5
D	305	HIS	-	expression tag	UNP V9HWJ5
E	298	LEU	-	expression tag	UNP V9HWJ5
E	299	GLU	-	expression tag	UNP V9HWJ5
E	300	HIS	-	expression tag	UNP V9HWJ5
E	301	HIS	-	expression tag	UNP V9HWJ5
E	302	HIS	-	expression tag	UNP V9HWJ5
E	303	HIS	-	expression tag	UNP V9HWJ5
E	304	HIS	-	expression tag	UNP V9HWJ5
E	305	HIS	-	expression tag	UNP V9HWJ5
F	298	LEU	-	expression tag	UNP V9HWJ5
F	299	GLU	-	expression tag	UNP V9HWJ5
F	300	HIS	-	expression tag	UNP V9HWJ5
F	301	HIS	-	expression tag	UNP V9HWJ5
F	302	HIS	-	expression tag	UNP V9HWJ5
F	303	HIS	-	expression tag	UNP V9HWJ5
F	304	HIS	-	expression tag	UNP V9HWJ5
F	305	HIS	-	expression tag	UNP V9HWJ5
G	298	LEU	-	expression tag	UNP V9HWJ5
G	299	GLU	-	expression tag	UNP V9HWJ5
G	300	HIS	-	expression tag	UNP V9HWJ5
G	301	HIS	-	expression tag	UNP V9HWJ5
G	302	HIS	-	expression tag	UNP V9HWJ5

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	303	HIS	-	expression tag	UNP V9HWJ5
G	304	HIS	-	expression tag	UNP V9HWJ5
G	305	HIS	-	expression tag	UNP V9HWJ5
H	298	LEU	-	expression tag	UNP V9HWJ5
H	299	GLU	-	expression tag	UNP V9HWJ5
H	300	HIS	-	expression tag	UNP V9HWJ5
H	301	HIS	-	expression tag	UNP V9HWJ5
H	302	HIS	-	expression tag	UNP V9HWJ5
H	303	HIS	-	expression tag	UNP V9HWJ5
H	304	HIS	-	expression tag	UNP V9HWJ5
H	305	HIS	-	expression tag	UNP V9HWJ5
I	298	LEU	-	expression tag	UNP V9HWJ5
I	299	GLU	-	expression tag	UNP V9HWJ5
I	300	HIS	-	expression tag	UNP V9HWJ5
I	301	HIS	-	expression tag	UNP V9HWJ5
I	302	HIS	-	expression tag	UNP V9HWJ5
I	303	HIS	-	expression tag	UNP V9HWJ5
I	304	HIS	-	expression tag	UNP V9HWJ5
I	305	HIS	-	expression tag	UNP V9HWJ5

- Molecule 2 is QUINOLINIC ACID (three-letter code: NTM) (formula:  $C_7H_5NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	7	1	4		
2	B	1	Total	C	N	O	0	0
			12	7	1	4		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			12	7	1	4		
2	D	1	Total	C	N	O	0	0
			12	7	1	4		
2	E	1	Total	C	N	O	0	0
			12	7	1	4		
2	F	1	Total	C	N	O	0	0
			12	7	1	4		
2	G	1	Total	C	N	O	0	0
			12	7	1	4		
2	H	1	Total	C	N	O	0	0
			12	7	1	4		
2	I	1	Total	C	N	O	0	0
			12	7	1	4		


- Molecule 3 is water.

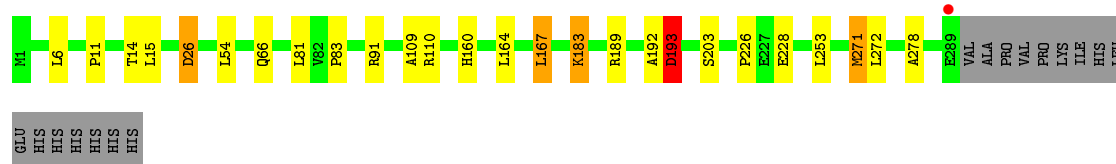
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		
3	C	5	Total	O	0	0
			5	5		
3	D	7	Total	O	0	0
			7	7		
3	E	6	Total	O	0	0
			6	6		
3	F	3	Total	O	0	0
			3	3		
3	G	1	Total	O	0	0
			1	1		
3	H	9	Total	O	0	0
			9	9		
3	I	4	Total	O	0	0
			4	4		

### 3 Residue-property plots


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.

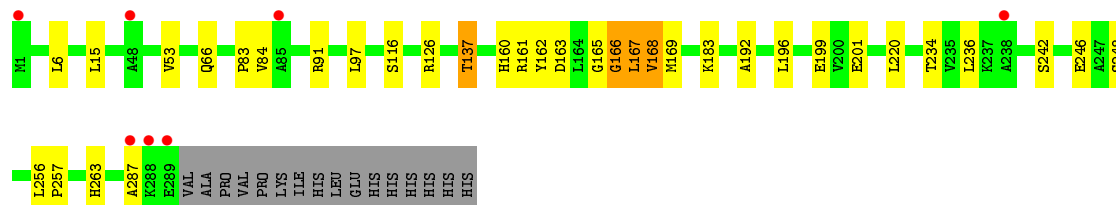
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain A: 




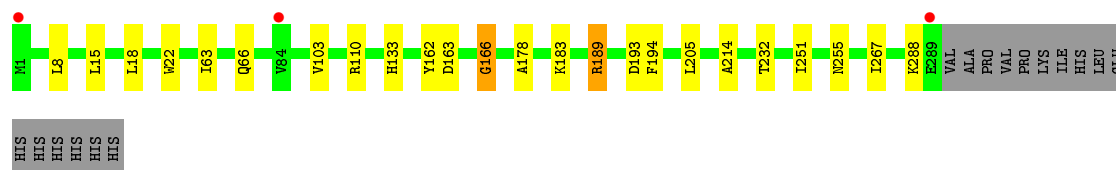
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain B: 




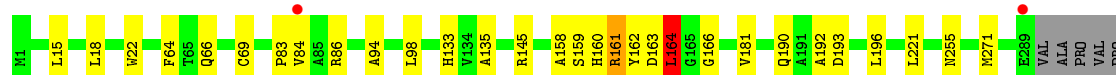
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain C: 




- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain D: 



LYS  
ILE  
HIS  
LEU  
GLU  
HIS  
HIS  
HIS  
HIS  
HIS


- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]


Chain E: 



PRO  
VAL  
PRO  
PRO  
LYS  
ILE  
HIS  
LEU  
GLU  
HIS  
HIS  
HIS  
HIS  
HIS


- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain F: 



GLU  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS


- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain G: 



M271  
L285  
E289  
VAL  
ALA  
PRO  
VAL  
PRO  
LYS  
HIS  
HIS  
HIS  
HIS  
HIS


- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain H: 



S248  
L279  
L283  
K284  
L285  
E289  
VAL  
ALA  
PRO  
PRO  
VAL  
LYS  
HIS  
HIS  
HIS  
HIS  
HIS

- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain I: 



HIS  
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.25Å 174.25Å 211.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.43 – 3.09 45.43 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.43-3.09) 98.9 (45.43-3.09)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.99 (at 3.12Å)	Xtriage
Refinement program	REFMAC 6.5.0	Depositor
R, $R_{free}$	0.185 , 0.239 0.180 , 0.236	Depositor DCC
$R_{free}$ test set	3421 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19117	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	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 26.58 % 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 2.5660e-03. 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: NTM

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	0.62	0/2151	0.83	2/2931 (0.1%)
1	B	0.58	0/2151	0.87	4/2931 (0.1%)
1	C	0.60	0/2151	0.81	0/2931
1	D	0.60	0/2151	0.82	2/2931 (0.1%)
1	E	0.58	0/2151	0.79	0/2931
1	F	0.58	0/2151	0.83	3/2931 (0.1%)
1	G	0.60	0/2151	0.90	8/2931 (0.3%)
1	H	0.62	0/2151	0.80	0/2931
1	I	0.61	0/2151	0.83	0/2931
All	All	0.60	0/19359	0.83	19/26379 (0.1%)

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	2
1	D	0	3
1	F	0	1
1	G	0	3
1	H	0	2
1	I	0	1
All	All	0	14

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	LEU	N-CA-C	10.33	138.88	111.00
1	B	287	ALA	CB-CA-C	10.21	125.41	110.10
1	G	161	ARG	N-CA-CB	8.73	126.31	110.60
1	F	189	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	G	161	ARG	N-CA-C	-7.36	91.14	111.00

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	PRO	Peptide
1	B	165	GLY	Peptide
1	C	162	TYR	Peptide
1	C	189	ARG	Sidechain
1	D	83	PRO	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	2108	0	2131	12	0
1	B	2108	0	2131	17	0
1	C	2108	0	2131	17	0
1	D	2108	0	2131	16	0
1	E	2108	0	2131	14	0
1	F	2108	0	2131	10	0
1	G	2108	0	2131	19	0
1	H	2108	0	2131	16	0
1	I	2108	0	2131	8	0
2	A	12	0	3	1	0
2	B	12	0	3	2	0
2	C	12	0	3	0	0
2	D	12	0	3	1	0
2	E	12	0	3	0	0
2	F	12	0	3	0	0
2	G	12	0	3	0	0
2	H	12	0	3	0	0
2	I	12	0	3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	5	0	0	0	0
3	D	7	0	0	2	0
3	E	6	0	0	1	0
3	F	3	0	0	0	0
3	G	1	0	0	0	0
3	H	9	0	0	1	0
3	I	4	0	0	0	0
All	All	19117	0	19206	120	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 3.

The worst 5 of 120 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:H:189:ARG:NH1	1:H:214:ALA:O	1.69	1.25
1:D:193:ASP:OD1	1:G:133:HIS:ND1	2.19	0.76
1:C:189:ARG:CB	1:C:189:ARG:HH21	1.99	0.75
1:H:189:ARG:CZ	1:H:214:ALA:O	2.37	0.72
1:B:167:LEU:O	1:B:168:VAL:C	2.31	0.69

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	287/305 (94%)	276 (96%)	10 (4%)	1 (0%)	41 73
1	B	287/305 (94%)	264 (92%)	21 (7%)	2 (1%)	22 57

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	287/305 (94%)	273 (95%)	13 (4%)	1 (0%)	41	73
1	D	287/305 (94%)	269 (94%)	16 (6%)	2 (1%)	22	57
1	E	287/305 (94%)	275 (96%)	11 (4%)	1 (0%)	41	73
1	F	287/305 (94%)	269 (94%)	16 (6%)	2 (1%)	22	57
1	G	287/305 (94%)	275 (96%)	11 (4%)	1 (0%)	41	73
1	H	287/305 (94%)	274 (96%)	12 (4%)	1 (0%)	41	73
1	I	287/305 (94%)	275 (96%)	9 (3%)	3 (1%)	15	49
All	All	2583/2745 (94%)	2450 (95%)	119 (5%)	14 (0%)	29	64

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	168	VAL
1	C	166	GLY
1	D	166	GLY
1	E	167	LEU
1	D	164	LEU

### 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	212/227 (93%)	198 (93%)	14 (7%)	16	47
1	B	212/227 (93%)	201 (95%)	11 (5%)	23	55
1	C	212/227 (93%)	208 (98%)	4 (2%)	57	81
1	D	212/227 (93%)	206 (97%)	6 (3%)	43	73
1	E	212/227 (93%)	209 (99%)	3 (1%)	67	86
1	F	212/227 (93%)	202 (95%)	10 (5%)	26	59
1	G	212/227 (93%)	203 (96%)	9 (4%)	30	62
1	H	212/227 (93%)	200 (94%)	12 (6%)	20	52
1	I	212/227 (93%)	204 (96%)	8 (4%)	33	66

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1908/2043 (93%)	1831 (96%)	77 (4%)	31 65

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	271	MET
1	F	196	LEU
1	I	84	VAL
1	E	66	GLN
1	F	6	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	133	HIS
1	I	95	HIS
1	D	190	GLN
1	B	160	HIS
1	G	239	GLN

### 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 ⓘ

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NTM	A	401	-	7,12,12	2.32	2 (28%)	8,16,16	2.53	3 (37%)
2	NTM	G	401	-	7,12,12	3.25	2 (28%)	8,16,16	1.29	1 (12%)
2	NTM	C	401	-	7,12,12	2.62	2 (28%)	8,16,16	1.53	2 (25%)
2	NTM	E	401	-	7,12,12	2.94	2 (28%)	8,16,16	2.00	2 (25%)
2	NTM	H	401	-	7,12,12	2.56	1 (14%)	8,16,16	1.46	1 (12%)
2	NTM	F	401	-	7,12,12	3.70	2 (28%)	8,16,16	1.78	2 (25%)
2	NTM	D	401	-	7,12,12	2.57	1 (14%)	8,16,16	1.54	1 (12%)
2	NTM	B	401	-	7,12,12	3.22	2 (28%)	8,16,16	1.76	2 (25%)
2	NTM	I	401	-	7,12,12	3.67	2 (28%)	8,16,16	1.98	3 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NTM	A	401	-	-	0/0/8/8	0/1/1/1
2	NTM	G	401	-	-	0/0/8/8	0/1/1/1
2	NTM	C	401	-	-	0/0/8/8	0/1/1/1
2	NTM	E	401	-	-	0/0/8/8	0/1/1/1
2	NTM	H	401	-	-	0/0/8/8	0/1/1/1
2	NTM	F	401	-	-	0/0/8/8	0/1/1/1
2	NTM	D	401	-	-	0/0/8/8	0/1/1/1
2	NTM	B	401	-	-	0/0/8/8	0/1/1/1
2	NTM	I	401	-	-	0/0/8/8	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	NTM	C3-C2	8.54	1.51	1.41
2	F	401	NTM	C3-C2	8.43	1.51	1.41
2	E	401	NTM	C3-C2	7.24	1.50	1.41
2	G	401	NTM	C3-C2	6.74	1.49	1.41
2	D	401	NTM	C3-C2	6.59	1.49	1.41

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	401	NTM	C3-C2-N1	-5.89	117.16	122.02
2	E	401	NTM	C3-C2-N1	-4.43	118.36	122.02
2	I	401	NTM	C3-C2-N1	-4.13	118.61	122.02
2	C	401	NTM	C3-C2-N1	-3.33	119.27	122.02
2	B	401	NTM	C3-C2-C7	-3.03	118.24	123.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NTM	1	0
2	D	401	NTM	1	0
2	B	401	NTM	2	0

## 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, 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	289/305 (94%)	-0.42	1 (0%) 94 88	32, 45, 70, 140	0
1	B	289/305 (94%)	-0.10	7 (2%) 59 37	48, 80, 113, 136	0
1	C	289/305 (94%)	-0.48	3 (1%) 82 67	29, 52, 83, 136	0
1	D	289/305 (94%)	-0.51	2 (0%) 87 75	31, 48, 71, 120	0
1	E	289/305 (94%)	-0.42	2 (0%) 87 75	37, 53, 77, 123	0
1	F	289/305 (94%)	-0.29	2 (0%) 87 75	40, 57, 81, 125	0
1	G	289/305 (94%)	-0.52	1 (0%) 94 88	32, 45, 65, 114	0
1	H	289/305 (94%)	-0.57	1 (0%) 94 88	29, 43, 62, 108	0
1	I	289/305 (94%)	-0.54	1 (0%) 94 88	30, 44, 69, 120	0
All	All	2601/2745 (94%)	-0.43	20 (0%) 86 72	29, 50, 91, 140	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	5.0
1	A	289	GLU	4.7
1	B	289	GLU	4.2
1	F	289	GLU	3.8
1	C	289	GLU	3.8

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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	NTM	B	401	12/12	0.90	0.22	58,73,76,78	5
2	NTM	F	401	12/12	0.91	0.28	45,56,71,82	6
2	NTM	A	401	12/12	0.91	0.23	35,48,66,72	5
2	NTM	G	401	12/12	0.95	0.25	37,46,63,65	5
2	NTM	E	401	12/12	0.95	0.18	58,63,72,75	3
2	NTM	I	401	12/12	0.96	0.15	60,65,70,72	0
2	NTM	H	401	12/12	0.97	0.16	32,33,34,35	4
2	NTM	D	401	12/12	0.97	0.18	28,29,29,31	4
2	NTM	C	401	12/12	0.98	0.15	43,45,50,53	2

## 6.5 Other polymers [i](#)

There are no such residues in this entry.