



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:47 pm GMT

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 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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
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)	:	trunk28620

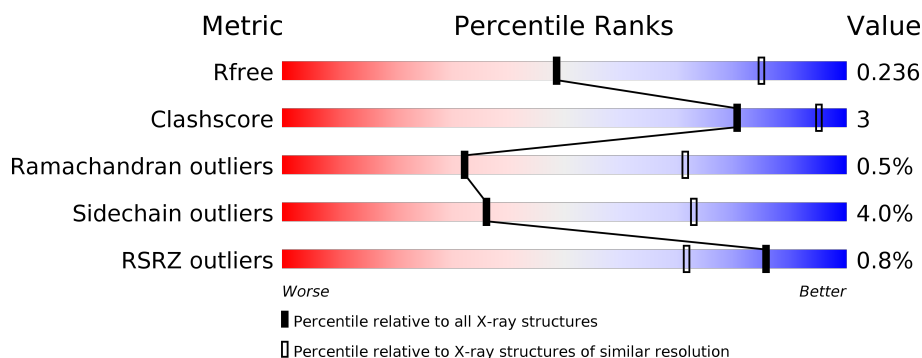
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	305	
1	B	305	
1	C	305	
1	D	305	
1	E	305	
1	F	305	

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

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	NTM	A	401	-	-	-	X
2	NTM	F	401	-	-	-	X

## 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

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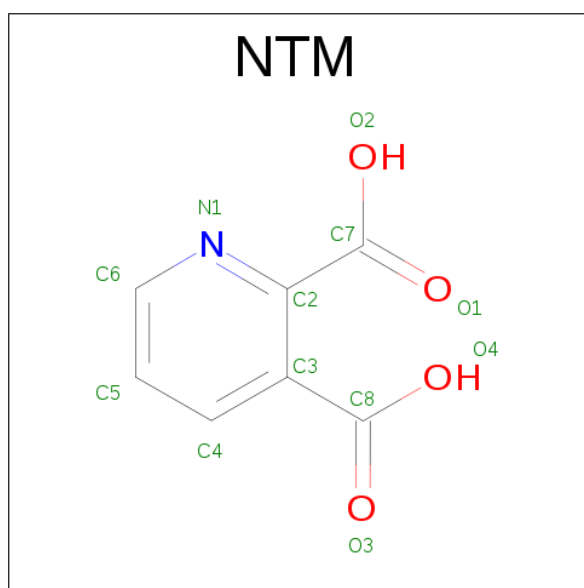
Chain	Residue	Modelled	Actual	Comment	Reference
B	301	HIS	-	expression tag	UNP V9HWJ5
B	302	HIS	-	expression tag	UNP V9HWJ5
B	303	HIS	-	expression tag	UNP V9HWJ5
B	304	HIS	-	expression tag	UNP V9HWJ5
B	305	HIS	-	expression tag	UNP V9HWJ5
C	298	LEU	-	expression tag	UNP V9HWJ5
C	299	GLU	-	expression tag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

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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		

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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		

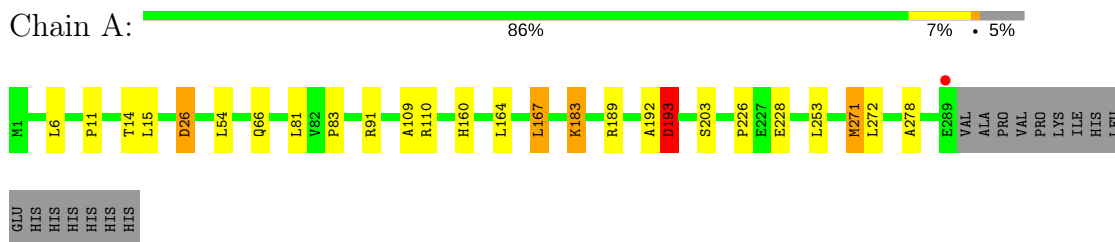
- Molecule 3 is water.

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		

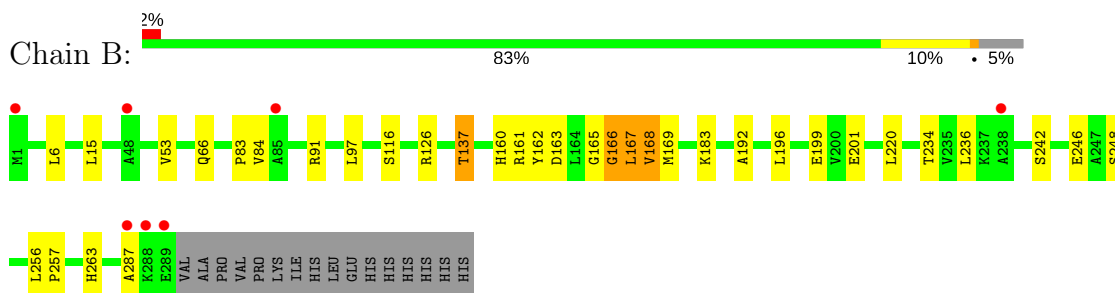
### 3 Residue-property plots

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.

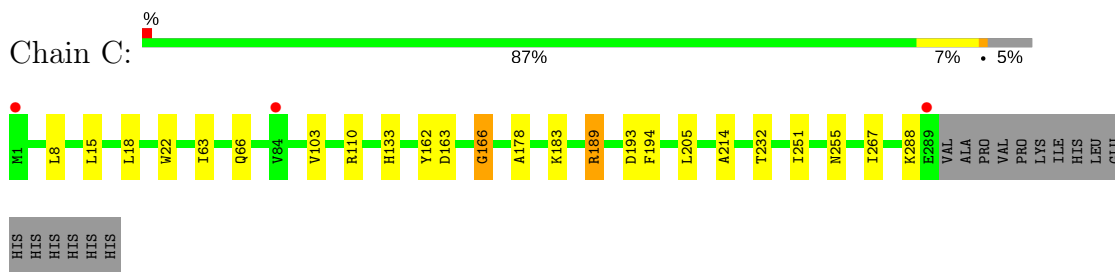
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]



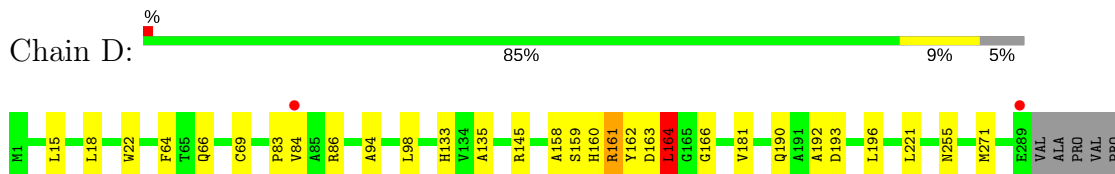
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]



- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]




- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

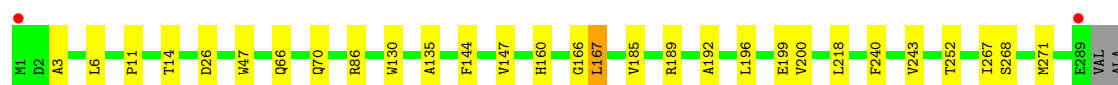




LYS  
ILE  
HIS  
LEU  
GLU  
HIS  
HIS  
HIS  
HIS


- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

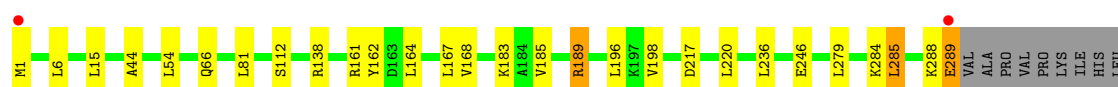
Chain E: 



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


- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

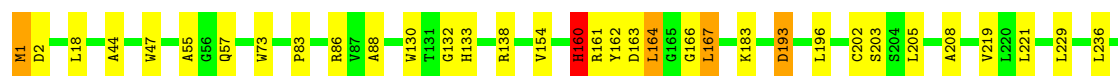
Chain F: 

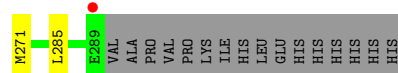


GLU  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS


- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

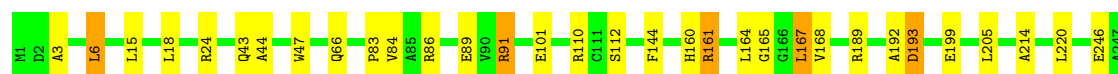
Chain G: 

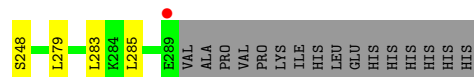





- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain H: 





- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain I: 



HIS  
STH

## 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 5.7.0029	Depositor
R, $R_{free}$	0.185 , 0.239 0.180 , 0.236	Depositor DCC
$R_{free}$ test set	3421 reflections (5.34%)	DCC
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.

All (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
1	G	160	HIS	CB-CA-C	-7.04	96.32	110.40
1	A	167	LEU	CA-CB-CG	6.94	131.26	115.30
1	F	138	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	G	193	ASP	N-CA-C	6.28	127.95	111.00
1	G	160	HIS	N-CA-C	6.07	127.39	111.00
1	B	162	TYR	CB-CA-C	-6.00	98.40	110.40
1	D	145	ARG	NE-CZ-NH2	5.81	123.20	120.30
1	B	163	ASP	N-CA-CB	5.66	120.80	110.60
1	G	164	LEU	CA-CB-CG	5.51	127.97	115.30
1	G	167	LEU	CA-CB-CG	5.47	127.88	115.30
1	F	189	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	G	138	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	86	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	A	26	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

All (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	162	TYR	Peptide
1	D	221	LEU	Peptide
1	D	83	PRO	Peptide
1	F	162	TYR	Peptide
1	G	160	HIS	Mainchain
1	G	166	GLY	Peptide
1	G	83	PRO	Peptide
1	H	165	GLY	Peptide
1	H	83	PRO	Peptide
1	I	165	GLY	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
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.

All (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
1:C:189:ARG:HH21	1:C:189:ARG:HB2	1.59	0.66
1:C:193:ASP:OD2	1:C:194:PHE:N	2.25	0.66
1:B:234:THR:HG22	1:B:263:HIS:CD2	2.31	0.65
1:D:193:ASP:OD1	1:G:133:HIS:CE1	2.52	0.63
1:A:26:ASP:O	1:G:163:ASP:O	2.18	0.62
1:A:183:LYS:H	1:A:183:LYS:HD2	1.64	0.61
1:B:137:THR:HG22	2:B:401:NTM:C6	2.31	0.61
1:F:185:VAL:O	1:F:189:ARG:HG2	2.00	0.61
1:C:193:ASP:OD2	1:C:194:PHE:HD1	1.86	0.59
1:A:271:MET:HG3	1:A:272:LEU:N	2.17	0.59
1:D:193:ASP:HB3	3:D:507:HOH:O	2.00	0.59
1:C:189:ARG:HB3	1:C:189:ARG:NH2	2.18	0.59
1:C:193:ASP:OD2	1:C:194:PHE:CD1	2.57	0.57
1:E:11:PRO:HG2	1:E:14:THR:OG1	2.04	0.57
1:E:160:HIS:HB3	3:E:501:HOH:O	2.05	0.57
1:B:192:ALA:HB1	1:B:196:LEU:HB2	1.86	0.57
1:D:84:VAL:O	1:D:84:VAL:HG12	2.04	0.57
1:B:83:PRO:O	1:B:84:VAL:HG22	2.05	0.57
1:D:190:GLN:NE2	1:G:1:MET:HB2	2.20	0.56
1:E:47:TRP:CZ3	1:E:86:ARG:HB2	2.42	0.54
1:H:112:SER:HB3	1:H:279:LEU:HD12	1.88	0.54
1:B:166:GLY:O	1:B:167:LEU:HB2	2.06	0.54
1:C:18:LEU:HG	1:C:22:TRP:CZ2	2.42	0.54
1:D:64:PHE:HB3	1:D:69:CYS:HB2	1.90	0.54
1:B:234:THR:HA	1:B:263:HIS:HD2	1.73	0.54
1:E:185:VAL:HG22	1:E:200:VAL:HG21	1.90	0.53
1:F:168:VAL:HB	1:F:198:VAL:HG22	1.90	0.53
1:G:44:ALA:HB2	1:G:285:LEU:HD23	1.90	0.53
1:D:163:ASP:O	1:D:164:LEU:HB2	2.09	0.53
1:C:189:ARG:CB	1:C:189:ARG:NH2	2.69	0.52
1:G:130:TRP:CZ2	1:G:132:GLY:HA3	2.44	0.52
1:H:44:ALA:HB2	1:H:285:LEU:HD23	1.91	0.52
1:A:160:HIS:CE1	2:A:401:NTM:H4	2.44	0.52
1:A:109:ALA:HB1	1:A:278:ALA:HB1	1.92	0.51
1:F:44:ALA:HA	1:F:285:LEU:HA	1.91	0.51
1:C:205:LEU:HB2	1:C:232:THR:HG23	1.92	0.51
1:G:163:ASP:O	1:G:164:LEU:CB	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1:MET:HG2	1:G:2:ASP:H	1.76	0.51
1:B:53:VAL:HG23	1:B:116:SER:HA	1.93	0.50
1:G:1:MET:CG	1:G:2:ASP:H	2.25	0.50
1:B:201:GLU:HG2	1:B:220:LEU:HD22	1.93	0.50
1:A:192:ALA:O	1:A:193:ASP:C	2.49	0.49
1:D:160:HIS:HB3	3:D:501:HOH:O	2.11	0.49
1:B:160:HIS:HE1	1:B:246:GLU:OE1	1.96	0.49
1:C:178:ALA:O	1:C:183:LYS:NZ	2.43	0.49
1:I:54:LEU:HB2	1:I:81:LEU:HD21	1.95	0.49
1:A:183:LYS:CD	1:A:183:LYS:H	2.26	0.49
1:I:171:LYS:O	1:I:172:ASP:C	2.50	0.49
1:H:101:GLU:HG3	1:H:283:LEU:HD23	1.94	0.48
1:B:160:HIS:CD2	2:B:401:NTM:H4	2.48	0.48
1:E:240:PHE:O	1:E:243:VAL:HG12	2.13	0.48
1:F:112:SER:HB3	1:F:279:LEU:HD12	1.96	0.48
1:I:18:LEU:HG	1:I:22:TRP:CZ2	2.49	0.48
1:E:144:PHE:CZ	1:E:147:VAL:HG11	2.48	0.48
1:F:54:LEU:HB2	1:F:81:LEU:HD21	1.95	0.48
1:H:161:ARG:NH2	1:H:164:LEU:HD12	2.29	0.47
1:G:47:TRP:CZ3	1:G:86:ARG:HB2	2.49	0.47
1:A:14:THR:HG22	1:H:24:ARG:HE	1.79	0.47
1:H:3:ALA:HA	1:H:6:LEU:HD22	1.96	0.47
1:B:234:THR:HG22	1:B:263:HIS:HD2	1.78	0.47
1:A:253:LEU:N	1:A:271:MET:HE3	2.30	0.46
1:H:168:VAL:HG21	1:H:192:ALA:HB2	1.97	0.46
1:E:26:ASP:O	1:F:164:LEU:HB3	2.16	0.46
1:G:162:TYR:HD2	1:G:163:ASP:HB3	1.80	0.46
1:A:11:PRO:HG2	1:A:14:THR:OG1	2.16	0.45
1:D:18:LEU:HG	1:D:22:TRP:CZ2	2.51	0.45
1:A:253:LEU:H	1:A:271:MET:CE	2.30	0.45
1:C:251:ILE:HD12	1:C:267:ILE:HG23	1.99	0.45
1:H:220:LEU:HD21	1:H:248:SER:HB3	1.97	0.45
1:D:133:HIS:CE1	1:G:193:ASP:OD1	2.70	0.45
1:B:167:LEU:O	1:B:169:MET:N	2.49	0.45
1:B:199:GLU:OE2	1:B:246:GLU:OE1	2.35	0.44
1:D:161:ARG:NH1	2:D:401:NTM:O4	2.50	0.44
1:I:3:ALA:HA	1:I:6:LEU:HD22	1.99	0.44
1:G:55:ALA:HB2	1:G:154:VAL:HG11	1.99	0.44
1:G:208:ALA:HB1	1:G:219:VAL:HG11	1.99	0.44
1:G:202:CYS:SG	1:G:208:ALA:HA	2.57	0.44
1:E:192:ALA:HB1	1:E:196:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ILE:HD13	1:C:103:VAL:HG12	2.01	0.43
1:H:199:GLU:OE2	1:H:246:GLU:OE1	2.36	0.43
1:B:161:ARG:HB2	1:B:166:GLY:O	2.19	0.43
1:D:192:ALA:HB1	1:D:196:LEU:HB2	2.00	0.43
1:F:220:LEU:HD12	1:F:246:GLU:CD	2.39	0.43
1:I:144:PHE:CZ	1:I:147:VAL:HG11	2.54	0.43
1:D:255:ASN:OD1	1:D:255:ASN:C	2.56	0.43
1:E:135:ALA:O	1:E:268:SER:HA	2.19	0.43
1:E:130:TRP:CH2	1:E:267:ILE:HD12	2.54	0.43
1:I:109:ALA:HB1	1:I:278:ALA:HB1	2.01	0.42
1:G:57:GLN:HG2	1:G:73:TRP:CZ2	2.54	0.42
1:E:166:GLY:O	1:E:167:LEU:HB2	2.19	0.42
1:C:8:LEU:HD22	1:I:39:ALA:HB2	2.01	0.42
1:F:288:LYS:HG2	1:F:289:GLU:N	2.35	0.42
1:F:189:ARG:HH11	1:F:198:VAL:HB	1.84	0.42
1:C:189:ARG:NH2	1:C:214:ALA:O	2.53	0.42
1:E:3:ALA:HA	1:E:6:LEU:HD22	2.02	0.42
1:G:221:LEU:HD12	1:G:229:LEU:HD12	2.01	0.42
1:H:89:GLU:OE1	1:H:91:ARG:NH1	2.51	0.42
1:G:73:TRP:CE3	1:G:88:ALA:HB2	2.55	0.42
1:C:133:HIS:CE1	1:H:193:ASP:OD1	2.73	0.41
1:B:256:LEU:HB3	1:B:257:PRO:HD3	2.02	0.41
1:B:168:VAL:HG21	1:B:192:ALA:HB2	2.02	0.41
1:E:199:GLU:HA	1:E:218:LEU:O	2.19	0.41
1:D:94:ALA:O	1:D:98:LEU:HG	2.21	0.41
1:D:135:ALA:HA	1:D:158:ALA:O	2.21	0.41
1:I:118:ALA:O	1:I:122:VAL:HG23	2.20	0.41
1:G:160:HIS:ND1	1:G:160:HIS:C	2.74	0.41
1:F:189:ARG:NH1	1:F:217:ASP:OD1	2.54	0.41
1:A:54:LEU:HB2	1:A:81:LEU:HD21	2.03	0.41
1:H:43:GLN:HG2	1:H:91:ARG:HE	1.85	0.41
1:D:159:SER:C	1:D:160:HIS:O	2.60	0.40
1:E:252:THR:HA	1:E:271:MET:HE2	2.03	0.40
1:H:160:HIS:HB3	3:H:502:HOH:O	2.21	0.40
1:C:163:ASP:HB3	1:C:166:GLY:H	1.87	0.40
1:C:255:ASN:OD1	1:C:255:ASN:C	2.60	0.40
1:H:47:TRP:CZ3	1:H:86:ARG:HB2	2.56	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	287/305 (94%)	276 (96%)	10 (4%)	1 (0%)	44	79
1	B	287/305 (94%)	264 (92%)	21 (7%)	2 (1%)	25	64
1	C	287/305 (94%)	273 (95%)	13 (4%)	1 (0%)	44	79
1	D	287/305 (94%)	269 (94%)	16 (6%)	2 (1%)	25	64
1	E	287/305 (94%)	275 (96%)	11 (4%)	1 (0%)	44	79
1	F	287/305 (94%)	269 (94%)	16 (6%)	2 (1%)	25	64
1	G	287/305 (94%)	275 (96%)	11 (4%)	1 (0%)	44	79
1	H	287/305 (94%)	274 (96%)	12 (4%)	1 (0%)	44	79
1	I	287/305 (94%)	275 (96%)	9 (3%)	3 (1%)	18	57
All	All	2583/2745 (94%)	2450 (95%)	119 (5%)	14 (0%)	32	71

All (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
1	I	166	GLY
1	F	167	LEU
1	G	160	HIS
1	H	167	LEU
1	A	193	ASP
1	B	166	GLY
1	I	193	ASP
1	F	161	ARG
1	I	165	GLY

### 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%)	19	54
1	B	212/227 (93%)	201 (95%)	11 (5%)	27	63
1	C	212/227 (93%)	208 (98%)	4 (2%)	62	87
1	D	212/227 (93%)	206 (97%)	6 (3%)	49	81
1	E	212/227 (93%)	209 (99%)	3 (1%)	71	90
1	F	212/227 (93%)	202 (95%)	10 (5%)	30	67
1	G	212/227 (93%)	203 (96%)	9 (4%)	34	71
1	H	212/227 (93%)	200 (94%)	12 (6%)	24	60
1	I	212/227 (93%)	204 (96%)	8 (4%)	38	74
All	All	1908/2043 (93%)	1831 (96%)	77 (4%)	36	73

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	15	LEU
1	A	66	GLN
1	A	91	ARG
1	A	110	ARG
1	A	164	LEU
1	A	167	LEU
1	A	183	LYS
1	A	189	ARG
1	A	193	ASP
1	A	203	SER
1	A	226	PRO
1	A	228	GLU
1	A	271	MET
1	B	6	LEU
1	B	15	LEU
1	B	66	GLN
1	B	91	ARG

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Mol	Chain	Res	Type
1	B	97	LEU
1	B	126	ARG
1	B	137	THR
1	B	183	LYS
1	B	236	LEU
1	B	242	SER
1	B	248	SER
1	C	15	LEU
1	C	66	GLN
1	C	110	ARG
1	C	288	LYS
1	D	15	LEU
1	D	66	GLN
1	D	161	ARG
1	D	164	LEU
1	D	181	VAL
1	D	271	MET
1	E	66	GLN
1	E	70	GLN
1	E	189	ARG
1	F	1	MET
1	F	6	LEU
1	F	15	LEU
1	F	66	GLN
1	F	183	LYS
1	F	196	LEU
1	F	236	LEU
1	F	284	LYS
1	F	285	LEU
1	F	289	GLU
1	G	1	MET
1	G	18	LEU
1	G	167	LEU
1	G	183	LYS
1	G	196	LEU
1	G	203	SER
1	G	205	LEU
1	G	236	LEU
1	G	271	MET
1	H	6	LEU
1	H	15	LEU
1	H	18	LEU

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Mol	Chain	Res	Type
1	H	66	GLN
1	H	84	VAL
1	H	91	ARG
1	H	110	ARG
1	H	144	PHE
1	H	161	ARG
1	H	167	LEU
1	H	193	ASP
1	H	205	LEU
1	I	6	LEU
1	I	15	LEU
1	I	84	VAL
1	I	110	ARG
1	I	186	ARG
1	I	193	ASP
1	I	254	ASP
1	I	289	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	GLN
1	B	160	HIS
1	B	263	HIS
1	C	133	HIS
1	D	190	GLN
1	G	239	GLN
1	I	95	HIS

### 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	-	6,12,12	2.24	1 (16%)	8,16,16	2.32	3 (37%)
2	NTM	B	401	-	6,12,12	2.54	1 (16%)	8,16,16	1.74	2 (25%)
2	NTM	C	401	-	6,12,12	2.57	1 (16%)	8,16,16	1.43	2 (25%)
2	NTM	D	401	-	6,12,12	2.70	1 (16%)	8,16,16	1.45	1 (12%)
2	NTM	E	401	-	6,12,12	2.90	1 (16%)	8,16,16	1.87	2 (25%)
2	NTM	F	401	-	6,12,12	3.42	1 (16%)	8,16,16	1.70	2 (25%)
2	NTM	G	401	-	6,12,12	2.69	1 (16%)	8,16,16	1.21	1 (12%)
2	NTM	H	401	-	6,12,12	2.68	1 (16%)	8,16,16	1.40	1 (12%)
2	NTM	I	401	-	6,12,12	3.40	1 (16%)	8,16,16	1.87	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	B	401	-	-	0/0/8/8	0/1/1/1
2	NTM	C	401	-	-	0/0/8/8	0/1/1/1
2	NTM	D	401	-	-	0/0/8/8	0/1/1/1
2	NTM	E	401	-	-	0/0/8/8	0/1/1/1
2	NTM	F	401	-	-	0/0/8/8	0/1/1/1
2	NTM	G	401	-	-	0/0/8/8	0/1/1/1
2	NTM	H	401	-	-	0/0/8/8	0/1/1/1
2	NTM	I	401	-	-	0/0/8/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NTM	C3-C2	5.41	1.48	1.41
2	B	401	NTM	C3-C2	6.11	1.49	1.41
2	C	401	NTM	C3-C2	6.15	1.49	1.41
2	H	401	NTM	C3-C2	6.34	1.49	1.41
2	D	401	NTM	C3-C2	6.40	1.49	1.41
2	G	401	NTM	C3-C2	6.55	1.49	1.41
2	E	401	NTM	C3-C2	7.03	1.50	1.41
2	F	401	NTM	C3-C2	8.18	1.51	1.41
2	I	401	NTM	C3-C2	8.29	1.51	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NTM	C3-C2-N1	-5.32	117.16	122.05
2	E	401	NTM	C3-C2-N1	-4.01	118.36	122.05
2	I	401	NTM	C3-C2-N1	-3.74	118.61	122.05
2	B	401	NTM	C3-C2-C7	-3.05	118.24	123.48
2	C	401	NTM	C3-C2-N1	-3.02	119.27	122.05
2	F	401	NTM	C3-C2-N1	-2.73	119.54	122.05
2	G	401	NTM	C3-C2-N1	-2.56	119.69	122.05
2	B	401	NTM	C4-C3-C2	-2.52	115.25	117.50
2	H	401	NTM	C4-C3-C8	-2.45	116.46	120.23
2	D	401	NTM	C3-C2-N1	-2.39	119.85	122.05
2	I	401	NTM	C4-C3-C8	-2.15	116.92	120.23
2	C	401	NTM	C6-N1-C2	2.13	121.03	116.77
2	E	401	NTM	C6-N1-C2	2.28	121.32	116.77
2	I	401	NTM	C6-N1-C2	2.30	121.36	116.77
2	F	401	NTM	C6-N1-C2	2.40	121.57	116.77
2	A	401	NTM	C4-C3-C2	2.47	119.71	117.50
2	A	401	NTM	C6-N1-C2	2.59	121.96	116.77

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	B	401	NTM	2	0
2	D	401	NTM	1	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%) 93 86	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%) 93 86	32, 45, 65, 114	0
1	H	289/305 (94%)	-0.58	1 (0%) 93 86	29, 43, 62, 108	0
1	I	289/305 (94%)	-0.54	1 (0%) 93 86	30, 44, 69, 120	0
All	All	2601/2745 (94%)	-0.43	20 (0%) 86 71	29, 50, 91, 140	0

All (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
1	G	289	GLU	3.2
1	E	289	GLU	3.1
1	B	1	MET	3.0
1	B	288	LYS	2.8
1	F	1	MET	2.8
1	I	289	GLU	2.8
1	B	238	ALA	2.6
1	B	85	ALA	2.6
1	B	48	ALA	2.4
1	D	84	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	1	MET	2.2
1	B	287	ALA	2.2
1	H	289	GLU	2.2
1	C	84	VAL	2.1
1	D	289	GLU	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	NTM	F	401	12/12	0.91	0.28	3.86	45,56,71,82	6
2	NTM	A	401	12/12	0.91	0.23	3.23	35,48,66,72	5
2	NTM	B	401	12/12	0.90	0.22	1.86	58,73,76,78	5
2	NTM	G	401	12/12	0.95	0.25	1.53	37,46,63,65	5
2	NTM	E	401	12/12	0.95	0.18	0.48	58,63,72,75	3
2	NTM	D	401	12/12	0.97	0.17	0.39	28,29,29,31	4
2	NTM	H	401	12/12	0.97	0.16	0.24	32,33,34,35	4
2	NTM	I	401	12/12	0.96	0.15	-0.15	60,65,70,72	0
2	NTM	C	401	12/12	0.98	0.14	-0.85	43,45,50,53	2

## 6.5 Other polymers [i](#)

There are no such residues in this entry.