



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:57 AM UTC

PDB ID : 5AYY / pdb_00005ayy
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)

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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
Mogul	:	2022.3.0, CSD as543be (2022)
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

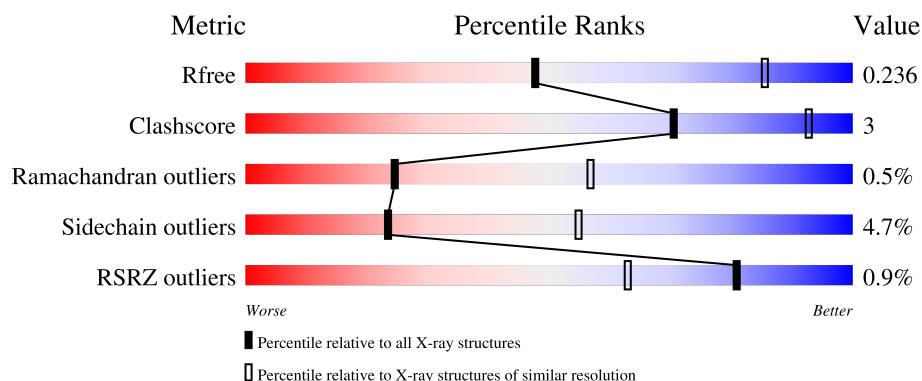
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 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	305	% 85% 9% • 5%
1	B	305	3% 82% 10% • 5%
1	C	305	% 86% 8% • 5%
1	D	305	% 84% 10% 5%

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Mol	Chain	Length	Quality of chain
1	E	305	84% 10%5%
1	F	305	85% 10%5%
1	G	305	% 82% 11%5%
1	H	305	82% 10%5%
1	I	305	% 84% 9%5%

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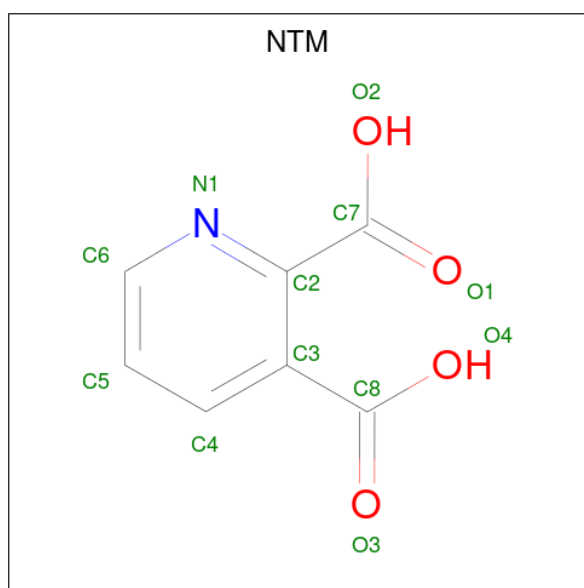
Chain	Residue	Modelled	Actual	Comment	Reference
B	301	HIS	-	expression tag	UNP V9HWJ5
B	302	HIS	-	expression tag	UNP V9HWJ5
B	303	HIS	-	expression tag	UNP V9HWJ5
B	304	HIS	-	expression tag	UNP V9HWJ5
B	305	HIS	-	expression tag	UNP V9HWJ5
C	298	LEU	-	expression tag	UNP V9HWJ5
C	299	GLU	-	expression tag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

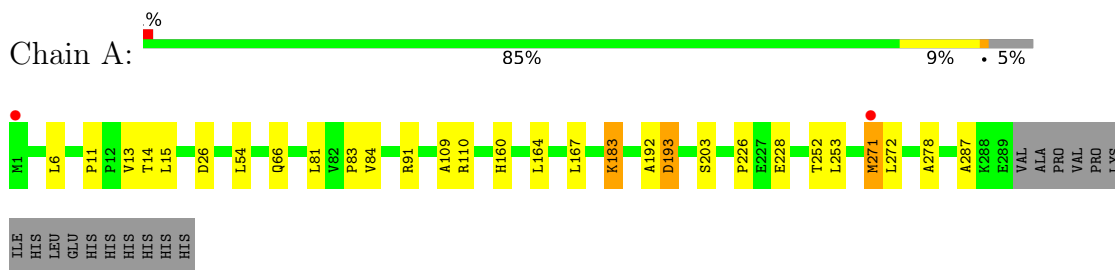
- Molecule 3 is water.

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		

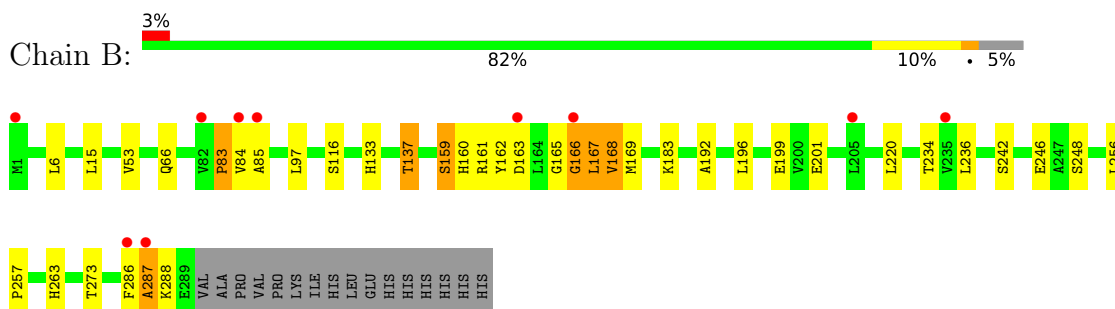
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

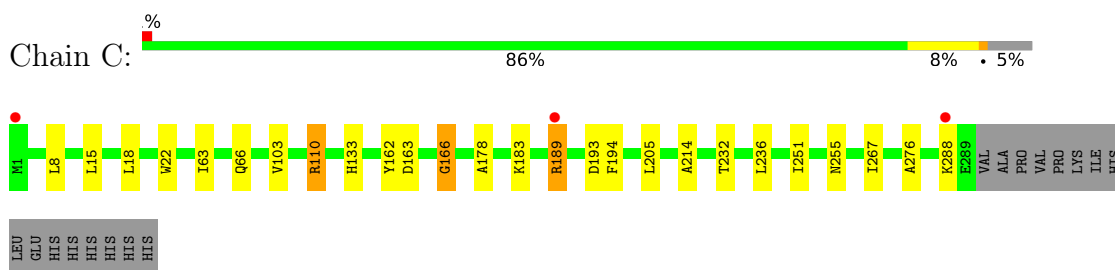
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]



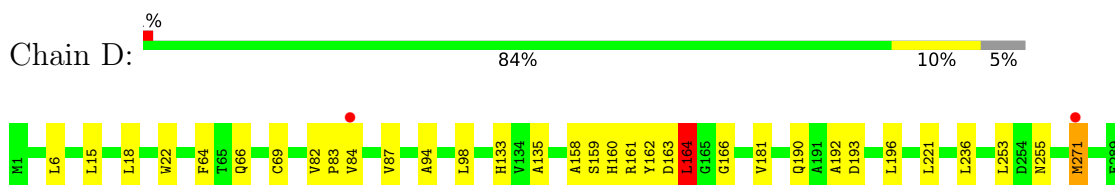
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]



- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]



- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]



VAL
ALA
PRO
VAL
PRO
PRO
LYS
TLE
HIS
LEU
GLU
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain E:  84% 10% • 5%

M1 D2 A3 L6 P11 T14 L18 S21 D26 W47 R86 W130 A135 F144 V147 S159 H160 R161 G166 L167 K183 A184 V185 A192 D193 F194 A195 L196 E199 V200 E213 L218 F240 V243 I267 S268 E289

VAL
ALA
PRO
VAL
PRO
PRO
LYS
TLE
HIS
LEU
GLU
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain F:  85% 10% • 5%

M1 L6 L15 S37 A44 L54 Q66 L81 V87 R91 S112 R161 Y162 D163 L164 L167 V168 K183 A184 V185 R189 A192 D193 L196 K197 V198 D217 L220 L236 E246 L279 K284 L285 K288 E289 VAL ALA

PRO
VAL
PRO
PRO
LYS
TLE
HIS
LEU
GLU
HIS
HIS
HIS
HIS
HIS

- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain G:  82% 11% • 5%

M1 D2 L6 L18 A44 W47 A55 Q57 Q66 W73 P83 V84 A85 R86 V87 A88 W130 T131 G132 H133 V154 H160 R161 Y162 D163 L164 G165 G166 L167 K183 D193 L196 C202 S203 S204 L205 A208 V219 L220 L221 L229

L236 A276 L285 E289 VAL
ALA
PRO
PRO
VAL
PRO
LYS
TLE
HIS
LEU
GLU
HIS
HIS
HIS
HIS

- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain H:  82% 10% • 5%

M1 D2 A3 E4 G5 L6 L15 L18 R24 Q43 A44 W47 Q66 P83 V84 A85 R86 E89 Y90 R91 E101 R110 C111 S112 A121 H180 R161 L164 G165 G166 L167 V168 K183 R199 A192 D193 E199 L205 A214 L220

E246 A247 S248 W269 L279 L283 K284 L285 E289 VAL
ALA
PRO
PRO
VAL
PRO
LYS
TLE
HIS
LEU
GLU
HIS
HIS
HIS
HIS

- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain I:  84% 9% • 5%

M1 D2 A3 L6 L15 L18 W22 A39 S42 L54 E77 L81 V82 P83 V84 R91 A109 R110 A118 V122 A135 F144 V147 Y150 G165 G166 K171 D172 K183 R186 D193 E213 D254 A278

1287	
1288	
E289	
VAL	
ALA	
PRO	
VAL	
PRO	
LYS	
ILE	
HIS	
LEU	
GLU	
HIS	
HIS	
HIS	
HIS	
HIS	
HIS	

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 98.8 (45.43-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.88	0/2151	1.11	2/2931 (0.1%)
1	B	0.85	0/2151	1.13	10/2931 (0.3%)
1	C	0.86	0/2151	1.07	3/2931 (0.1%)
1	D	0.86	0/2151	1.07	2/2931 (0.1%)
1	E	0.83	0/2151	1.07	2/2931 (0.1%)
1	F	0.84	0/2151	1.04	0/2931
1	G	0.84	0/2151	1.16	10/2931 (0.3%)
1	H	0.88	0/2151	1.05	1/2931 (0.0%)
1	I	0.89	0/2151	1.10	3/2931 (0.1%)
All	All	0.86	0/19359	1.09	33/26379 (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 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	LEU	N-CA-C	13.18	138.88	110.80
1	B	287	ALA	CB-CA-C	10.59	125.41	110.16
1	G	161	ARG	N-CA-CB	9.36	126.31	110.49
1	G	161	ARG	N-CA-C	-9.23	91.14	110.80
1	E	194	PHE	N-CA-C	-8.47	103.81	114.56

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	13	0
1	B	2108	0	2131	19	0
1	C	2108	0	2131	17	0
1	D	2108	0	2131	19	0
1	E	2108	0	2131	15	0
1	F	2108	0	2131	11	0
1	G	2108	0	2131	20	0
1	H	2108	0	2131	17	0
1	I	2108	0	2131	9	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

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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	131	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 131 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:HH21	1:C:189:ARG:CB	1.99	0.75
1:B:167:LEU:O	1:B:168:VAL:C	2.31	0.73
1:H:189:ARG:CZ	1:H:214:ALA:O	2.37	0.72

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%)	36 67
1	B	287/305 (94%)	264 (92%)	21 (7%)	2 (1%)	18 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	287/305 (94%)	273 (95%)	13 (4%)	1 (0%)	36	67
1	D	287/305 (94%)	269 (94%)	16 (6%)	2 (1%)	18	49
1	E	287/305 (94%)	275 (96%)	11 (4%)	1 (0%)	36	67
1	F	287/305 (94%)	269 (94%)	16 (6%)	2 (1%)	18	49
1	G	287/305 (94%)	275 (96%)	11 (4%)	1 (0%)	36	67
1	H	287/305 (94%)	274 (96%)	12 (4%)	1 (0%)	36	67
1	I	287/305 (94%)	275 (96%)	9 (3%)	3 (1%)	12	41
All	All	2583/2745 (94%)	2450 (95%)	119 (5%)	14 (0%)	24	57

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%)	199 (94%)	13 (6%)	17	46
1	B	212/227 (93%)	202 (95%)	10 (5%)	23	55
1	C	212/227 (93%)	207 (98%)	5 (2%)	43	69
1	D	212/227 (93%)	204 (96%)	8 (4%)	29	60
1	E	212/227 (93%)	208 (98%)	4 (2%)	50	73
1	F	212/227 (93%)	200 (94%)	12 (6%)	18	49
1	G	212/227 (93%)	201 (95%)	11 (5%)	21	51
1	H	212/227 (93%)	197 (93%)	15 (7%)	13	41
1	I	212/227 (93%)	200 (94%)	12 (6%)	18	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1908/2043 (93%)	1818 (95%)	90 (5%)	23 55

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	167	LEU
1	H	91	ARG
1	G	196	LEU
1	H	15	LEU
1	H	183	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	70	GLN
1	I	95	HIS
1	I	258	GLN
1	I	210	GLN
1	C	210	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 oligosaccharides 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	D	401	-	12,12,12	1.73	2 (16%)	15,16,16	1.02	0
2	NTM	G	401	-	12,12,12	1.70	2 (16%)	15,16,16	1.20	1 (6%)
2	NTM	F	401	-	12,12,12	1.86	1 (8%)	15,16,16	1.51	3 (20%)
2	NTM	C	401	-	12,12,12	1.67	2 (16%)	15,16,16	1.25	2 (13%)
2	NTM	B	401	-	12,12,12	1.64	2 (16%)	15,16,16	1.63	2 (13%)
2	NTM	H	401	-	12,12,12	1.82	3 (25%)	15,16,16	1.07	1 (6%)
2	NTM	A	401	-	12,12,12	1.50	2 (16%)	15,16,16	1.36	2 (13%)
2	NTM	I	401	-	12,12,12	1.88	2 (16%)	15,16,16	1.16	2 (13%)
2	NTM	E	401	-	12,12,12	1.65	1 (8%)	15,16,16	1.23	2 (13%)

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	D	401	-	-	6/8/8/8	0/1/1/1
2	NTM	G	401	-	-	0/8/8/8	0/1/1/1
2	NTM	F	401	-	-	6/8/8/8	0/1/1/1
2	NTM	C	401	-	-	6/8/8/8	0/1/1/1
2	NTM	B	401	-	-	4/8/8/8	0/1/1/1
2	NTM	H	401	-	-	6/8/8/8	0/1/1/1
2	NTM	A	401	-	-	0/8/8/8	0/1/1/1
2	NTM	I	401	-	-	4/8/8/8	0/1/1/1
2	NTM	E	401	-	-	0/8/8/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	NTM	C3-C2	5.57	1.51	1.40
2	F	401	NTM	C3-C2	5.51	1.51	1.40
2	E	401	NTM	C3-C2	4.82	1.50	1.40
2	G	401	NTM	C3-C2	4.53	1.49	1.40
2	D	401	NTM	C3-C2	4.44	1.49	1.40

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NTM	O1-C7-C2	-3.44	113.73	120.80
2	A	401	NTM	C3-C2-N1	-3.13	117.16	122.61
2	A	401	NTM	C6-N1-C2	2.65	121.96	116.80
2	F	401	NTM	O4-C8-C3	2.48	122.33	115.28
2	H	401	NTM	O1-C7-C2	-2.47	115.72	120.80

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	NTM	N1-C2-C7-O1
2	C	401	NTM	N1-C2-C7-O2
2	C	401	NTM	C3-C2-C7-O2
2	B	401	NTM	C2-C3-C8-O3
2	C	401	NTM	C3-C2-C7-O1

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	NTM	1	0
2	B	401	NTM	2	0
2	A	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 [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, 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	289/305 (94%)	-0.57	2 (0%) 84 68	32, 45, 70, 140	0
1	B	289/305 (94%)	0.23	10 (3%) 47 27	48, 80, 113, 136	0
1	C	289/305 (94%)	-0.45	3 (1%) 79 61	29, 52, 83, 136	0
1	D	289/305 (94%)	-0.54	2 (0%) 84 68	32, 48, 71, 120	0
1	E	289/305 (94%)	-0.50	1 (0%) 90 80	37, 53, 77, 123	0
1	F	289/305 (94%)	-0.37	1 (0%) 90 80	40, 57, 81, 125	0
1	G	289/305 (94%)	-0.58	2 (0%) 84 68	32, 45, 65, 114	0
1	H	289/305 (94%)	-0.63	1 (0%) 90 80	29, 43, 62, 108	0
1	I	289/305 (94%)	-0.60	2 (0%) 84 68	30, 44, 69, 120	0
All	All	2601/2745 (94%)	-0.45	24 (0%) 81 63	29, 50, 91, 140	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	166	GLY	3.7
1	B	287	ALA	3.6
1	A	1	MET	3.4
1	B	82	VAL	3.0
1	B	84	VAL	2.9

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

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(Å ²)	Q<0.9
2	NTM	F	401	12/12	0.88	0.15	45,56,71,82	6
2	NTM	B	401	12/12	0.90	0.11	58,73,76,78	5
2	NTM	A	401	12/12	0.91	0.13	35,48,66,72	5
2	NTM	E	401	12/12	0.94	0.09	58,63,72,75	3
2	NTM	G	401	12/12	0.95	0.11	37,46,63,65	5
2	NTM	C	401	12/12	0.96	0.07	43,45,50,53	2
2	NTM	I	401	12/12	0.96	0.09	60,65,70,72	0
2	NTM	H	401	12/12	0.97	0.07	32,33,34,35	4
2	NTM	D	401	12/12	0.97	0.06	28,29,29,31	4

6.5 Other polymers

There are no such residues in this entry.