



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 11:22 pm BST

PDB ID : 3L0G  
Title : Crystal structure of Nicotinate-nucleotide pyrophosphorylase from *Ehrlichia chaffeensis* at 2.05Å resolution  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2009-12-09  
Resolution : 2.05 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (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

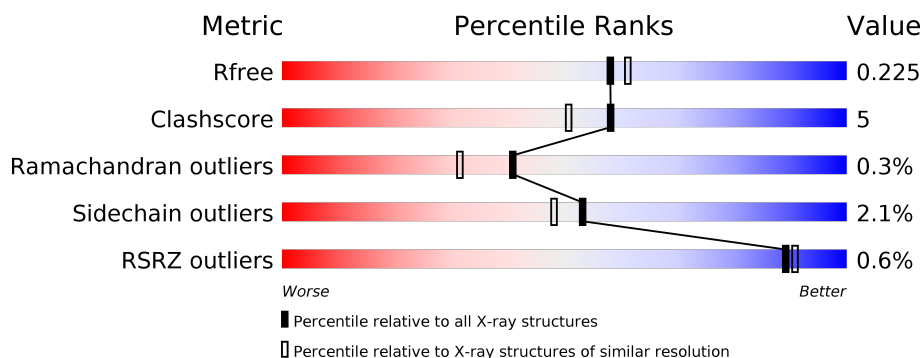
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	300	<div> <div>82%</div> <div>8%</div> <div>9%</div> </div>
1	B	300	<div> <div>81%</div> <div>9%</div> <div>9%</div> </div>
1	C	300	<div> <div>82%</div> <div>9%</div> <div>9%</div> </div>
1	D	300	<div> <div>81%</div> <div>10%</div> <div>9%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9292 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	5	0
			2098	1315	357	414	12			
1	B	273	Total	C	N	O	S	6	7	0
			2110	1325	361	413	11			
1	C	274	Total	C	N	O	S	0	8	0
			2109	1322	356	417	14			
1	D	274	Total	C	N	O	S	0	5	0
			2094	1310	355	416	13			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q2GI74
A	-19	ALA	-	EXPRESSION TAG	UNP Q2GI74
A	-18	HIS	-	EXPRESSION TAG	UNP Q2GI74
A	-17	HIS	-	EXPRESSION TAG	UNP Q2GI74
A	-16	HIS	-	EXPRESSION TAG	UNP Q2GI74
A	-15	HIS	-	EXPRESSION TAG	UNP Q2GI74
A	-14	HIS	-	EXPRESSION TAG	UNP Q2GI74
A	-13	HIS	-	EXPRESSION TAG	UNP Q2GI74
A	-12	MET	-	EXPRESSION TAG	UNP Q2GI74
A	-11	GLY	-	EXPRESSION TAG	UNP Q2GI74
A	-10	THR	-	EXPRESSION TAG	UNP Q2GI74
A	-9	LEU	-	EXPRESSION TAG	UNP Q2GI74
A	-8	GLU	-	EXPRESSION TAG	UNP Q2GI74
A	-7	ALA	-	EXPRESSION TAG	UNP Q2GI74
A	-6	GLN	-	EXPRESSION TAG	UNP Q2GI74
A	-5	THR	-	EXPRESSION TAG	UNP Q2GI74
A	-4	GLN	-	EXPRESSION TAG	UNP Q2GI74
A	-3	GLY	-	EXPRESSION TAG	UNP Q2GI74
A	-2	PRO	-	EXPRESSION TAG	UNP Q2GI74
A	-1	GLY	-	EXPRESSION TAG	UNP Q2GI74
A	0	SER	-	EXPRESSION TAG	UNP Q2GI74

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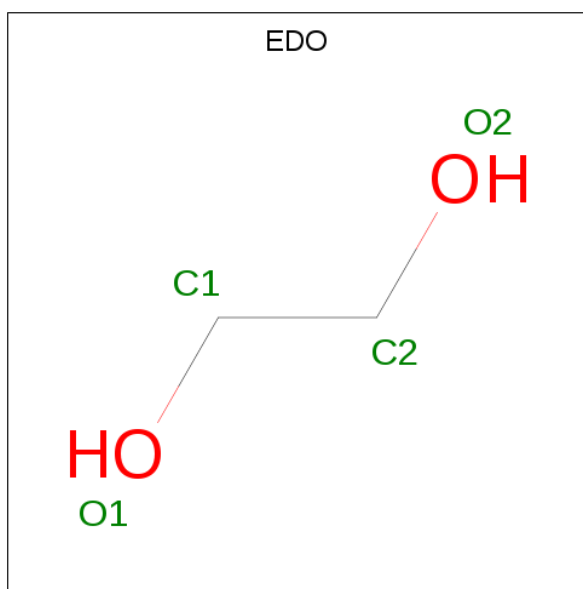
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	EXPRESSION TAG	UNP Q2GI74
B	-19	ALA	-	EXPRESSION TAG	UNP Q2GI74
B	-18	HIS	-	EXPRESSION TAG	UNP Q2GI74
B	-17	HIS	-	EXPRESSION TAG	UNP Q2GI74
B	-16	HIS	-	EXPRESSION TAG	UNP Q2GI74
B	-15	HIS	-	EXPRESSION TAG	UNP Q2GI74
B	-14	HIS	-	EXPRESSION TAG	UNP Q2GI74
B	-13	HIS	-	EXPRESSION TAG	UNP Q2GI74
B	-12	MET	-	EXPRESSION TAG	UNP Q2GI74
B	-11	GLY	-	EXPRESSION TAG	UNP Q2GI74
B	-10	THR	-	EXPRESSION TAG	UNP Q2GI74
B	-9	LEU	-	EXPRESSION TAG	UNP Q2GI74
B	-8	GLU	-	EXPRESSION TAG	UNP Q2GI74
B	-7	ALA	-	EXPRESSION TAG	UNP Q2GI74
B	-6	GLN	-	EXPRESSION TAG	UNP Q2GI74
B	-5	THR	-	EXPRESSION TAG	UNP Q2GI74
B	-4	GLN	-	EXPRESSION TAG	UNP Q2GI74
B	-3	GLY	-	EXPRESSION TAG	UNP Q2GI74
B	-2	PRO	-	EXPRESSION TAG	UNP Q2GI74
B	-1	GLY	-	EXPRESSION TAG	UNP Q2GI74
B	0	SER	-	EXPRESSION TAG	UNP Q2GI74
C	-20	MET	-	EXPRESSION TAG	UNP Q2GI74
C	-19	ALA	-	EXPRESSION TAG	UNP Q2GI74
C	-18	HIS	-	EXPRESSION TAG	UNP Q2GI74
C	-17	HIS	-	EXPRESSION TAG	UNP Q2GI74
C	-16	HIS	-	EXPRESSION TAG	UNP Q2GI74
C	-15	HIS	-	EXPRESSION TAG	UNP Q2GI74
C	-14	HIS	-	EXPRESSION TAG	UNP Q2GI74
C	-13	HIS	-	EXPRESSION TAG	UNP Q2GI74
C	-12	MET	-	EXPRESSION TAG	UNP Q2GI74
C	-11	GLY	-	EXPRESSION TAG	UNP Q2GI74
C	-10	THR	-	EXPRESSION TAG	UNP Q2GI74
C	-9	LEU	-	EXPRESSION TAG	UNP Q2GI74
C	-8	GLU	-	EXPRESSION TAG	UNP Q2GI74
C	-7	ALA	-	EXPRESSION TAG	UNP Q2GI74
C	-6	GLN	-	EXPRESSION TAG	UNP Q2GI74
C	-5	THR	-	EXPRESSION TAG	UNP Q2GI74
C	-4	GLN	-	EXPRESSION TAG	UNP Q2GI74
C	-3	GLY	-	EXPRESSION TAG	UNP Q2GI74
C	-2	PRO	-	EXPRESSION TAG	UNP Q2GI74
C	-1	GLY	-	EXPRESSION TAG	UNP Q2GI74
C	0	SER	-	EXPRESSION TAG	UNP Q2GI74

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	EXPRESSION TAG	UNP Q2GI74
D	-19	ALA	-	EXPRESSION TAG	UNP Q2GI74
D	-18	HIS	-	EXPRESSION TAG	UNP Q2GI74
D	-17	HIS	-	EXPRESSION TAG	UNP Q2GI74
D	-16	HIS	-	EXPRESSION TAG	UNP Q2GI74
D	-15	HIS	-	EXPRESSION TAG	UNP Q2GI74
D	-14	HIS	-	EXPRESSION TAG	UNP Q2GI74
D	-13	HIS	-	EXPRESSION TAG	UNP Q2GI74
D	-12	MET	-	EXPRESSION TAG	UNP Q2GI74
D	-11	GLY	-	EXPRESSION TAG	UNP Q2GI74
D	-10	THR	-	EXPRESSION TAG	UNP Q2GI74
D	-9	LEU	-	EXPRESSION TAG	UNP Q2GI74
D	-8	GLU	-	EXPRESSION TAG	UNP Q2GI74
D	-7	ALA	-	EXPRESSION TAG	UNP Q2GI74
D	-6	GLN	-	EXPRESSION TAG	UNP Q2GI74
D	-5	THR	-	EXPRESSION TAG	UNP Q2GI74
D	-4	GLN	-	EXPRESSION TAG	UNP Q2GI74
D	-3	GLY	-	EXPRESSION TAG	UNP Q2GI74
D	-2	PRO	-	EXPRESSION TAG	UNP Q2GI74
D	-1	GLY	-	EXPRESSION TAG	UNP Q2GI74
D	0	SER	-	EXPRESSION TAG	UNP Q2GI74

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



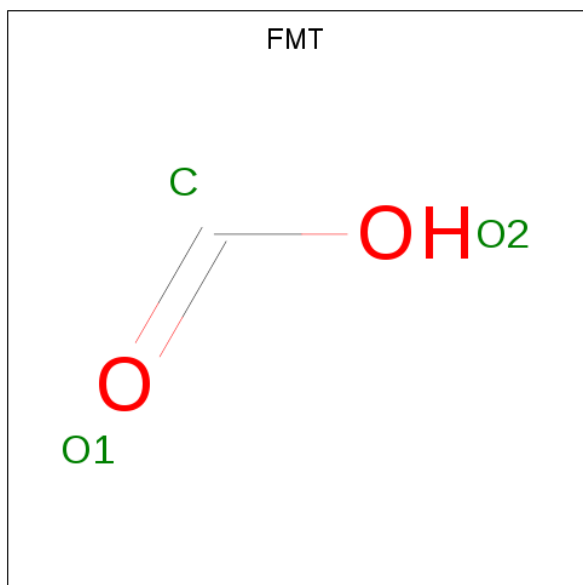
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	222	Total	O	0	0
			222	222		
4	B	216	Total	O	0	0
			216	216		

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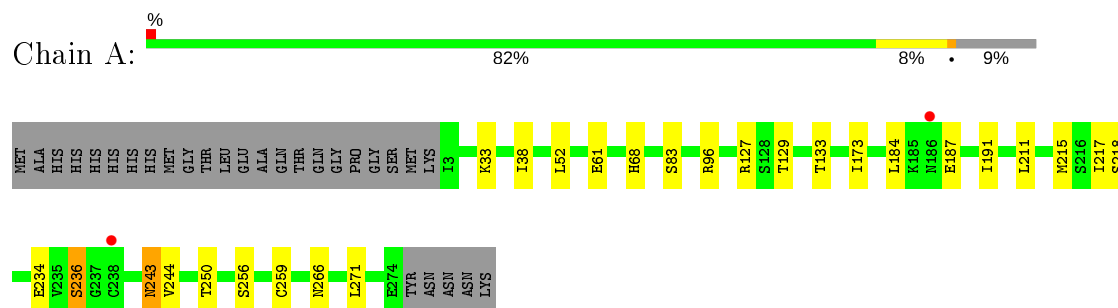
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	221	Total 221	O 221	0	0
4	D	194	Total 194	O 194	0	0

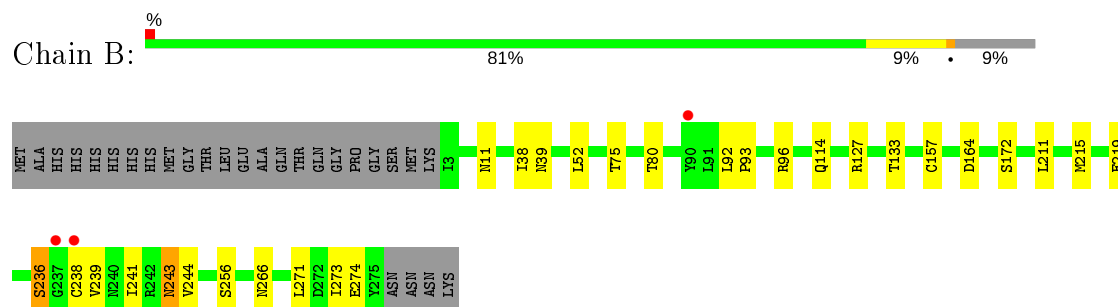
### 3 Residue-property plots [i](#)

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.

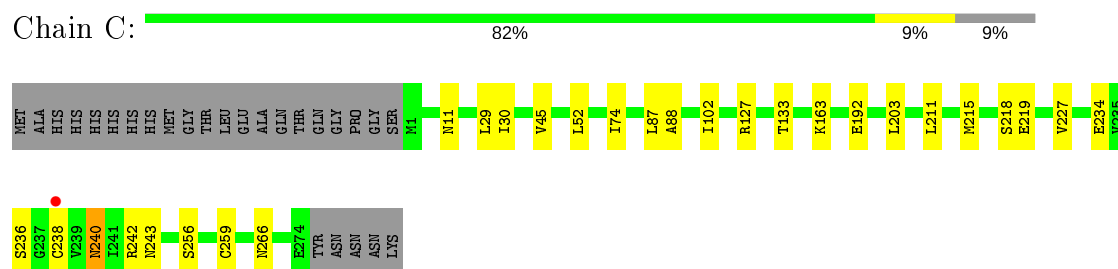
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase



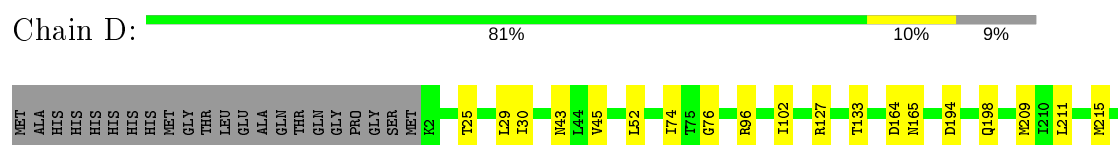
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase



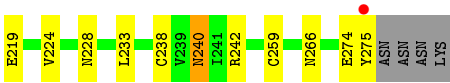
- Molecule 1: Nicotinate-nucleotide pyrophosphorylase



- Molecule 1: Nicotinate-nucleotide pyrophosphorylase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.53Å 77.32Å 78.32Å 113.01° 91.82° 111.68°	Depositor
Resolution (Å)	50.00 – 2.05 46.99 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-2.05) 96.8 (46.99-2.05)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0104	Depositor
R, $R_{free}$	0.174 , 0.226 0.175 , 0.225	Depositor DCC
$R_{free}$ test set	3640 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.1	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.136 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, EDO

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	0.71	0/2132	0.74	1/2882 (0.0%)
1	B	0.70	1/2150 (0.0%)	0.78	4/2906 (0.1%)
1	C	0.71	0/2152	0.71	0/2911
1	D	0.66	0/2128	0.73	4/2880 (0.1%)
All	All	0.70	1/8562 (0.0%)	0.74	9/11579 (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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	157	CYS	CB-SG	-5.04	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	D	127	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	B	164	ASP	CB-CG-OD1	5.93	123.64	118.30
1	D	96	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	96	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	96	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	127	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	127	ARG	NE-CZ-NH2	5.07	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	238	CYS	Peptide

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2098	0	2137	21	0
1	B	2110	0	2160	24	0
1	C	2109	0	2136	17	0
1	D	2094	0	2105	22	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
2	D	4	0	6	1	0
3	A	3	0	1	0	0
3	B	3	0	1	0	0
3	C	3	0	1	0	0
3	D	3	0	1	0	0
4	A	222	0	0	2	0
4	B	216	0	0	2	0
4	C	221	0	0	1	0
4	D	194	0	0	0	0
All	All	9292	0	8566	78	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 5.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:GLU:HA	1:D:275:TYR:CB	1.95	0.96
1:C:240:ASN:HD22	1:C:242:ARG:H	1.24	0.86
1:D:215:MET:HE3	1:D:219:GLU:HB3	1.59	0.82
1:C:215:MET:HE3	1:C:219:GLU:HB3	1.62	0.80
1:D:238[A]:CYS:HG	1:D:259[A]:CYS:HG	1.09	0.75
1:A:133:THR:HG21	1:C:133:THR:HG21	1.71	0.72
1:D:238[B]:CYS:HG	1:D:259[B]:CYS:CB	2.03	0.71
1:D:45:VAL:HG22	1:D:74:ILE:HD13	1.73	0.70
1:B:211:LEU:HD21	1:B:236:SER:HB2	1.73	0.70
1:B:133:THR:HG21	1:D:133:THR:HG21	1.76	0.68
1:B:38:ILE:CD1	1:B:271[B]:LEU:HD23	2.24	0.66
1:B:39:ASN:HD22	1:B:80:THR:HA	1.60	0.66
1:A:133:THR:HG21	1:C:133:THR:CG2	2.26	0.65
1:D:274:GLU:CA	1:D:275:TYR:CB	2.74	0.64
1:A:217:ILE:HD11	1:A:250:THR:CG2	2.28	0.63
1:A:68:HIS:HE1	1:A:83:SER:OG	1.80	0.63
1:A:243:ASN:C	1:A:243:ASN:HD22	2.02	0.63
1:A:211:LEU:HD21	1:A:236:SER:HB2	1.81	0.63
1:B:243:ASN:C	1:B:243:ASN:HD22	2.04	0.60
1:A:243:ASN:HD22	1:A:244:VAL:N	2.00	0.59
1:D:194:ASP:H	1:D:198:GLN:NE2	2.01	0.59
1:B:243:ASN:HD22	1:B:244:VAL:N	2.01	0.58
1:A:133:THR:CG2	1:C:133:THR:HG21	2.32	0.58
1:B:38:ILE:HD13	1:B:271[B]:LEU:HD23	1.84	0.58
1:B:38:ILE:HD11	1:B:271[B]:LEU:HD23	1.87	0.56
1:A:38:ILE:HD13	1:A:271:LEU:HD13	1.87	0.56
1:B:271[B]:LEU:HD11	1:B:273:ILE:HD11	1.88	0.56
1:C:163:LYS:HA	1:C:192:GLU:CG	2.36	0.56
1:B:215:MET:CE	1:B:219:GLU:HB3	2.37	0.55
1:D:45:VAL:HG22	1:D:74:ILE:CD1	2.35	0.55
1:B:243:ASN:HB3	4:B:286:HOH:O	2.07	0.54
1:A:33:LYS:NZ	4:A:628:HOH:O	2.39	0.54
1:C:240:ASN:ND2	1:C:242:ARG:H	2.01	0.53
1:C:203:LEU:HD11	1:C:227:VAL:HA	1.90	0.53
1:D:52:LEU:HB2	1:D:102[B]:ILE:HD11	1.91	0.53
1:D:209:MET:CE	1:D:211:LEU:HD11	2.39	0.52
1:D:211:LEU:HD21	2:D:300:EDO:H12	1.92	0.51
1:B:274:GLU:CB	4:B:550:HOH:O	2.58	0.51
1:B:215:MET:HE2	1:B:219:GLU:HB3	1.92	0.50
1:C:52:LEU:HB2	1:C:102[B]:ILE:HD11	1.93	0.50
1:A:38:ILE:CD1	1:A:271:LEU:HD13	2.42	0.49
1:C:52:LEU:C	1:C:52:LEU:HD23	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:MET:HE3	1:D:211:LEU:HD11	1.95	0.49
1:A:217:ILE:CD1	1:A:250:THR:CG2	2.92	0.48
1:A:243:ASN:C	1:A:243:ASN:ND2	2.67	0.47
1:A:127:ARG:NH1	1:A:234:GLU:OE1	2.37	0.47
1:B:133:THR:HG21	1:D:133:THR:CG2	2.43	0.47
1:B:38:ILE:HD13	1:B:271[B]:LEU:CD2	2.44	0.47
1:C:11:ASN:ND2	4:C:357:HOH:O	2.47	0.47
1:A:38:ILE:HD13	1:A:271:LEU:CD1	2.46	0.46
1:B:133:THR:CG2	1:D:133:THR:HG21	2.45	0.46
1:D:164:ASP:OD1	1:D:165:ASN:N	2.49	0.46
1:B:243:ASN:C	1:B:243:ASN:ND2	2.69	0.46
1:C:45:VAL:HG22	1:C:74:ILE:HG12	1.98	0.46
1:B:39:ASN:ND2	1:B:80:THR:HA	2.29	0.45
1:A:173:ILE:HG23	1:A:191:ILE:HD13	1.99	0.45
1:A:184:LEU:HD13	1:A:187:GLU:HG3	1.99	0.45
1:B:211:LEU:HD23	1:B:211:LEU:C	2.38	0.44
1:B:114:GLN:HG2	1:B:241:ILE:HD13	1.98	0.44
1:A:129:THR:HG22	1:A:256:SER:HB2	1.99	0.44
1:D:238[B]:CYS:HG	1:D:259[B]:CYS:HB3	1.80	0.44
1:C:127:ARG:NH2	1:C:234:GLU:OE2	2.47	0.44
1:D:25:THR:HG23	1:D:29:LEU:HD12	2.00	0.44
1:D:43:ASN:ND2	1:D:76:GLY:HA2	2.33	0.44
1:B:92:LEU:N	1:B:93:PRO:CD	2.82	0.43
1:C:163:LYS:HA	1:C:192:GLU:HG2	2.00	0.43
1:D:240:ASN:HD22	1:D:242:ARG:H	1.66	0.43
1:A:52:LEU:C	1:A:52:LEU:HD23	2.39	0.42
1:C:29:LEU:HD13	1:C:88:ALA:HB3	2.02	0.42
1:D:238[B]:CYS:SG	1:D:259[B]:CYS:HB3	2.61	0.41
1:B:215:MET:HE3	1:B:219:GLU:HB3	2.02	0.41
1:B:11:ASN:HD22	1:B:11:ASN:HA	1.75	0.41
1:D:224:VAL:HG22	1:D:233:LEU:HD23	2.02	0.41
1:A:61:GLU:CB	4:A:740:HOH:O	2.69	0.40
1:B:52:LEU:HD23	1:B:52:LEU:C	2.41	0.40
1:C:238[B]:CYS:SG	1:C:259[B]:CYS:CB	3.09	0.40
1:A:215:MET:HE2	1:A:215:MET:HB3	1.85	0.40
1:C:211:LEU:HD21	1:C:236:SER:CB	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/300 (92%)	271 (98%)	4 (2%)	0	100	100
1	B	278/300 (93%)	273 (98%)	4 (1%)	1 (0%)	34	24
1	C	280/300 (93%)	276 (99%)	3 (1%)	1 (0%)	34	24
1	D	277/300 (92%)	271 (98%)	5 (2%)	1 (0%)	34	24
All	All	1110/1200 (92%)	1091 (98%)	16 (1%)	3 (0%)	41	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	239	VAL
1	C	30	ILE
1	D	30	ILE

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/265 (91%)	235 (98%)	6 (2%)	47	40
1	B	242/265 (91%)	235 (97%)	7 (3%)	42	35
1	C	242/265 (91%)	235 (97%)	7 (3%)	42	35
1	D	238/265 (90%)	235 (99%)	3 (1%)	69	67
All	All	963/1060 (91%)	940 (98%)	23 (2%)	53	42

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	SER
1	A	236	SER
1	A	243	ASN
1	A	259[A]	CYS
1	A	259[B]	CYS
1	A	266	ASN
1	B	75	THR
1	B	172	SER
1	B	236	SER
1	B	243	ASN
1	B	256[A]	SER
1	B	256[B]	SER
1	B	266	ASN
1	C	87	LEU
1	C	218	SER
1	C	240	ASN
1	C	243	ASN
1	C	256[A]	SER
1	C	256[B]	SER
1	C	266	ASN
1	D	228	ASN
1	D	240	ASN
1	D	266	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	57	ASN
1	A	68	HIS
1	A	165	ASN
1	A	178	GLN
1	A	228	ASN
1	A	243	ASN
1	A	246	ASN
1	A	266	ASN
1	B	11	ASN
1	B	26	ASN
1	B	35	ASN
1	B	39	ASN
1	B	114	GLN
1	B	165	ASN
1	B	228	ASN

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Mol	Chain	Res	Type
1	B	243	ASN
1	B	266	ASN
1	C	11	ASN
1	C	57	ASN
1	C	103	GLN
1	C	114	GLN
1	C	165	ASN
1	C	178	GLN
1	C	205	ASN
1	C	228	ASN
1	C	240	ASN
1	C	246	ASN
1	C	266	ASN
1	D	11	ASN
1	D	43	ASN
1	D	57	ASN
1	D	78	ASN
1	D	114	GLN
1	D	165	ASN
1	D	198	GLN
1	D	228	ASN
1	D	240	ASN
1	D	246	ASN
1	D	266	ASN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

8 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	$\# Z  > 2$
3	FMT	B	301	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	301	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	301	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	301	-	0,2,2	0.00	-	0,1,1	0.00	-
2	EDO	A	300	-	3,3,3	0.42	0	2,2,2	0.45	0
2	EDO	B	300	-	3,3,3	0.49	0	2,2,2	0.40	0
2	EDO	C	300	-	3,3,3	0.52	0	2,2,2	0.17	0
2	EDO	D	300	-	3,3,3	0.45	0	2,2,2	0.57	0

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	EDO	C	300	-	-	0/1/1/1	-
2	EDO	A	300	-	-	0/1/1/1	-
2	EDO	D	300	-	-	0/1/1/1	-
2	EDO	B	300	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	300	EDO	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	272/300 (90%)	-0.54	2 (0%) 87 89	4, 11, 21, 28	0
1	B	273/300 (91%)	-0.53	3 (1%) 80 82	5, 12, 22, 30	0
1	C	274/300 (91%)	-0.50	1 (0%) 92 93	5, 12, 22, 29	0
1	D	274/300 (91%)	-0.46	1 (0%) 92 93	4, 12, 22, 28	0
All	All	1093/1200 (91%)	-0.50	7 (0%) 89 91	4, 12, 22, 30	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	CYS	4.2
1	A	238	CYS	2.9
1	D	275	TYR	2.9
1	B	90	TYR	2.4
1	C	238[A]	CYS	2.2
1	A	186	ASN	2.0
1	B	237	GLY	2.0

### 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( $\text{\AA}^2$ )	Q<0.9
2	EDO	D	300	4/4	0.96	0.11	11,17,18,19	0
2	EDO	B	300	4/4	0.97	0.10	12,13,14,19	0
2	EDO	C	300	4/4	0.97	0.08	16,16,19,20	0
2	EDO	A	300	4/4	0.97	0.11	9,10,12,18	0
3	FMT	B	301	3/3	0.98	0.08	10,10,10,11	0
3	FMT	D	301	3/3	0.99	0.10	11,11,12,12	0
3	FMT	C	301	3/3	0.99	0.08	12,12,12,12	0
3	FMT	A	301	3/3	0.99	0.12	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.