Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:48 PM GMT

PDB ID	:	5AYZ
Title	:	CRYSTAL STRUCTURE OF HUMAN QUINOLINATE PHOSPHORIBOSYLTRANSFERASE IN COMPLEX WITH THE PRODUCT NICOTINATE MONONUCLEOTIDE
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	:	2.60 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

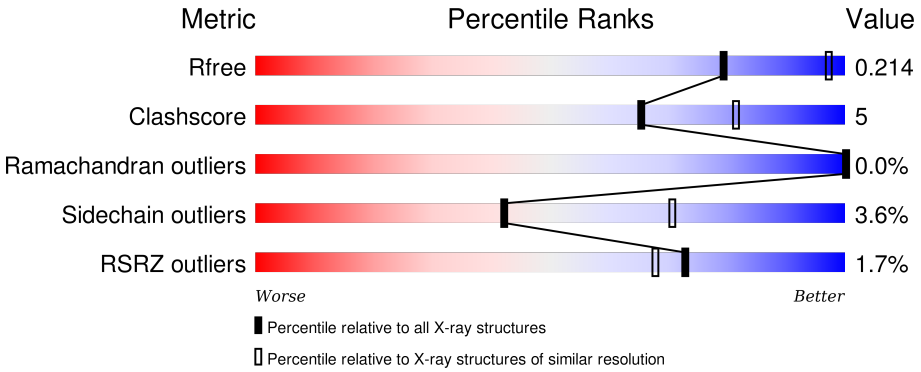
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 >=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 <=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	79% 15% • 5%
1	B	305	84% 9% •• 5%
1	C	305	3% 83% 10% • 5%
1	D	305	81% 13% • 5%
1	E	305	86% 8% • 5%

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Mol	Chain	Length	Quality of chain
1	F	305	3% 83% 10% • 5%
1	G	305	% 84% 9% • 5%
1	H	305	2% 82% 10% • • 5%
1	I	305	% 85% 9% • 5%
1	J	305	2% 82% 11% • 5%
1	K	305	% 86% 8% 5%
1	L	305	2% 81% 12% • 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	NCN	J	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25814 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			
1	J	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	K	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			
1	L	289	Total	C	N	O	S	0	0	0
			2108	1343	365	390	10			

There are 96 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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

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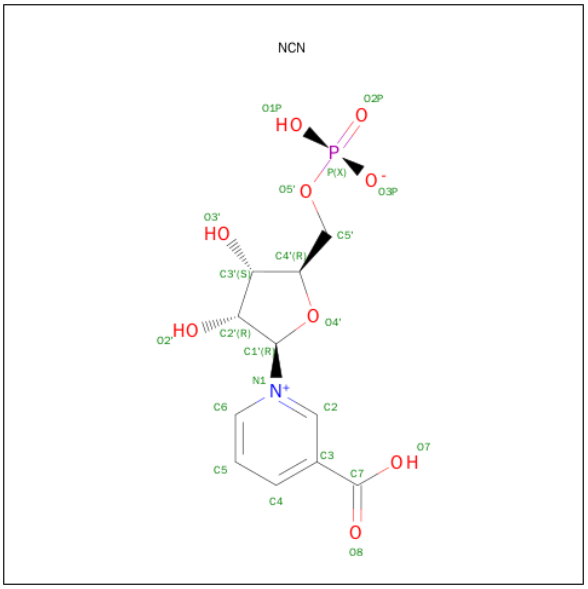
Chain	Residue	Modelled	Actual	Comment	Reference
L	299	GLU	-	expression tag	UNP V9HWJ5
L	300	HIS	-	expression tag	UNP V9HWJ5
L	301	HIS	-	expression tag	UNP V9HWJ5
L	302	HIS	-	expression tag	UNP V9HWJ5
L	303	HIS	-	expression tag	UNP V9HWJ5
L	304	HIS	-	expression tag	UNP V9HWJ5
L	305	HIS	-	expression tag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

- Molecule 2 is NICOTINATE MONONUCLEOTIDE (three-letter code: NCN) (formula: $C_{11}H_{14}NO_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	C	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	D	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	E	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	F	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	G	1	Total	C	N	O	P	0	0
			22	11	1	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	I	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	J	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	K	1	Total	C	N	O	P	0	0
			22	11	1	9	1		
2	L	1	Total	C	N	O	P	0	0
			22	11	1	9	1		

- Molecule 3 is water.

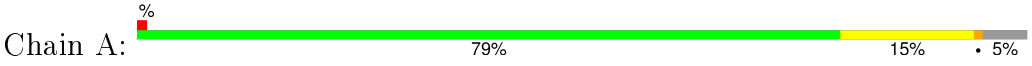
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	25	Total	O	0	0
			25	25		
3	C	20	Total	O	0	0
			20	20		
3	D	23	Total	O	0	0
			23	23		
3	E	17	Total	O	0	0
			17	17		
3	F	14	Total	O	0	0
			14	14		
3	G	26	Total	O	0	0
			26	26		
3	H	28	Total	O	0	0
			28	28		
3	I	20	Total	O	0	0
			20	20		
3	J	26	Total	O	0	0
			26	26		
3	K	16	Total	O	0	0
			16	16		
3	L	12	Total	O	0	0
			12	12		

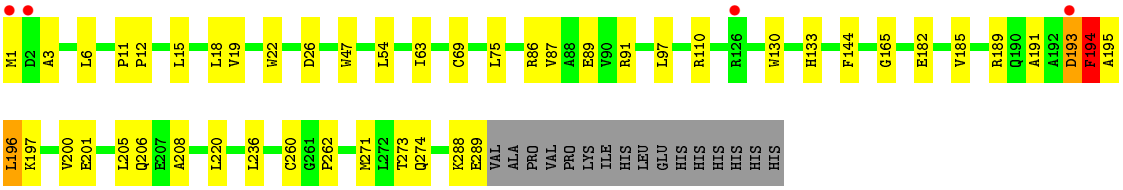
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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]

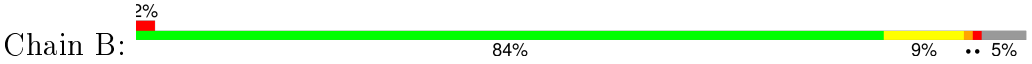
Chain A:

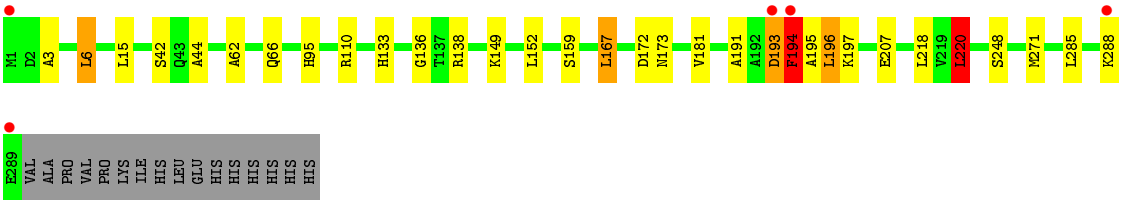




- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

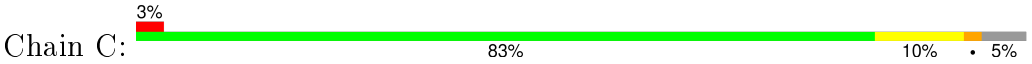
Chain B:

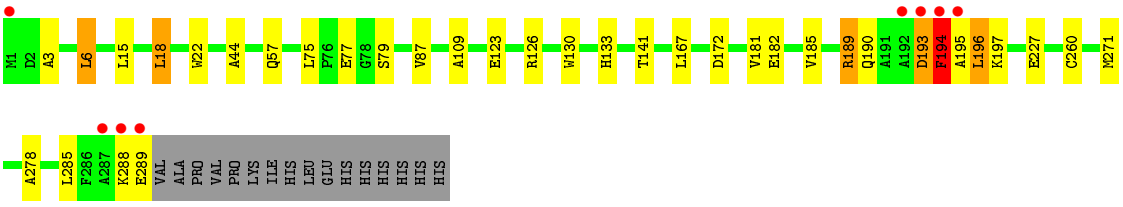




- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

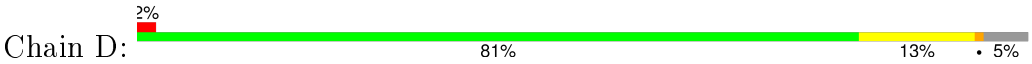
Chain C:

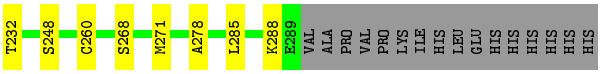




- Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

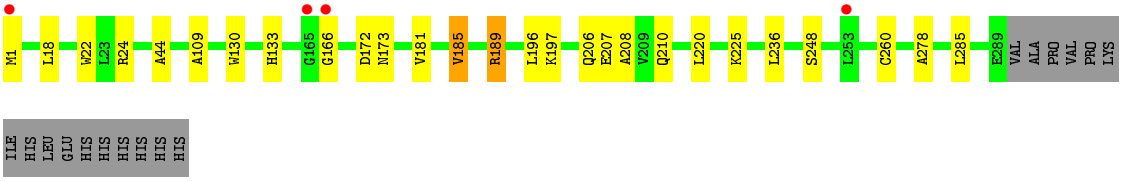
Chain D:





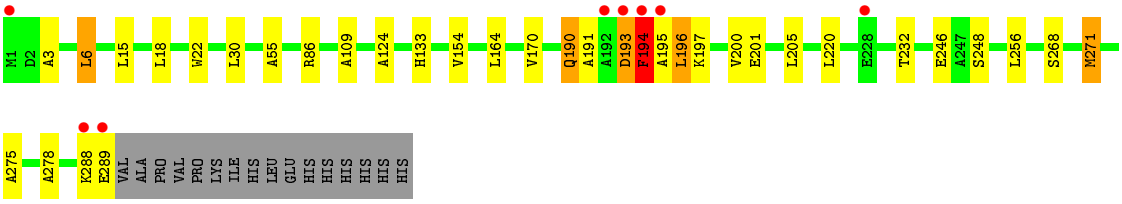
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain E:



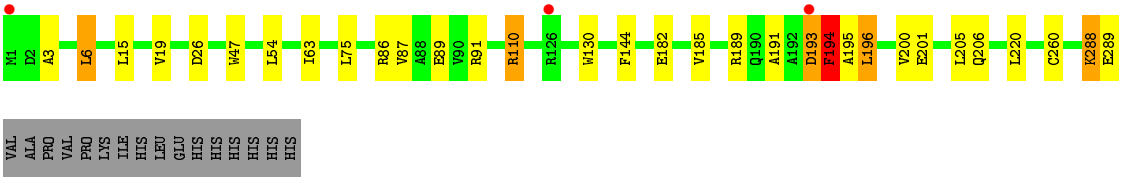
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain F:



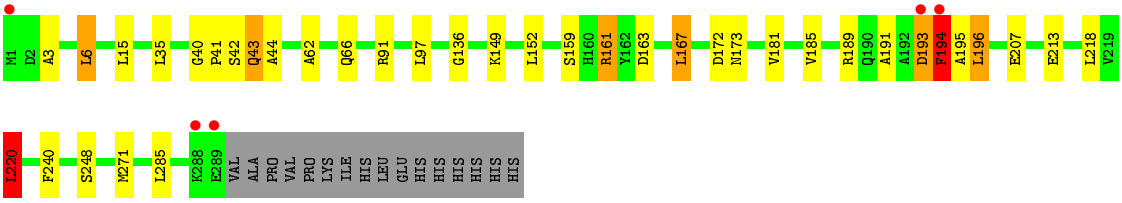
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain G:



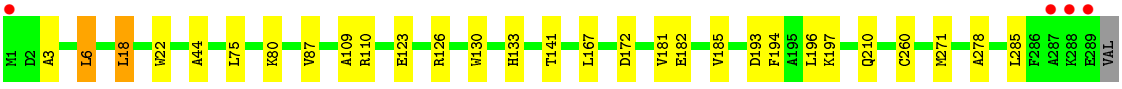
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain H:



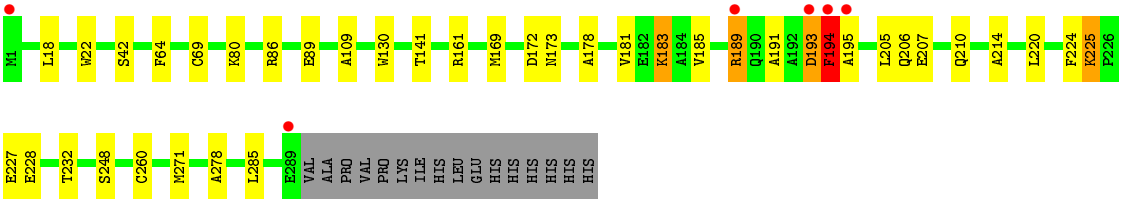
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain I:



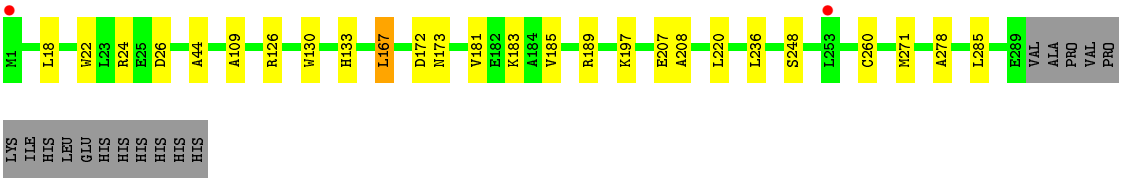
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain J:



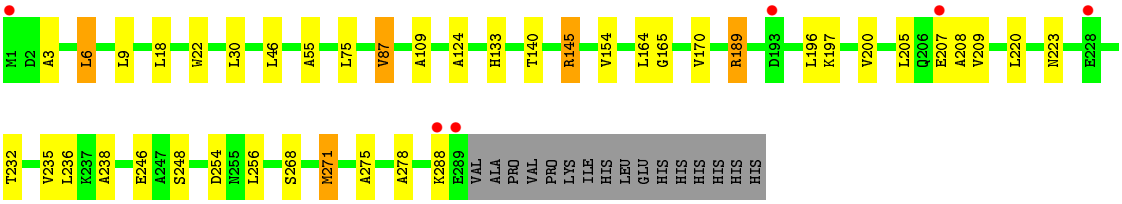
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain K:



• Molecule 1: Nicotinate-nucleotide pyrophosphorylase [carboxylating]

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.19Å 101.16Å 151.64Å 90.00° 92.49° 90.00°	Depositor
Resolution (Å)	44.14 – 2.60 44.14 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.14-2.60) 99.2 (44.14-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.17 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.226 , 0.256 0.212 , 0.214	Depositor DCC
R_{free} test set	5036 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 31.5	EDS
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	3 of 100763 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	25814	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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 99.73 % 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 5.0737e-14.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NCN

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	0.54	0/2151	0.69	3/2931 (0.1%)
1	B	0.50	0/2151	0.67	4/2931 (0.1%)
1	C	0.50	0/2151	0.66	4/2931 (0.1%)
1	D	0.52	0/2151	0.66	3/2931 (0.1%)
1	E	0.42	0/2151	0.60	0/2931
1	F	0.49	0/2151	0.65	3/2931 (0.1%)
1	G	0.52	0/2151	0.68	4/2931 (0.1%)
1	H	0.50	0/2151	0.66	4/2931 (0.1%)
1	I	0.45	0/2151	0.61	2/2931 (0.1%)
1	J	0.51	0/2151	0.66	2/2931 (0.1%)
1	K	0.40	0/2151	0.59	1/2931 (0.0%)
1	L	0.45	0/2151	0.62	0/2931
All	All	0.48	0/25812	0.65	30/35172 (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	2
1	B	0	2
1	C	0	1
1	D	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	J	0	2
All	All	0	15

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	167	LEU	CB-CA-C	7.07	123.64	110.20
1	G	196	LEU	CA-CB-CG	6.61	130.50	115.30
1	G	196	LEU	N-CA-C	-6.21	94.23	111.00
1	A	165	GLY	N-CA-C	6.11	128.36	113.10
1	C	172	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	194	PHE	N-CA-C	-5.77	95.43	111.00
1	A	194	PHE	N-CA-C	-5.77	95.43	111.00
1	C	194	PHE	N-CA-C	-5.77	95.43	111.00
1	G	194	PHE	N-CA-C	-5.77	95.43	111.00
1	H	194	PHE	N-CA-C	-5.76	95.45	111.00
1	D	194	PHE	N-CA-C	-5.76	95.45	111.00
1	F	194	PHE	N-CA-C	-5.76	95.45	111.00
1	J	194	PHE	N-CA-C	-5.75	95.47	111.00
1	D	285	LEU	CA-CB-CG	5.64	128.28	115.30
1	I	172	ASP	CB-CG-OD1	5.63	123.37	118.30
1	J	285	LEU	CA-CB-CG	5.53	128.03	115.30
1	H	167	LEU	CA-CB-CG	5.52	128.00	115.30
1	B	167	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	196	LEU	CA-CB-CG	5.44	127.81	115.30
1	D	196	LEU	CA-CB-CG	5.44	127.81	115.30
1	C	196	LEU	CA-CB-CG	5.43	127.79	115.30
1	F	196	LEU	CA-CB-CG	5.43	127.78	115.30
1	A	196	LEU	CA-CB-CG	5.42	127.77	115.30
1	H	196	LEU	CA-CB-CG	5.42	127.77	115.30
1	I	18	LEU	CA-CB-CG	5.25	127.37	115.30
1	F	196	LEU	N-CA-C	-5.24	96.85	111.00
1	B	220	LEU	CA-CB-CG	5.22	127.31	115.30
1	C	18	LEU	CA-CB-CG	5.12	127.08	115.30
1	H	220	LEU	CA-CB-CG	5.10	127.03	115.30
1	G	196	LEU	CB-CG-CD1	5.07	119.61	111.00

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	ALA	Peptide
1	A	194	PHE	Peptide
1	B	191	ALA	Peptide
1	B	194	PHE	Peptide
1	C	194	PHE	Peptide
1	D	191	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	D	194	PHE	Peptide
1	F	191	ALA	Peptide
1	F	194	PHE	Peptide
1	G	191	ALA	Peptide
1	G	194	PHE	Peptide
1	H	191	ALA	Peptide
1	H	194	PHE	Peptide
1	J	191	ALA	Peptide
1	J	194	PHE	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	2108	0	2131	34	0
1	B	2108	0	2131	22	0
1	C	2108	0	2131	29	0
1	D	2108	0	2131	27	0
1	E	2108	0	2131	20	0
1	F	2108	0	2131	27	0
1	G	2108	0	2131	19	0
1	H	2108	0	2131	23	0
1	I	2108	0	2131	17	0
1	J	2108	0	2131	36	0
1	K	2108	0	2131	17	0
1	L	2108	0	2131	27	0
2	A	22	0	12	0	0
2	B	22	0	12	0	0
2	C	22	0	12	0	0
2	D	22	0	12	0	0
2	E	22	0	12	0	0
2	F	22	0	12	0	0
2	G	22	0	12	0	0
2	H	22	0	12	0	0
2	I	22	0	12	0	0
2	J	22	0	12	8	0
2	K	22	0	12	0	0
2	L	22	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	0	1	0
3	B	25	0	0	0	0
3	C	20	0	0	0	0
3	D	23	0	0	0	0
3	E	17	0	0	1	0
3	F	14	0	0	0	0
3	G	26	0	0	0	0
3	H	28	0	0	0	0
3	I	20	0	0	0	0
3	J	26	0	0	0	0
3	K	16	0	0	0	0
3	L	12	0	0	0	0
All	All	25814	0	25716	258	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 (258) 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:A:133:HIS:HE1	1:F:193:ASP:OD2	1.30	1.12
1:A:193:ASP:OD2	1:F:133:HIS:HE1	1.34	1.11
1:C:189:ARG:HH11	1:C:189:ARG:HG3	1.12	1.09
1:J:169:MET:CE	2:J:401:NCN:C7	2.30	1.08
1:D:193:ASP:OD2	1:E:133:HIS:NE2	1.86	1.08
1:G:193:ASP:OD2	1:L:133:HIS:HE1	1.34	1.07
1:D:205:LEU:HD12	1:D:232:THR:HG23	1.28	1.06
1:A:133:HIS:CE1	1:F:193:ASP:OD2	2.12	1.02
1:J:169:MET:HE3	2:J:401:NCN:C7	1.88	1.00
1:J:193:ASP:OD2	1:K:133:HIS:NE2	1.94	0.99
1:A:193:ASP:OD2	1:F:133:HIS:CE1	2.18	0.97
1:G:193:ASP:OD2	1:L:133:HIS:CE1	2.18	0.95
1:B:133:HIS:HE1	1:C:193:ASP:OD2	1.50	0.93
1:B:197:LYS:HD2	1:C:195:ALA:HB1	1.51	0.89
1:A:3:ALA:HA	1:A:6:LEU:HD23	1.55	0.88
1:B:193:ASP:OD2	1:C:133:HIS:HE1	1.56	0.88
1:E:189:ARG:NH2	1:E:189:ARG:O	2.06	0.88
1:J:189:ARG:NH2	1:J:193:ASP:HB2	1.89	0.87
1:A:197:LYS:HD2	1:F:195:ALA:HB1	1.57	0.87
1:C:189:ARG:HH12	1:C:193:ASP:HA	1.39	0.86
1:D:181:VAL:HG21	1:D:207:GLU:HG2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:HIS:CE1	1:C:193:ASP:OD2	2.29	0.83
1:D:205:LEU:CD1	1:D:232:THR:HG23	2.10	0.81
1:I:182:GLU:OE1	1:I:210:GLN:NE2	2.14	0.81
1:J:181:VAL:HG21	1:J:207:GLU:HG2	1.62	0.81
1:C:189:ARG:NH1	1:C:189:ARG:HG3	1.91	0.80
1:A:3:ALA:HA	1:A:6:LEU:CD2	2.12	0.79
1:L:246:GLU:OE1	1:L:268:SER:OG	2.01	0.78
1:I:193:ASP:OD1	1:I:194:PHE:N	2.14	0.77
1:H:195:ALA:HB1	1:I:197:LYS:HD2	1.67	0.76
1:H:193:ASP:OD2	1:I:133:HIS:HE1	1.68	0.76
1:J:169:MET:HE1	2:J:401:NCN:C7	2.14	0.75
1:J:189:ARG:HH22	1:J:193:ASP:HB2	1.49	0.75
1:B:197:LYS:CD	1:C:195:ALA:HB1	2.18	0.74
1:K:26:ASP:OD1	1:L:145:ARG:NH1	2.23	0.70
1:B:193:ASP:OD2	1:C:133:HIS:CE1	2.44	0.70
1:G:195:ALA:HB1	1:L:197:LYS:HD2	1.75	0.69
1:J:169:MET:CE	2:J:401:NCN:O8	2.42	0.67
1:H:195:ALA:HB1	1:I:197:LYS:CD	2.24	0.67
1:A:89:GLU:OE2	1:A:91:ARG:NH1	2.28	0.65
1:A:197:LYS:CD	1:F:195:ALA:HB1	2.26	0.65
1:B:195:ALA:HB1	1:C:197:LYS:CD	2.27	0.65
1:L:220:LEU:HD21	1:L:248:SER:HB3	1.79	0.64
1:H:193:ASP:OD2	1:I:133:HIS:CE1	2.50	0.64
1:B:181:VAL:HG21	1:B:207:GLU:HG3	1.79	0.64
1:J:169:MET:HE1	2:J:401:NCN:O8	1.98	0.64
1:H:181:VAL:HG21	1:H:207:GLU:HG3	1.80	0.64
1:I:123:GLU:OE2	1:I:126:ARG:NH2	2.31	0.62
1:L:3:ALA:HA	1:L:6:LEU:HD22	1.81	0.62
1:G:110:ARG:HG2	1:G:144:PHE:HE2	1.65	0.62
1:G:89:GLU:OE2	1:G:91:ARG:NH1	2.27	0.62
1:F:3:ALA:HA	1:F:6:LEU:HD22	1.80	0.62
1:J:169:MET:HE3	2:J:401:NCN:C3	2.31	0.61
1:F:288:LYS:O	1:F:289:GLU:HB2	2.01	0.60
1:C:3:ALA:HA	1:C:6:LEU:HD22	1.84	0.60
1:F:220:LEU:HD21	1:F:248:SER:HB3	1.83	0.60
1:C:189:ARG:NH1	1:C:193:ASP:HA	2.15	0.59
1:C:18:LEU:HG	1:C:22:TRP:CZ2	2.38	0.59
1:A:288:LYS:HD3	1:A:289:GLU:N	2.17	0.59
1:I:3:ALA:HA	1:I:6:LEU:HD22	1.83	0.59
1:I:18:LEU:HG	1:I:22:TRP:CZ2	2.37	0.59
1:A:195:ALA:HB1	1:F:197:LYS:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:MET:HG2	3:A:510:HOH:O	2.04	0.58
1:A:110:ARG:NH1	1:A:273:THR:O	2.37	0.58
1:J:86:ARG:NH2	1:J:89:GLU:OE2	2.36	0.57
1:E:206:GLN:O	1:E:210:GLN:HG3	2.04	0.57
1:H:43:GLN:HG2	1:H:91:ARG:HG2	1.86	0.57
1:K:220:LEU:HD21	1:K:248:SER:HB3	1.86	0.57
1:J:169:MET:CE	2:J:401:NCN:C3	2.83	0.56
1:H:185:VAL:O	1:H:189:ARG:HG3	2.04	0.56
1:K:183:LYS:H	1:K:183:LYS:HE2	1.71	0.56
1:D:43:GLN:HG2	1:D:91:ARG:NH2	2.21	0.55
1:D:205:LEU:HD12	1:D:232:THR:CG2	2.19	0.55
1:B:195:ALA:HB1	1:C:197:LYS:HD3	1.88	0.55
1:H:44:ALA:HB2	1:H:285:LEU:HD23	1.87	0.55
1:K:189:ARG:NH1	1:K:189:ARG:O	2.39	0.55
1:B:44:ALA:HB2	1:B:285:LEU:HD23	1.88	0.55
1:E:220:LEU:HD21	1:E:248:SER:HB3	1.88	0.54
1:D:190:GLN:HE22	1:E:1:MET:N	2.06	0.54
1:E:166:GLY:O	1:E:196:LEU:HD22	2.07	0.54
1:C:44:ALA:HB2	1:C:285:LEU:HD23	1.89	0.54
1:L:205:LEU:HD23	1:L:232:THR:HG23	1.90	0.54
1:G:206:GLN:H	1:G:206:GLN:CD	2.11	0.54
1:I:193:ASP:OD1	1:I:194:PHE:CD1	2.61	0.54
1:K:44:ALA:HB2	1:K:285:LEU:HD23	1.89	0.54
1:E:44:ALA:HB2	1:E:285:LEU:HD23	1.89	0.53
1:H:194:PHE:HA	1:H:195:ALA:HB2	1.91	0.53
1:A:206:GLN:H	1:A:206:GLN:CD	2.11	0.53
1:A:194:PHE:HA	1:A:195:ALA:HB2	1.91	0.53
1:J:205:LEU:HD13	1:J:232:THR:HG23	1.90	0.53
1:E:181:VAL:HG21	1:E:207:GLU:HG2	1.91	0.53
1:E:189:ARG:HB3	1:E:189:ARG:HH21	1.73	0.53
1:F:194:PHE:HA	1:F:195:ALA:HB2	1.91	0.53
1:D:89:GLU:OE1	1:D:91:ARG:NH1	2.41	0.53
1:K:109:ALA:HB1	1:K:278:ALA:HB1	1.91	0.53
1:G:194:PHE:HA	1:G:195:ALA:HB2	1.91	0.52
1:H:3:ALA:HA	1:H:6:LEU:HD22	1.92	0.52
1:D:194:PHE:HA	1:D:195:ALA:HB2	1.91	0.52
1:A:3:ALA:CA	1:A:6:LEU:HD23	2.36	0.52
1:C:194:PHE:HA	1:C:195:ALA:HB2	1.91	0.52
1:G:3:ALA:HA	1:G:6:LEU:HD22	1.90	0.52
1:B:194:PHE:HA	1:B:195:ALA:HB2	1.91	0.52
1:L:124:ALA:HB3	1:L:256:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:194:PHE:HA	1:J:195:ALA:HB2	1.91	0.52
1:D:205:LEU:HD13	1:D:232:THR:HA	1.92	0.51
1:G:195:ALA:HB1	1:L:197:LYS:CD	2.38	0.51
1:D:18:LEU:HG	1:D:22:TRP:CZ2	2.45	0.51
1:H:43:GLN:CG	1:H:91:ARG:HG2	2.40	0.51
1:C:182:GLU:H	1:C:182:GLU:CD	2.14	0.51
1:J:169:MET:HE3	2:J:401:NCN:O7	2.09	0.51
1:J:172:ASP:OD1	1:J:173:ASN:N	2.44	0.51
1:J:18:LEU:HG	1:J:22:TRP:CZ2	2.45	0.51
1:G:201:GLU:HG3	1:G:220:LEU:HD22	1.93	0.50
1:D:172:ASP:OD1	1:D:173:ASN:N	2.45	0.50
1:K:181:VAL:HG21	1:K:207:GLU:HG2	1.92	0.50
1:F:205:LEU:HD23	1:F:232:THR:HG23	1.94	0.50
1:I:44:ALA:HB2	1:I:285:LEU:HD23	1.93	0.50
1:I:141:THR:HG21	1:J:141:THR:HG21	1.93	0.50
1:E:1:MET:N	3:E:502:HOH:O	2.44	0.49
1:B:149:LYS:HD2	1:B:159:SER:HB2	1.93	0.49
1:J:178:ALA:O	1:J:183:LYS:HD2	2.12	0.49
1:L:207:GLU:OE1	1:L:207:GLU:N	2.29	0.49
1:F:55:ALA:HB2	1:F:154:VAL:HG11	1.95	0.49
1:L:75:LEU:HD12	1:L:87:VAL:HB	1.95	0.49
1:E:109:ALA:HB1	1:E:278:ALA:HB1	1.95	0.49
1:L:208:ALA:HB1	1:L:236:LEU:HD11	1.93	0.49
1:H:62:ALA:O	1:H:66:GLN:HG2	2.12	0.49
1:F:124:ALA:HB3	1:F:256:LEU:HD23	1.94	0.49
1:F:18:LEU:HG	1:F:22:TRP:CZ2	2.48	0.49
1:D:185:VAL:HG21	1:D:214:ALA:HB3	1.95	0.49
1:H:172:ASP:OD1	1:H:173:ASN:N	2.46	0.48
1:B:172:ASP:OD1	1:B:173:ASN:N	2.46	0.48
1:J:109:ALA:HB1	1:J:278:ALA:HB1	1.94	0.48
1:B:3:ALA:HA	1:B:6:LEU:HD22	1.95	0.48
1:D:109:ALA:HB1	1:D:278:ALA:HB1	1.95	0.48
1:H:149:LYS:HD2	1:H:159:SER:HB2	1.95	0.48
1:B:62:ALA:O	1:B:66:GLN:HG2	2.14	0.48
1:A:195:ALA:HB1	1:F:197:LYS:CD	2.44	0.48
1:C:57:GLN:HG3	1:C:77:GLU:OE1	2.14	0.48
1:J:161:ARG:CZ	1:J:169:MET:HE2	2.43	0.48
1:L:189:ARG:HA	1:L:189:ARG:HE	1.78	0.47
1:K:172:ASP:OD1	1:K:173:ASN:N	2.47	0.47
1:K:167:LEU:HD13	1:K:197:LYS:HB2	1.96	0.47
1:D:190:GLN:HE22	1:E:1:MET:H1	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:55:ALA:HB2	1:L:154:VAL:HG11	1.95	0.47
1:J:220:LEU:HD21	1:J:248:SER:HB3	1.97	0.47
1:J:161:ARG:NE	1:J:169:MET:HE2	2.30	0.47
1:I:181:VAL:O	1:I:185:VAL:HG13	2.13	0.47
1:C:181:VAL:O	1:C:185:VAL:HG13	2.14	0.47
1:J:185:VAL:HG21	1:J:214:ALA:HB3	1.97	0.47
1:A:47:TRP:CZ3	1:A:86:ARG:HB2	2.49	0.47
1:L:140:THR:OG1	1:L:145:ARG:HD3	2.15	0.47
1:C:15:LEU:HD23	1:C:15:LEU:HA	1.56	0.47
1:G:47:TRP:CZ3	1:G:86:ARG:HB2	2.50	0.47
1:E:172:ASP:OD1	1:E:173:ASN:N	2.46	0.47
1:D:220:LEU:HD21	1:D:248:SER:HB3	1.97	0.47
1:G:19:VAL:HG22	1:G:63:ILE:HG13	1.97	0.47
1:C:141:THR:HG21	1:D:141:THR:HG21	1.96	0.46
1:H:15:LEU:HD23	1:H:15:LEU:HA	1.66	0.46
1:I:75:LEU:HD12	1:I:87:VAL:HG12	1.97	0.46
1:J:195:ALA:HB1	1:K:197:LYS:HD2	1.97	0.46
1:A:201:GLU:HG3	1:A:220:LEU:HD22	1.98	0.46
1:J:189:ARG:HH22	1:J:193:ASP:CB	2.22	0.46
1:K:167:LEU:HD12	1:K:197:LYS:O	2.15	0.46
1:C:288:LYS:HG3	1:C:289:GLU:H	1.79	0.46
1:A:18:LEU:HG	1:A:22:TRP:CZ2	2.50	0.46
1:I:182:GLU:CD	1:I:182:GLU:H	2.19	0.45
1:A:19:VAL:HG22	1:A:63:ILE:HG13	1.98	0.45
1:L:18:LEU:HG	1:L:22:TRP:CZ2	2.51	0.45
1:A:1:MET:HG3	1:F:190:GLN:HE22	1.81	0.45
1:J:224:PHE:CD2	1:J:228:GLU:HG3	2.52	0.45
1:J:189:ARG:NH2	1:J:193:ASP:CB	2.71	0.45
1:G:15:LEU:HA	1:G:15:LEU:HD23	1.68	0.45
1:B:288:LYS:N	1:B:288:LYS:HD2	2.32	0.45
1:G:130:TRP:HB2	1:G:260:CYS:HB3	1.98	0.45
1:A:110:ARG:HG2	1:A:144:PHE:HE2	1.81	0.44
1:G:288:LYS:HE3	1:G:289:GLU:H	1.83	0.44
1:F:271:MET:HG2	1:F:275:ALA:HB3	2.00	0.44
1:J:130:TRP:HB2	1:J:260:CYS:HB3	1.99	0.44
1:A:75:LEU:HD12	1:A:87:VAL:HB	1.98	0.44
1:C:123:GLU:OE2	1:C:126:ARG:NH1	2.37	0.44
1:H:213:GLU:HG3	1:H:240:PHE:CZ	2.53	0.44
1:D:130:TRP:HB2	1:D:260:CYS:HB3	1.99	0.44
1:A:274:GLN:HE21	1:B:110:ARG:HH12	1.66	0.44
1:B:15:LEU:HA	1:B:15:LEU:HD23	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:246:GLU:OE2	1:F:268:SER:OG	2.29	0.44
1:H:97:LEU:HA	1:H:97:LEU:HD23	1.83	0.43
1:L:170:VAL:CG2	1:L:200:VAL:HG13	2.49	0.43
1:E:130:TRP:HB2	1:E:260:CYS:HB3	2.00	0.43
1:K:181:VAL:O	1:K:185:VAL:HG13	2.18	0.43
1:L:288:LYS:HE2	1:L:288:LYS:HB3	1.92	0.43
1:J:161:ARG:NH2	1:J:169:MET:HE2	2.34	0.43
1:D:181:VAL:O	1:D:185:VAL:HG13	2.19	0.43
1:G:75:LEU:HD12	1:G:87:VAL:HB	2.00	0.43
1:A:26:ASP:OD2	1:B:138:ARG:NH2	2.37	0.43
1:G:185:VAL:HG22	1:G:200:VAL:HG21	2.01	0.43
1:I:109:ALA:HB1	1:I:278:ALA:HB1	2.00	0.43
1:K:208:ALA:HB1	1:K:236:LEU:HD11	2.00	0.43
1:J:181:VAL:CG2	1:J:207:GLU:HG2	2.42	0.43
1:C:130:TRP:HB2	1:C:260:CYS:HB3	2.01	0.43
1:A:130:TRP:HB2	1:A:260:CYS:HB3	1.99	0.43
1:A:195:ALA:HB1	1:F:197:LYS:NZ	2.33	0.43
1:D:195:ALA:HB1	1:E:197:LYS:HD2	1.99	0.43
1:D:135:ALA:O	1:D:268:SER:HA	2.19	0.43
1:L:46:LEU:HD23	1:L:87:VAL:HG22	2.01	0.42
1:L:223:ASN:O	1:L:223:ASN:ND2	2.51	0.42
1:C:227:GLU:CD	1:C:227:GLU:H	2.23	0.42
1:K:130:TRP:HB2	1:K:260:CYS:HB3	1.99	0.42
1:A:208:ALA:HB1	1:A:236:LEU:HD11	2.00	0.42
1:D:224:PHE:CD2	1:D:228:GLU:HG3	2.53	0.42
1:F:170:VAL:CG2	1:F:200:VAL:HG13	2.49	0.42
1:J:225:LYS:HB3	1:J:227:GLU:OE1	2.20	0.42
1:E:208:ALA:HB1	1:E:236:LEU:HD11	2.00	0.42
1:J:224:PHE:HD2	1:J:228:GLU:HG3	1.85	0.42
1:C:109:ALA:HB1	1:C:278:ALA:HB1	2.01	0.42
1:I:130:TRP:HB2	1:I:260:CYS:HB3	2.02	0.42
1:B:195:ALA:HB1	1:C:197:LYS:HD2	2.01	0.42
1:A:185:VAL:HG22	1:A:200:VAL:HG21	2.02	0.42
1:H:220:LEU:HD11	1:H:248:SER:HB3	2.02	0.42
1:E:18:LEU:HG	1:E:22:TRP:CZ2	2.55	0.41
1:A:69:CYS:SG	1:A:97:LEU:HD23	2.60	0.41
1:H:136:GLY:HA3	1:H:152:LEU:HD13	2.01	0.41
1:G:288:LYS:HE3	1:G:289:GLU:N	2.35	0.41
1:L:170:VAL:HG22	1:L:200:VAL:HG22	2.01	0.41
1:B:220:LEU:HD11	1:B:248:SER:HB3	2.01	0.41
1:C:288:LYS:HG3	1:C:289:GLU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:GLU:OE2	1:D:186:ARG:CZ	2.68	0.41
1:D:64:PHE:HB3	1:D:69:CYS:HB2	2.02	0.41
1:E:189:ARG:NH2	1:E:189:ARG:C	2.70	0.41
1:L:271:MET:HG2	1:L:275:ALA:HB3	2.02	0.41
1:G:26:ASP:O	1:H:163:ASP:HB2	2.20	0.41
1:F:164:LEU:HA	1:F:164:LEU:HD23	1.93	0.41
1:A:11:PRO:HA	1:A:12:PRO:HD3	1.94	0.41
1:K:183:LYS:H	1:K:183:LYS:CE	2.32	0.41
1:D:130:TRP:CZ2	1:D:132:GLY:HA3	2.56	0.41
1:J:64:PHE:HB3	1:J:69:CYS:HB2	2.03	0.41
1:F:15:LEU:HA	1:F:15:LEU:HD23	1.77	0.41
1:E:225:LYS:HD3	1:E:225:LYS:HA	1.84	0.41
1:C:75:LEU:HD12	1:C:87:VAL:HG12	2.02	0.41
1:F:201:GLU:HG2	1:F:220:LEU:HD22	2.02	0.41
1:F:271:MET:HE3	1:F:271:MET:HB3	1.89	0.41
1:D:169:MET:HG2	1:D:171:LYS:HE2	2.03	0.41
1:B:136:GLY:HA3	1:B:152:LEU:HD13	2.02	0.41
1:H:35:LEU:HG	1:L:9:LEU:HD21	2.03	0.41
1:K:18:LEU:HG	1:K:22:TRP:CZ2	2.56	0.41
1:D:224:PHE:HD2	1:D:228:GLU:HG3	1.86	0.41
1:L:109:ALA:HB1	1:L:278:ALA:HB1	2.02	0.40
1:H:40:GLY:HA2	1:H:41:PRO:HD3	1.96	0.40
1:H:161:ARG:O	1:H:161:ARG:HG2	2.20	0.40
1:L:235:VAL:O	1:L:238:ALA:HB3	2.21	0.40
1:L:205:LEU:O	1:L:209:VAL:HG23	2.21	0.40
1:F:170:VAL:HG22	1:F:200:VAL:HG22	2.04	0.40
1:A:110:ARG:HG2	1:A:144:PHE:CE2	2.55	0.40
1:E:181:VAL:O	1:E:185:VAL:HG13	2.22	0.40
1:F:109:ALA:HB1	1:F:278:ALA:HB1	2.02	0.40
1:J:206:GLN:O	1:J:210:GLN:HG3	2.22	0.40
1:A:15:LEU:HD23	1:A:15:LEU:HA	1.68	0.40
1:J:80:LYS:HE3	1:J:80:LYS:HB3	1.90	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	287/305 (94%)	283 (99%)	4 (1%)	0	100	100
1	B	287/305 (94%)	282 (98%)	5 (2%)	0	100	100
1	C	287/305 (94%)	280 (98%)	7 (2%)	0	100	100
1	D	287/305 (94%)	283 (99%)	4 (1%)	0	100	100
1	E	287/305 (94%)	285 (99%)	2 (1%)	0	100	100
1	F	287/305 (94%)	278 (97%)	9 (3%)	0	100	100
1	G	287/305 (94%)	283 (99%)	4 (1%)	0	100	100
1	H	287/305 (94%)	284 (99%)	3 (1%)	0	100	100
1	I	287/305 (94%)	281 (98%)	6 (2%)	0	100	100
1	J	287/305 (94%)	282 (98%)	5 (2%)	0	100	100
1	K	287/305 (94%)	283 (99%)	4 (1%)	0	100	100
1	L	287/305 (94%)	277 (96%)	9 (3%)	1 (0%)	46	72
All	All	3444/3660 (94%)	3381 (98%)	62 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	165	GLY

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	212/227 (93%)	204 (96%)	8 (4%)	40	68
1	B	212/227 (93%)	202 (95%)	10 (5%)	32	59
1	C	212/227 (93%)	203 (96%)	9 (4%)	36	65
1	D	212/227 (93%)	205 (97%)	7 (3%)	45	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	212/227 (93%)	209 (99%)	3 (1%)	74 90
1	F	212/227 (93%)	204 (96%)	8 (4%)	40 68
1	G	212/227 (93%)	202 (95%)	10 (5%)	32 59
1	H	212/227 (93%)	201 (95%)	11 (5%)	29 54
1	I	212/227 (93%)	206 (97%)	6 (3%)	51 78
1	J	212/227 (93%)	205 (97%)	7 (3%)	45 73
1	K	212/227 (93%)	209 (99%)	3 (1%)	74 90
1	L	212/227 (93%)	203 (96%)	9 (4%)	36 65
All	All	2544/2724 (93%)	2453 (96%)	91 (4%)	42 71

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	182	GLU
1	A	189	ARG
1	A	193	ASP
1	A	194	PHE
1	A	196	LEU
1	A	205	LEU
1	A	262	PRO
1	B	6	LEU
1	B	42	SER
1	B	95	HIS
1	B	167	LEU
1	B	193	ASP
1	B	194	PHE
1	B	196	LEU
1	B	218	LEU
1	B	220	LEU
1	B	271	MET
1	C	6	LEU
1	C	79	SER
1	C	167	LEU
1	C	189	ARG
1	C	190	GLN
1	C	193	ASP
1	C	194	PHE
1	C	196	LEU

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Mol	Chain	Res	Type
1	C	271	MET
1	D	42	SER
1	D	189	ARG
1	D	193	ASP
1	D	194	PHE
1	D	196	LEU
1	D	271	MET
1	D	288	LYS
1	E	24	ARG
1	E	185	VAL
1	E	189	ARG
1	F	6	LEU
1	F	30	LEU
1	F	86	ARG
1	F	190	GLN
1	F	193	ASP
1	F	194	PHE
1	F	196	LEU
1	F	271	MET
1	G	6	LEU
1	G	54	LEU
1	G	110	ARG
1	G	182	GLU
1	G	189	ARG
1	G	193	ASP
1	G	194	PHE
1	G	196	LEU
1	G	205	LEU
1	G	288	LYS
1	H	6	LEU
1	H	42	SER
1	H	43	GLN
1	H	161	ARG
1	H	167	LEU
1	H	193	ASP
1	H	194	PHE
1	H	196	LEU
1	H	218	LEU
1	H	220	LEU
1	H	271	MET
1	I	6	LEU
1	I	80	LYS

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Mol	Chain	Res	Type
1	I	110	ARG
1	I	167	LEU
1	I	196	LEU
1	I	271	MET
1	J	42	SER
1	J	183	LYS
1	J	189	ARG
1	J	193	ASP
1	J	194	PHE
1	J	225	LYS
1	J	271	MET
1	K	24	ARG
1	K	126	ARG
1	K	271	MET
1	L	6	LEU
1	L	30	LEU
1	L	87	VAL
1	L	145	ARG
1	L	164	LEU
1	L	189	ARG
1	L	196	LEU
1	L	254	ASP
1	L	271	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	HIS
1	A	274	GLN
1	B	133	HIS
1	B	190	GLN
1	C	133	HIS
1	D	190	GLN
1	F	133	HIS
1	F	190	GLN
1	H	43	GLN
1	I	133	HIS
1	I	239	GLN
1	J	190	GLN
1	K	57	GLN
1	L	133	HIS
1	L	223	ASN

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

12 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	NCN	A	401	-	19,23,23	0.57	0	26,34,34	0.85	1 (3%)
2	NCN	B	401	-	19,23,23	0.58	0	26,34,34	0.90	1 (3%)
2	NCN	C	401	-	19,23,23	0.63	0	26,34,34	0.86	0
2	NCN	D	401	-	19,23,23	0.58	0	26,34,34	0.88	0
2	NCN	E	401	-	19,23,23	0.65	0	26,34,34	0.90	1 (3%)
2	NCN	F	401	-	19,23,23	0.68	0	26,34,34	0.93	1 (3%)
2	NCN	G	401	-	19,23,23	0.58	0	26,34,34	1.24	3 (11%)
2	NCN	H	401	-	19,23,23	0.68	0	26,34,34	1.06	2 (7%)
2	NCN	I	401	-	19,23,23	0.58	0	26,34,34	0.80	0
2	NCN	J	401	-	19,23,23	0.56	0	26,34,34	0.86	0
2	NCN	K	401	-	19,23,23	0.63	0	26,34,34	0.80	1 (3%)
2	NCN	L	401	-	19,23,23	0.67	0	26,34,34	0.86	1 (3%)

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	NCN	A	401	-	-	0/6/30/30	0/2/2/2
2	NCN	B	401	-	-	0/6/30/30	0/2/2/2
2	NCN	C	401	-	-	0/6/30/30	0/2/2/2
2	NCN	D	401	-	-	0/6/30/30	0/2/2/2
2	NCN	E	401	-	-	0/6/30/30	0/2/2/2
2	NCN	F	401	-	-	0/6/30/30	0/2/2/2
2	NCN	G	401	-	-	0/6/30/30	0/2/2/2
2	NCN	H	401	-	-	0/6/30/30	0/2/2/2
2	NCN	I	401	-	-	0/6/30/30	0/2/2/2
2	NCN	J	401	-	-	0/6/30/30	0/2/2/2
2	NCN	K	401	-	-	0/6/30/30	0/2/2/2
2	NCN	L	401	-	-	0/6/30/30	0/2/2/2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	401	NCN	O3P-P-O5'	-3.14	98.26	108.00
2	B	401	NCN	O3P-P-O5'	-2.86	99.14	108.00
2	K	401	NCN	O3P-P-O5'	-2.06	101.62	108.00
2	L	401	NCN	O1P-P-O2P	2.14	118.73	110.97
2	A	401	NCN	O1P-P-O2P	2.22	119.04	110.97
2	G	401	NCN	O1P-P-O2P	2.25	119.12	110.97
2	H	401	NCN	O1P-P-O5'	2.25	110.82	105.33
2	H	401	NCN	O1P-P-O2P	2.40	119.68	110.97
2	F	401	NCN	O1P-P-O2P	2.74	120.90	110.97
2	E	401	NCN	O1P-P-O5'	2.97	112.56	105.33
2	G	401	NCN	O1P-P-O5'	3.46	113.76	105.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	401	NCN	8	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	289/305 (94%)	-0.42	4 (1%)	78	74	15, 27, 46, 94	0
1	B	289/305 (94%)	-0.46	5 (1%)	73	68	16, 26, 44, 100	0
1	C	289/305 (94%)	-0.36	8 (2%)	56	49	19, 27, 44, 119	0
1	D	289/305 (94%)	-0.24	5 (1%)	73	68	15, 29, 52, 104	0
1	E	289/305 (94%)	-0.23	4 (1%)	78	74	21, 32, 49, 94	0
1	F	289/305 (94%)	-0.20	8 (2%)	56	49	21, 33, 64, 104	0
1	G	289/305 (94%)	-0.43	3 (1%)	84	81	15, 27, 46, 97	0
1	H	289/305 (94%)	-0.46	5 (1%)	73	68	16, 26, 45, 105	0
1	I	289/305 (94%)	-0.44	4 (1%)	78	74	19, 28, 44, 114	0
1	J	289/305 (94%)	-0.24	6 (2%)	67	61	15, 29, 52, 102	0
1	K	289/305 (94%)	-0.25	2 (0%)	89	87	21, 32, 49, 91	0
1	L	289/305 (94%)	-0.24	6 (2%)	67	61	21, 32, 64, 106	0
All	All	3468/3660 (94%)	-0.33	60 (1%)	73	68	15, 29, 53, 119	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	193	ASP	10.5
1	I	287	ALA	10.1
1	C	1	MET	7.2
1	F	193	ASP	7.1
1	B	1	MET	6.8
1	D	1	MET	6.8
1	I	1	MET	6.7
1	J	1	MET	6.7
1	B	193	ASP	6.6
1	H	1	MET	6.2
1	C	289	GLU	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	287	ALA	6.1
1	H	193	ASP	5.8
1	G	1	MET	5.5
1	A	1	MET	5.2
1	J	193	ASP	4.9
1	I	289	GLU	4.8
1	I	288	LYS	4.6
1	C	194	PHE	4.6
1	L	289	GLU	4.5
1	C	195	ALA	4.4
1	D	193	ASP	4.4
1	F	289	GLU	4.1
1	G	193	ASP	4.1
1	L	288	LYS	3.8
1	B	288	LYS	3.7
1	A	193	ASP	3.7
1	K	1	MET	3.5
1	F	195	ALA	3.5
1	F	288	LYS	3.5
1	E	1	MET	3.4
1	H	288	LYS	3.4
1	J	189	ARG	3.3
1	L	228	GLU	3.2
1	B	289	GLU	3.2
1	C	192	ALA	3.1
1	J	195	ALA	3.1
1	F	228	GLU	3.1
1	E	166	GLY	3.0
1	D	195	ALA	3.0
1	D	186	ARG	3.0
1	E	253	LEU	2.9
1	J	289	GLU	2.7
1	F	194	PHE	2.7
1	C	288	LYS	2.7
1	E	165	GLY	2.6
1	A	126	ARG	2.6
1	H	289	GLU	2.5
1	L	1	MET	2.5
1	F	192	ALA	2.5
1	A	2	ASP	2.5
1	G	126	ARG	2.4
1	L	207	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	194	PHE	2.2
1	B	194	PHE	2.2
1	L	193	ASP	2.2
1	H	194	PHE	2.2
1	F	1	MET	2.1
1	J	194	PHE	2.1
1	K	253	LEU	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^{th} 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^2)	Q<0.9
2	NCN	I	401	22/22	0.98	0.13	0.09	21,24,28,37	0
2	NCN	C	401	22/22	0.97	0.13	-0.01	21,24,27,37	0
2	NCN	G	401	22/22	0.97	0.13	-0.13	19,25,28,37	0
2	NCN	E	401	22/22	0.97	0.12	-0.47	27,31,37,39	0
2	NCN	A	401	22/22	0.98	0.12	-0.57	19,22,28,36	0
2	NCN	K	401	22/22	0.97	0.12	-0.57	26,31,36,40	0
2	NCN	H	401	22/22	0.98	0.11	-0.65	18,24,27,33	0
2	NCN	D	401	22/22	0.97	0.13	-0.69	24,30,37,44	0
2	NCN	J	401	22/22	0.97	0.12	-0.73	23,31,37,45	0
2	NCN	B	401	22/22	0.98	0.11	-0.73	18,23,27,33	0
2	NCN	L	401	22/22	0.97	0.11	-1.16	29,34,39,44	0
2	NCN	F	401	22/22	0.97	0.11	-1.38	31,33,37,43	0

6.5 Other polymers (i)

There are no such residues in this entry.