Full wwPDB EM Validation Report

May 19, 2025 – 04:21 AM EDT

PDB ID	:	6UA2 / pdb_00006ua2
EMDB ID	:	EMD-20704
Title	:	Human IMPDH2 treated with ATP, IMP, NAD+, and 2 mM GTP. Bent (2/4 compressed, 2/4 extended) segment reconstruction.
Authors	:	Johnson, M.C.; Kollman, J.M.
Deposited on	:	2019-09-10
Resolution	:	4.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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:

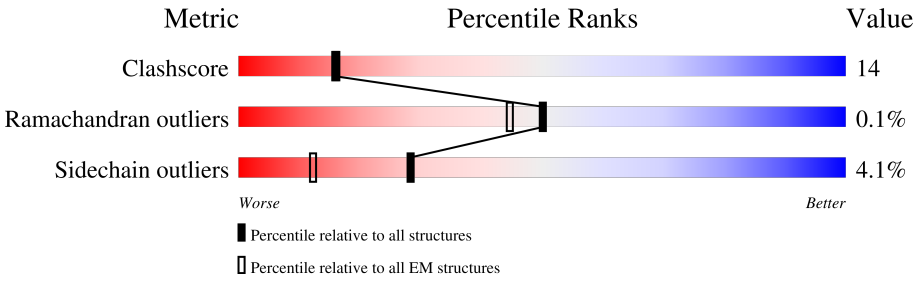
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	519	60% 32% • 6%
1	B	519	64% 28% • 6%
1	C	519	62% 31% • 6%
1	D	519	60% 33% • 6%
1	E	519	61% 31% • 6%
1	F	519	63% 29% • 6%
1	G	519	62% 30% • 6%
1	H	519	61% 32% • 6%

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Mol	Chain	Length	Quality of chain
1	I	519	97%
1	J	519	97%
1	K	519	97%
1	L	519	97%
1	M	519	97%
1	N	519	97%
1	O	519	97%
1	P	519	97%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 31660 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Inosine-5'-monophosphate dehydrogenase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	B	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	C	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	D	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	M	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	N	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	O	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	P	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	E	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	F	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	G	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	H	488	Total	C	N	O	S	0	0
			3710	2340	640	709	21		
1	I	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	J	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	K	14	Total	C	N	O	S	0	0
			102	66	14	21	1		
1	L	14	Total	C	N	O	S	0	0
			102	66	14	21	1		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP P12268
A	-3	GLU	-	expression tag	UNP P12268
A	-2	PHE	-	expression tag	UNP P12268
A	-1	GLU	-	expression tag	UNP P12268
A	0	LEU	-	expression tag	UNP P12268
B	-4	SER	-	expression tag	UNP P12268
B	-3	GLU	-	expression tag	UNP P12268
B	-2	PHE	-	expression tag	UNP P12268
B	-1	GLU	-	expression tag	UNP P12268
B	0	LEU	-	expression tag	UNP P12268
C	-4	SER	-	expression tag	UNP P12268
C	-3	GLU	-	expression tag	UNP P12268
C	-2	PHE	-	expression tag	UNP P12268
C	-1	GLU	-	expression tag	UNP P12268
C	0	LEU	-	expression tag	UNP P12268
D	-4	SER	-	expression tag	UNP P12268
D	-3	GLU	-	expression tag	UNP P12268
D	-2	PHE	-	expression tag	UNP P12268
D	-1	GLU	-	expression tag	UNP P12268
D	0	LEU	-	expression tag	UNP P12268
M	-4	SER	-	expression tag	UNP P12268
M	-3	GLU	-	expression tag	UNP P12268
M	-2	PHE	-	expression tag	UNP P12268
M	-1	GLU	-	expression tag	UNP P12268
M	0	LEU	-	expression tag	UNP P12268
N	-4	SER	-	expression tag	UNP P12268
N	-3	GLU	-	expression tag	UNP P12268
N	-2	PHE	-	expression tag	UNP P12268
N	-1	GLU	-	expression tag	UNP P12268
N	0	LEU	-	expression tag	UNP P12268
O	-4	SER	-	expression tag	UNP P12268
O	-3	GLU	-	expression tag	UNP P12268
O	-2	PHE	-	expression tag	UNP P12268
O	-1	GLU	-	expression tag	UNP P12268
O	0	LEU	-	expression tag	UNP P12268
P	-4	SER	-	expression tag	UNP P12268
P	-3	GLU	-	expression tag	UNP P12268
P	-2	PHE	-	expression tag	UNP P12268
P	-1	GLU	-	expression tag	UNP P12268
P	0	LEU	-	expression tag	UNP P12268
E	-4	SER	-	expression tag	UNP P12268
E	-3	GLU	-	expression tag	UNP P12268
E	-2	PHE	-	expression tag	UNP P12268

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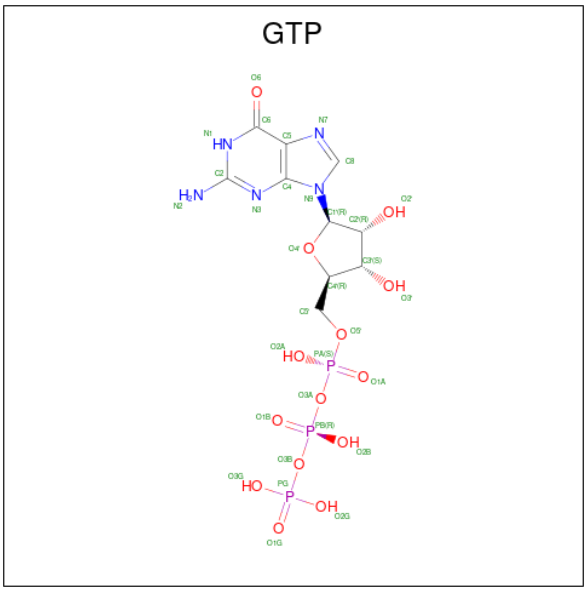
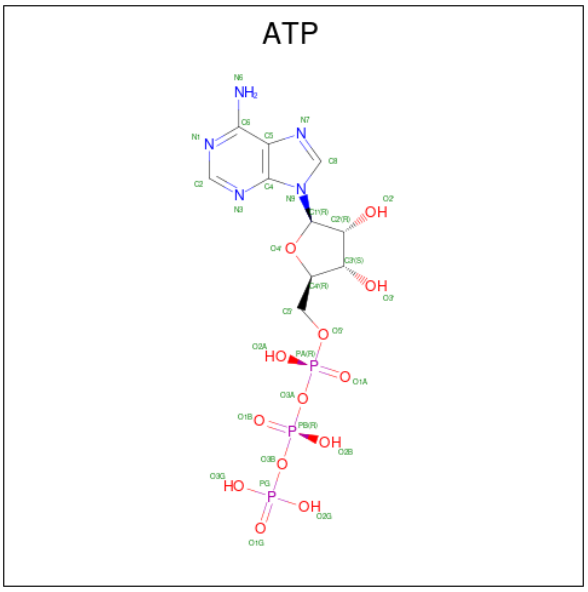
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLU	-	expression tag	UNP P12268
E	0	LEU	-	expression tag	UNP P12268
F	-4	SER	-	expression tag	UNP P12268
F	-3	GLU	-	expression tag	UNP P12268
F	-2	PHE	-	expression tag	UNP P12268
F	-1	GLU	-	expression tag	UNP P12268
F	0	LEU	-	expression tag	UNP P12268
G	-4	SER	-	expression tag	UNP P12268
G	-3	GLU	-	expression tag	UNP P12268
G	-2	PHE	-	expression tag	UNP P12268
G	-1	GLU	-	expression tag	UNP P12268
G	0	LEU	-	expression tag	UNP P12268
H	-4	SER	-	expression tag	UNP P12268
H	-3	GLU	-	expression tag	UNP P12268
H	-2	PHE	-	expression tag	UNP P12268
H	-1	GLU	-	expression tag	UNP P12268
H	0	LEU	-	expression tag	UNP P12268
I	-4	SER	-	expression tag	UNP P12268
I	-3	GLU	-	expression tag	UNP P12268
I	-2	PHE	-	expression tag	UNP P12268
I	-1	GLU	-	expression tag	UNP P12268
I	0	LEU	-	expression tag	UNP P12268
J	-4	SER	-	expression tag	UNP P12268
J	-3	GLU	-	expression tag	UNP P12268
J	-2	PHE	-	expression tag	UNP P12268
J	-1	GLU	-	expression tag	UNP P12268
J	0	LEU	-	expression tag	UNP P12268
K	-4	SER	-	expression tag	UNP P12268
K	-3	GLU	-	expression tag	UNP P12268
K	-2	PHE	-	expression tag	UNP P12268
K	-1	GLU	-	expression tag	UNP P12268
K	0	LEU	-	expression tag	UNP P12268
L	-4	SER	-	expression tag	UNP P12268
L	-3	GLU	-	expression tag	UNP P12268
L	-2	PHE	-	expression tag	UNP P12268
L	-1	GLU	-	expression tag	UNP P12268
L	0	LEU	-	expression tag	UNP P12268

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



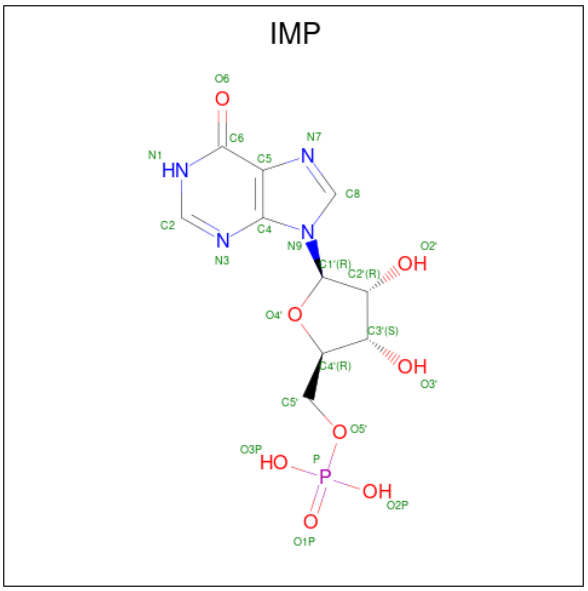
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	F	1	Total	C	N	O	P	0
			32	10	5	14	3	
2	F	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



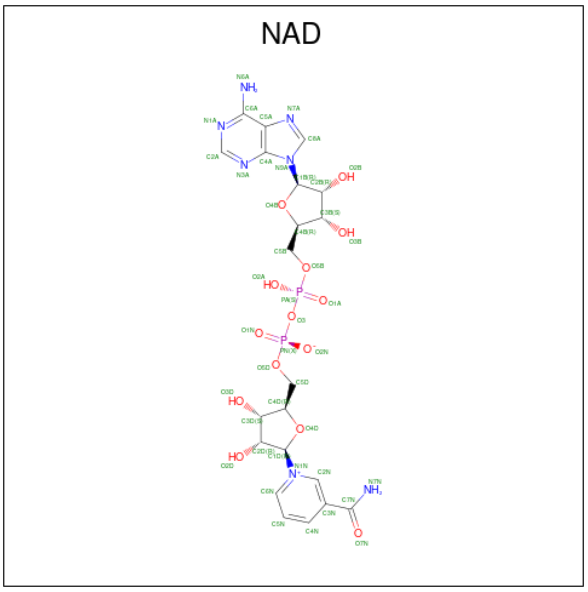
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
3	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 4 is INOSINIC ACID (CCD ID: IMP) (formula: $C_{10}H_{13}N_4O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	B	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	C	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	D	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	E	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	F	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	G	1	Total	C	N	O	P	0
			23	10	4	8	1	
4	H	1	Total	C	N	O	P	0
			23	10	4	8	1	

- Molecule 5 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



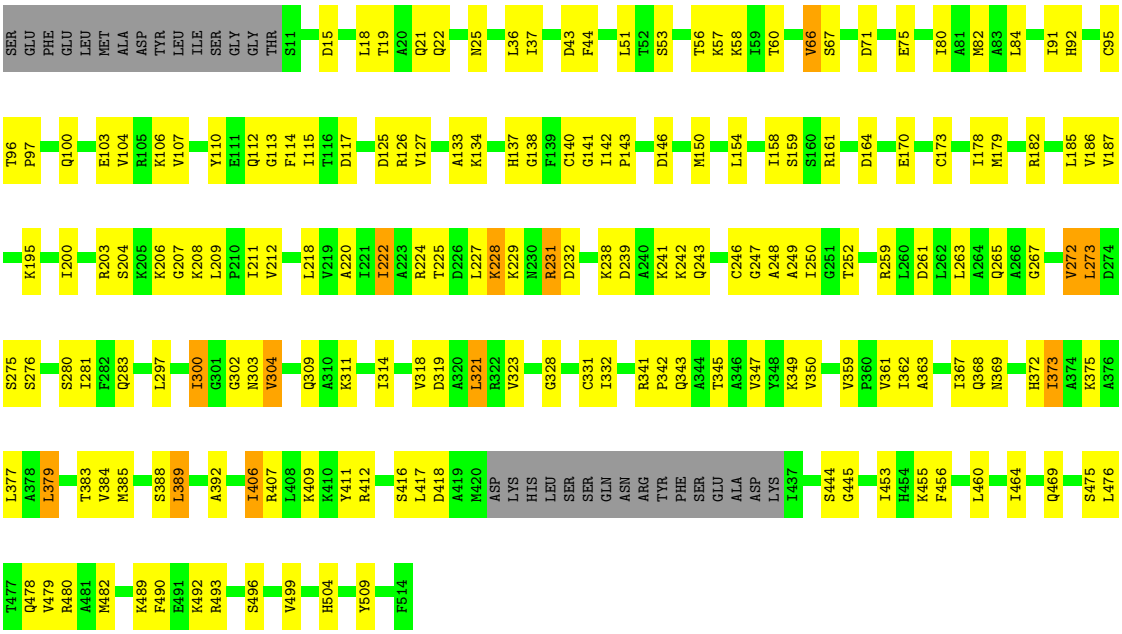
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	B	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	C	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	D	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	E	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	F	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	G	1	Total	C	N	O	P	0
			44	21	7	14	2	
5	H	1	Total	C	N	O	P	0
			44	21	7	14	2	

3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

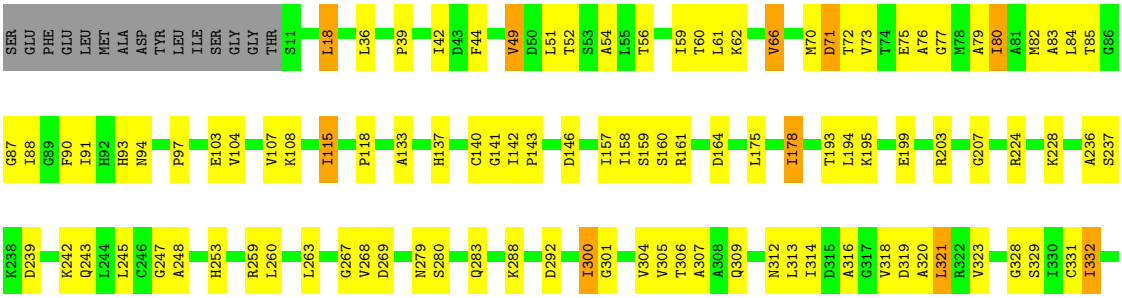
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

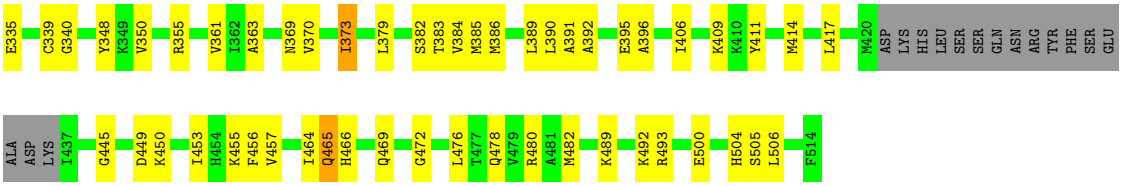
Chain A:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

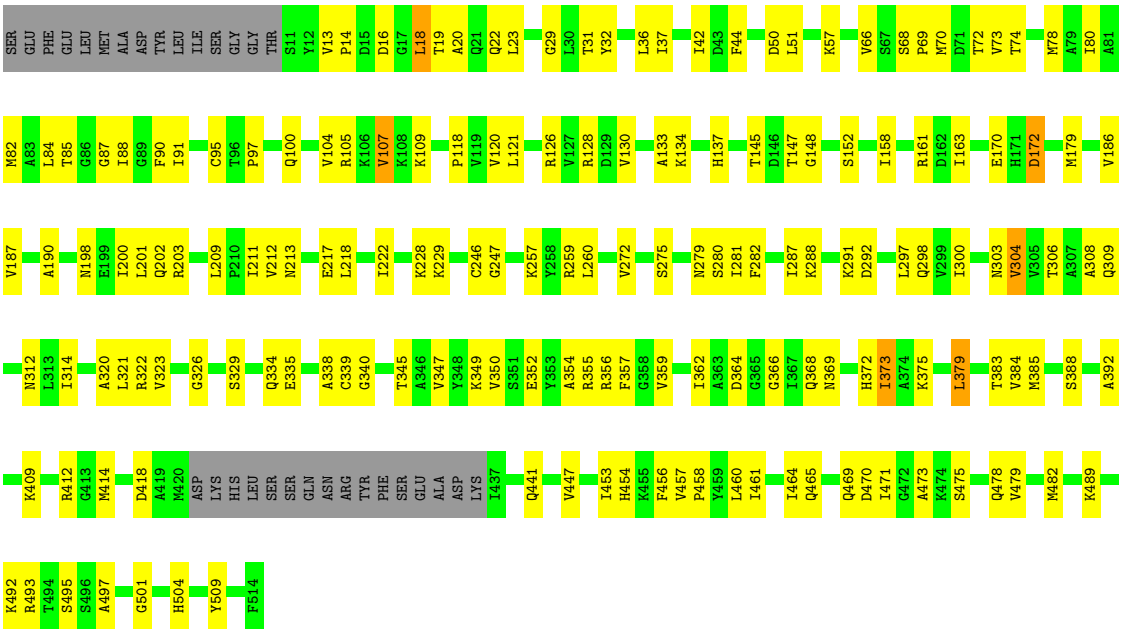
Chain B:





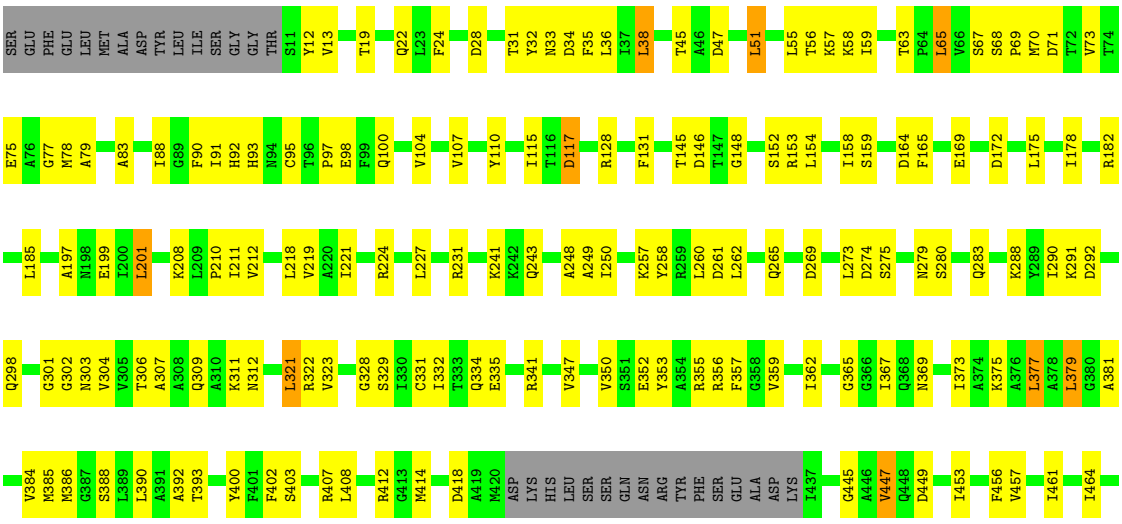
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

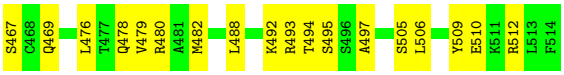
Chain C:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

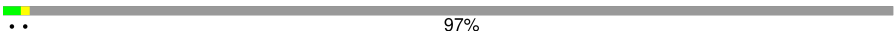
Chain D:

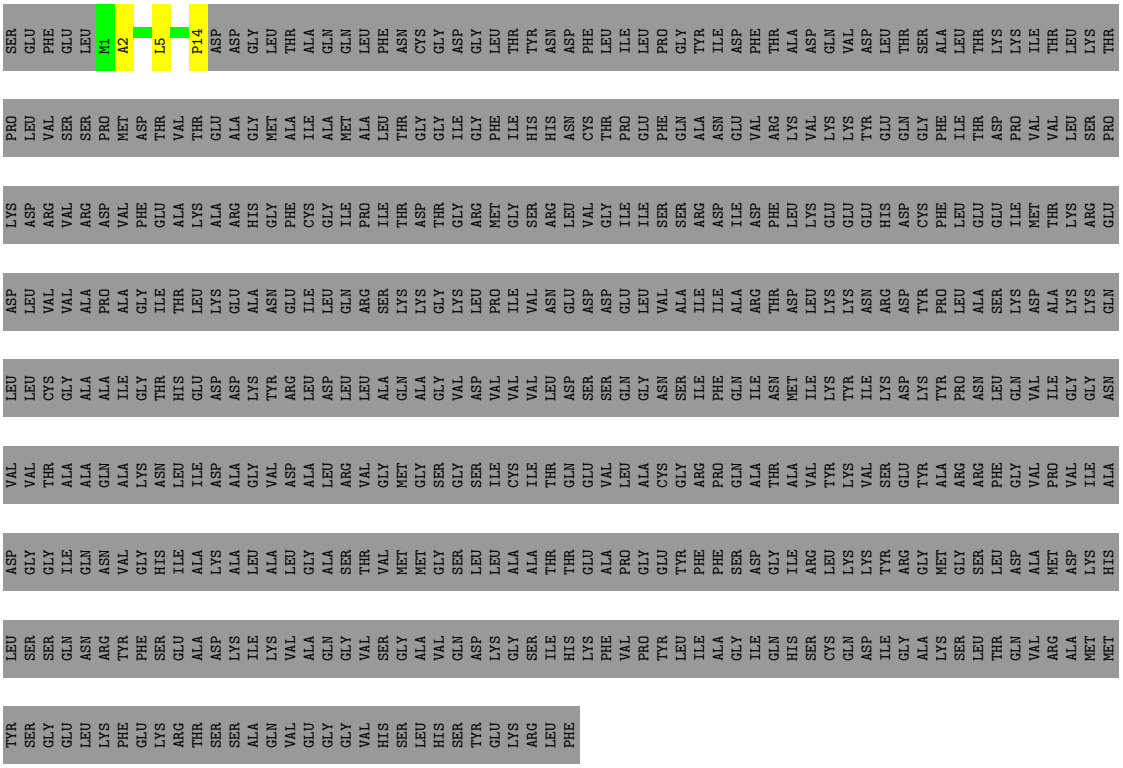




• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

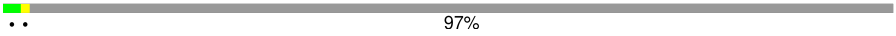
Chain M:

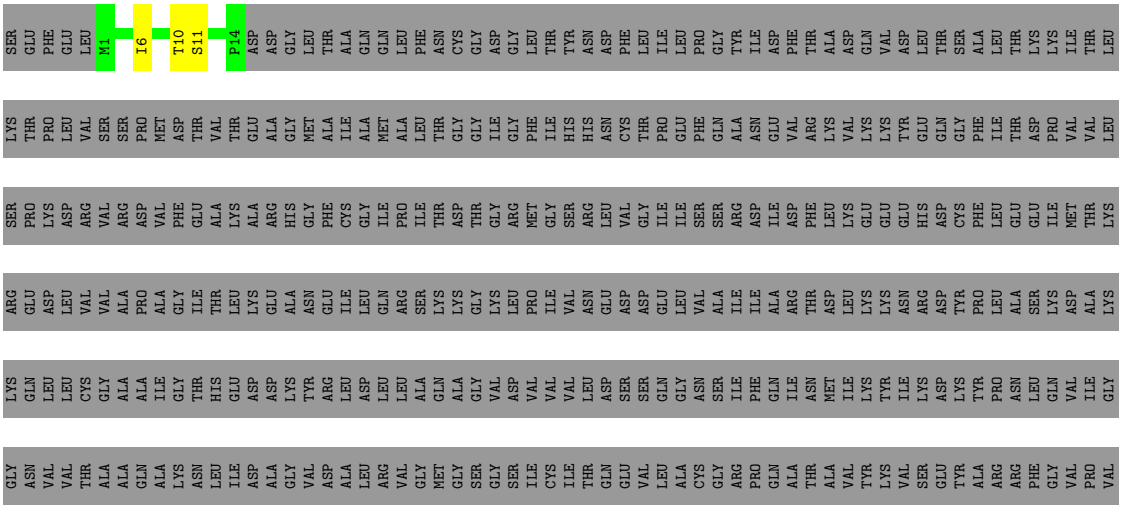


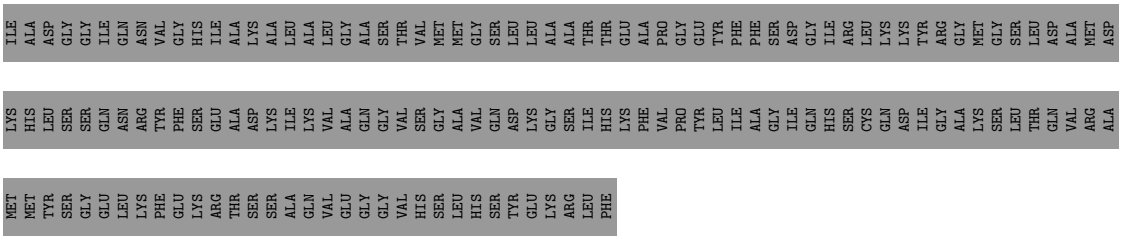


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain N:

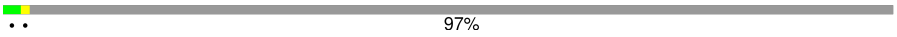






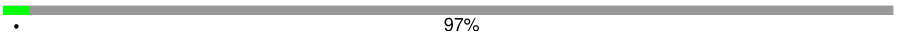
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

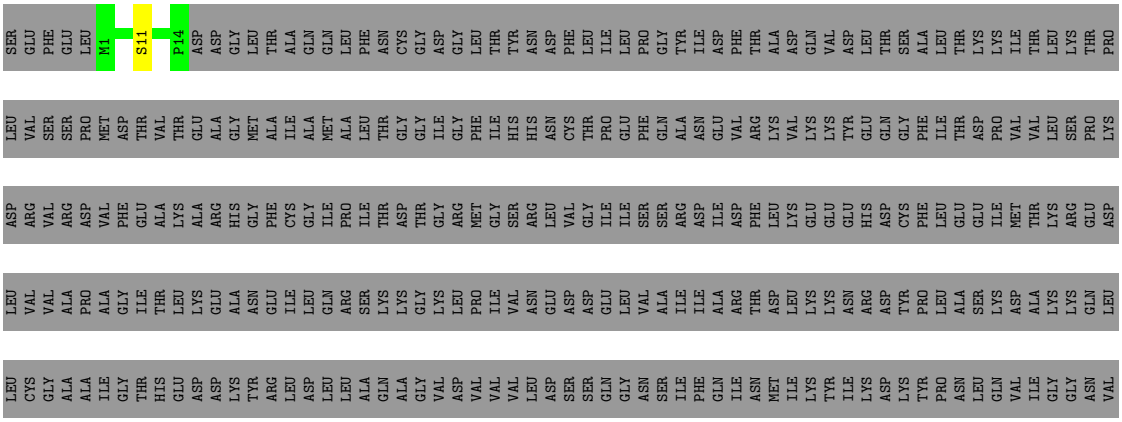
Chain O:

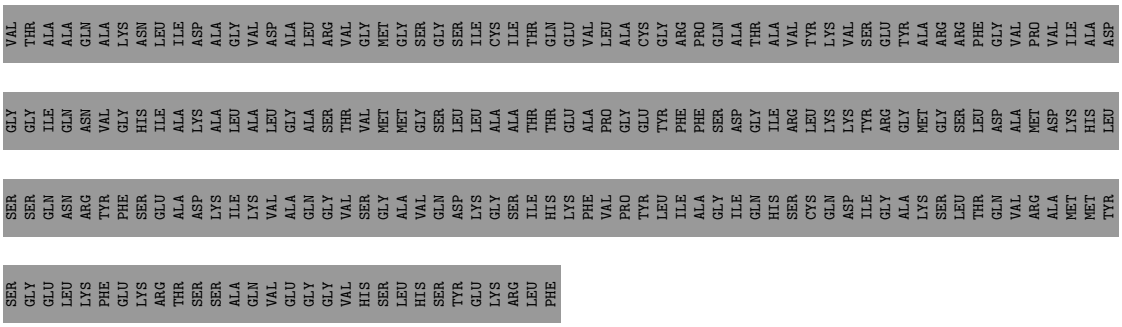


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain P:

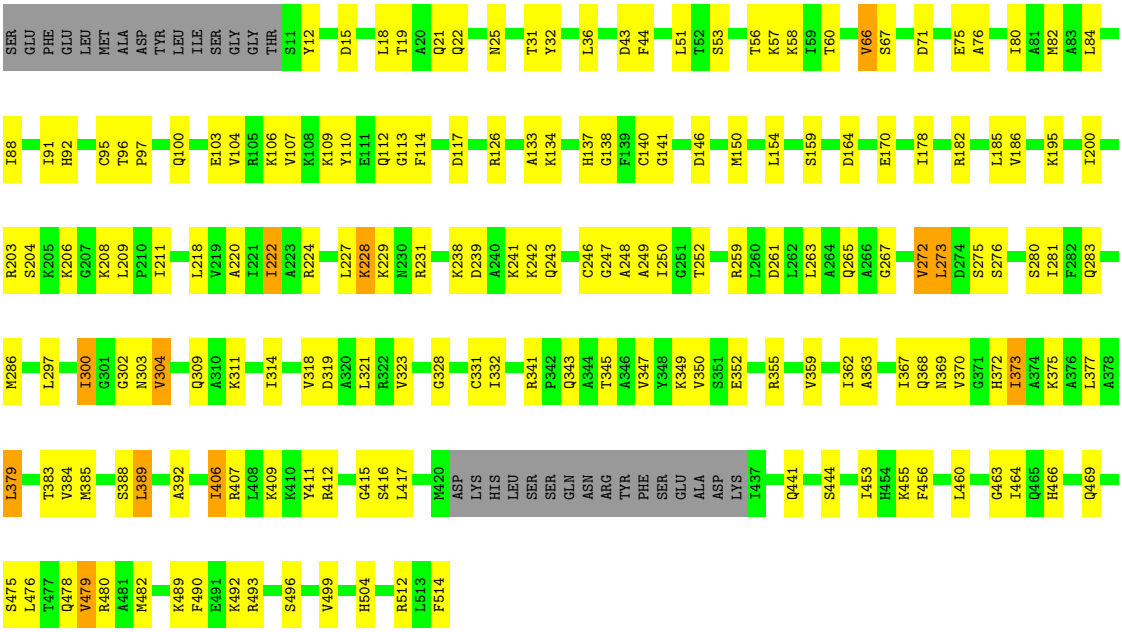






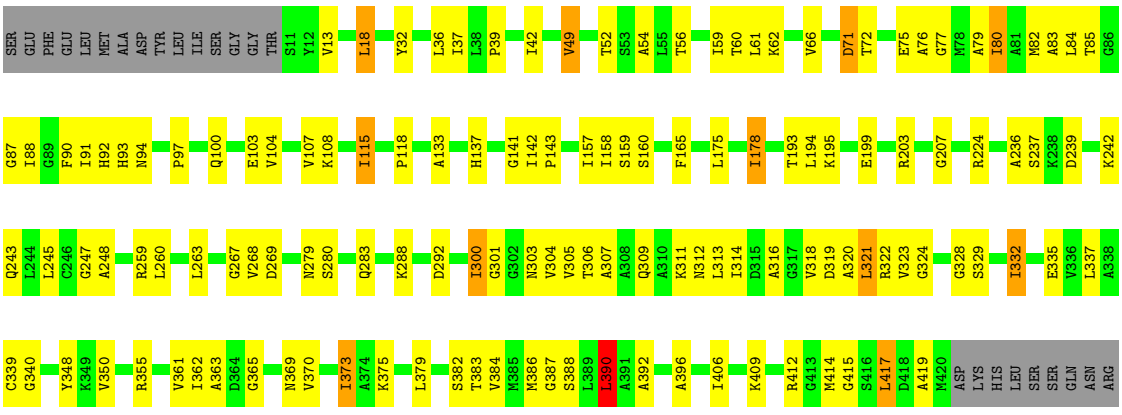
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain E:



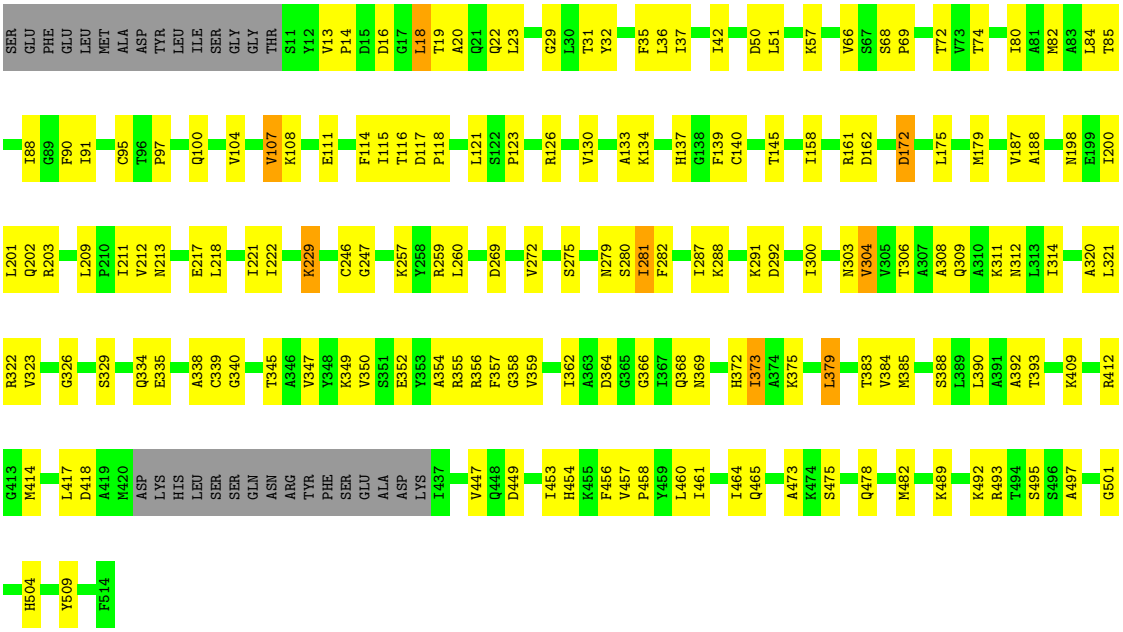
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain F:



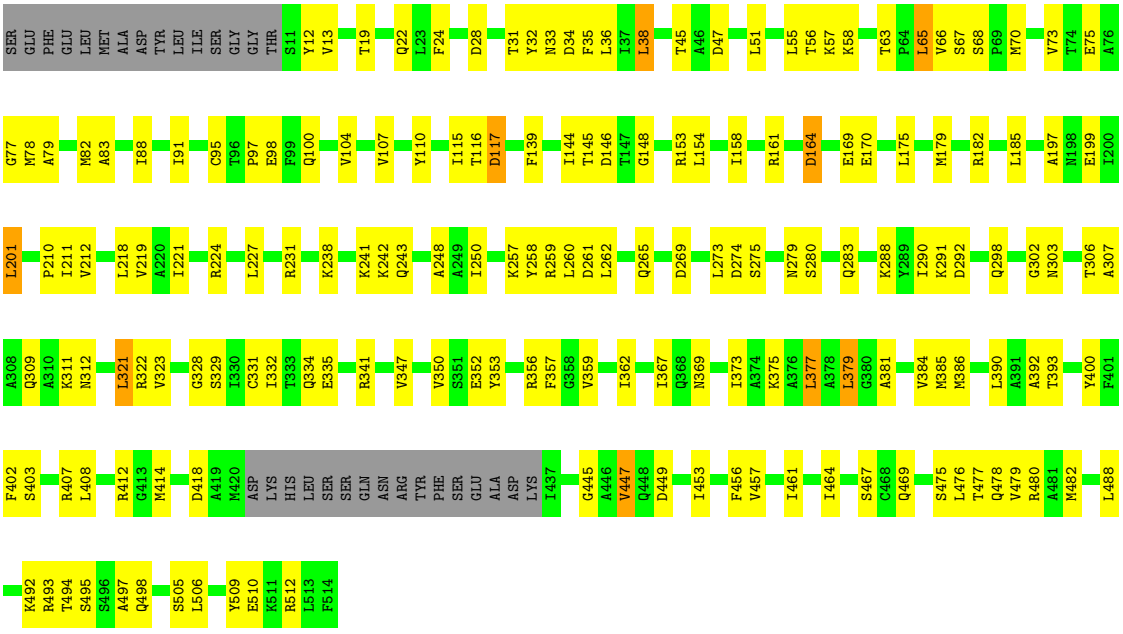
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain G:



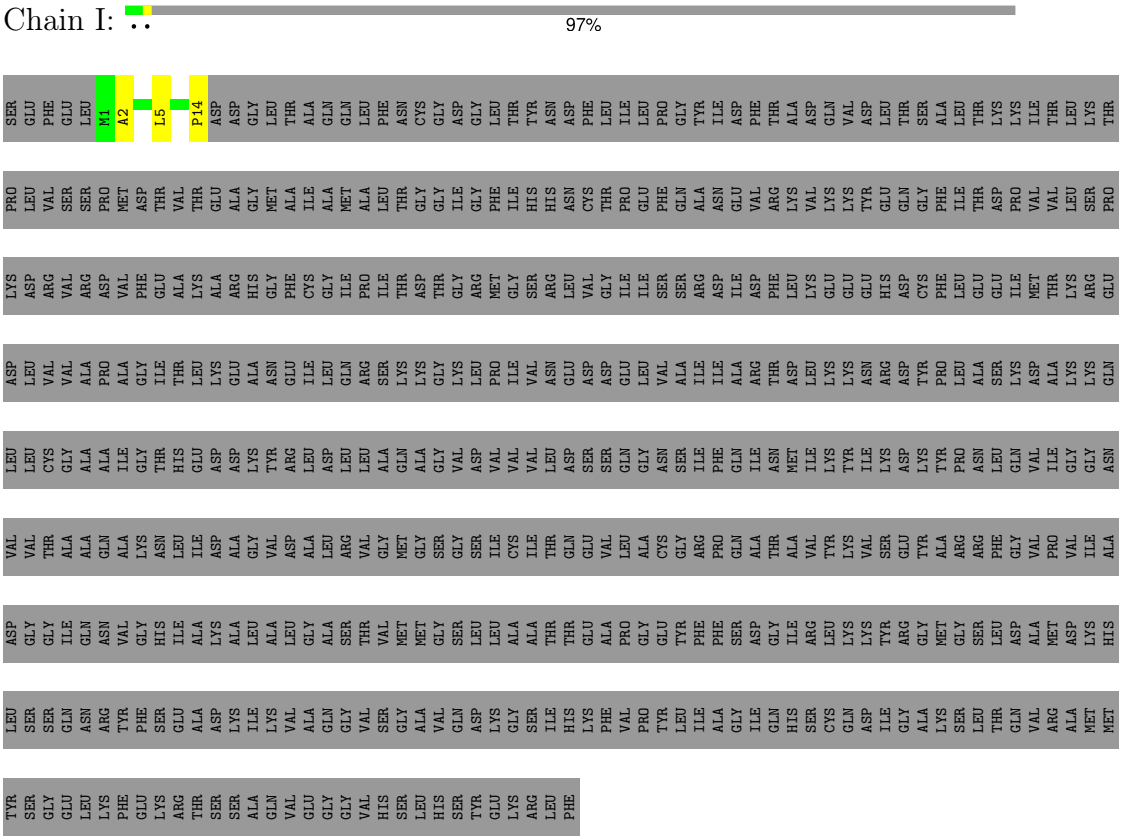
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain H:



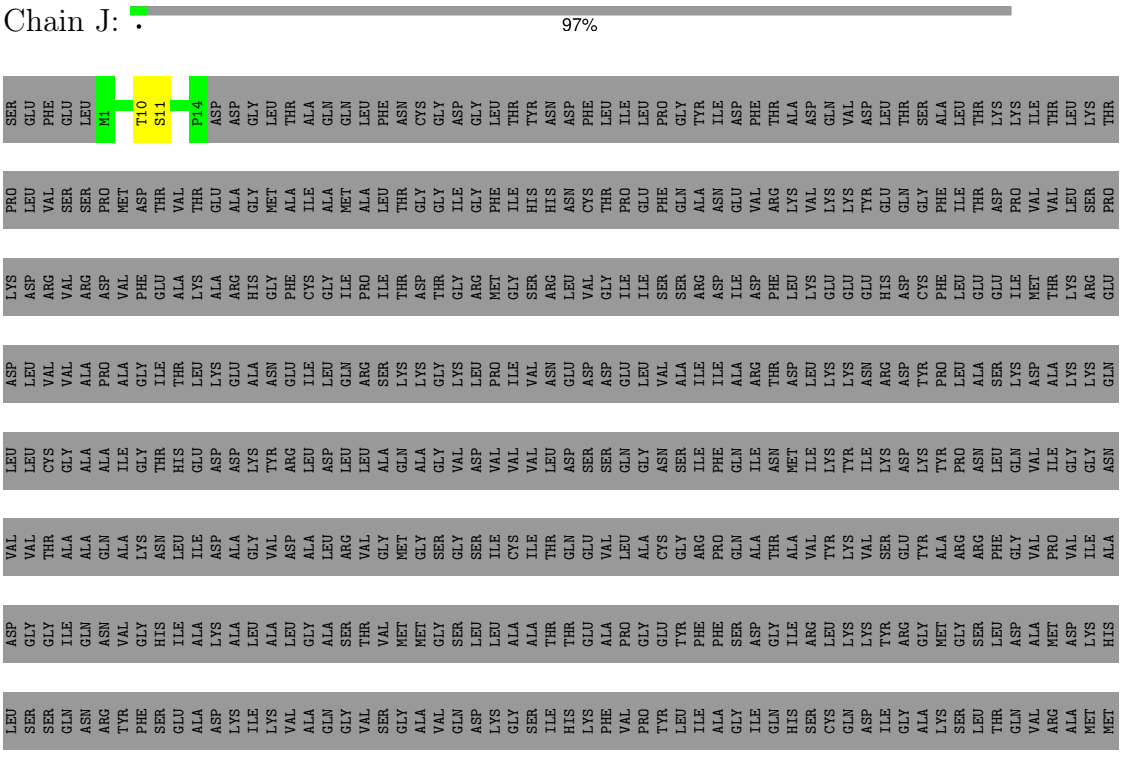
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain I:



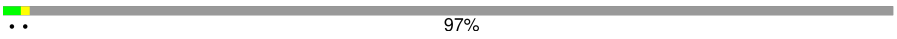
• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

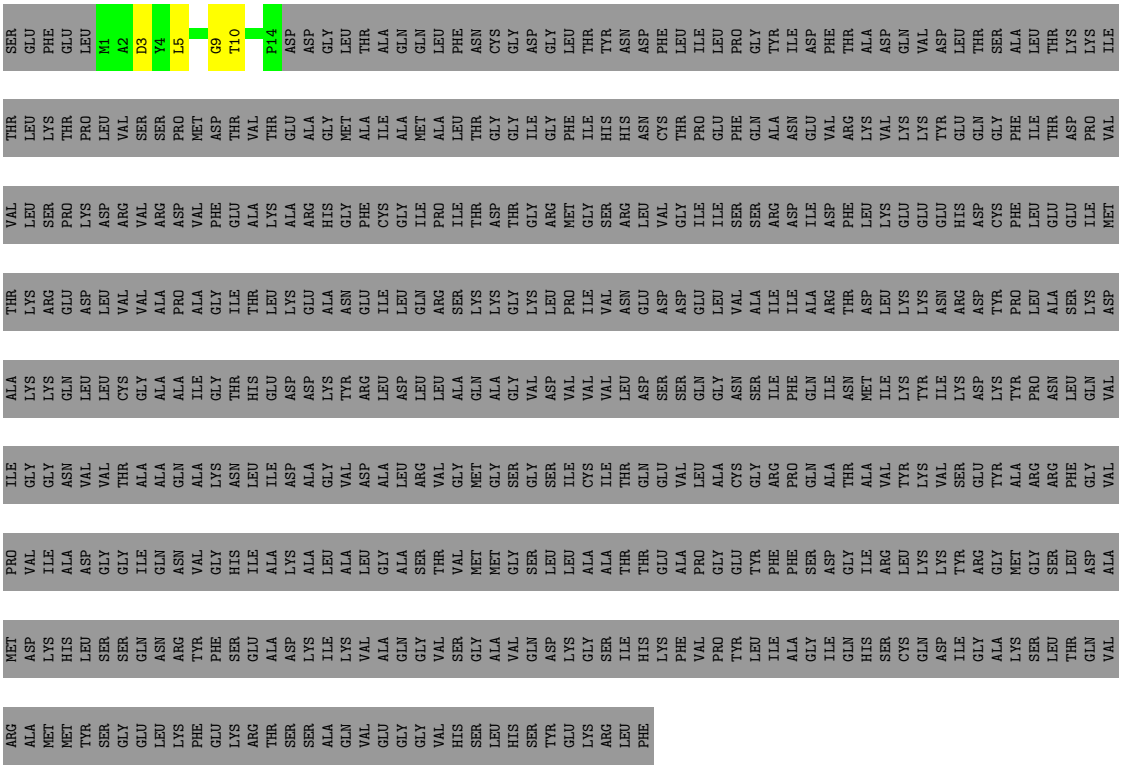
Chain J:



• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

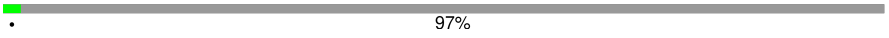
Chain K:

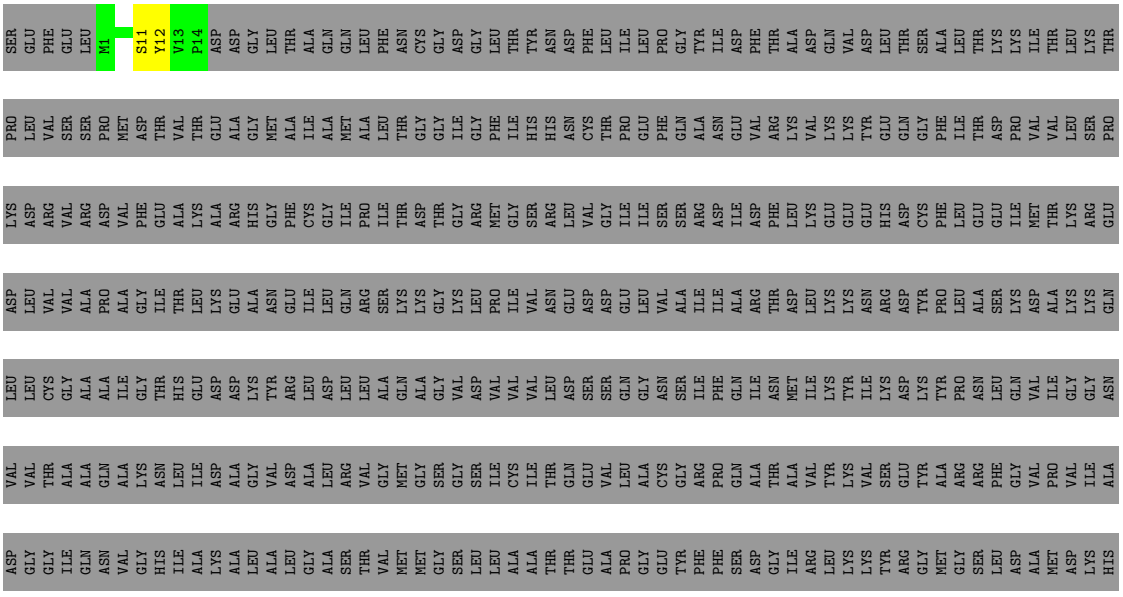


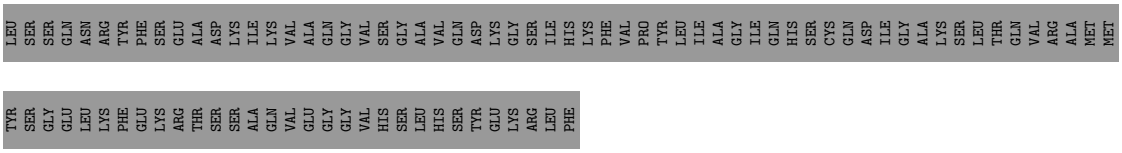


• Molecule 1: Inosine-5'-monophosphate dehydrogenase 2

Chain L:






LEU SER SER GLN ASN ARG TYR PHE SER GLU ALA ASP LYS ILE LYS VAL ALA GLN GLY VAL SER GLY ALA VAL GLN ASP LYS GLY SER ILE HIS LYS PHE VAL PRO TYR LEU ILE ALA GLY ILE GLN HIS SER CYS GLN ASP ILE GLY ALA LYS SER LEU THR GLN VAL ARG ALA MET MET
TYR SER GLY GLU LEU LYS PHE GLU LYS ARG THR SER SER ALA GLN VAL GLU GLY GLY VAL HIS SER LEU HIS SER TYR GLU LYS ARG LEU PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	31660	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	80.505	Depositor
Minimum map value	-55.496	Depositor
Average map value	0.091	Depositor
Map value standard deviation	2.383	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

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: GTP, IMP, ATP, NAD

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	0.50	1/3766 (0.0%)	0.80	0/5078
1	B	0.52	0/3766	0.84	0/5078
1	C	0.44	0/3766	0.78	1/5078 (0.0%)
1	D	0.43	0/3766	0.82	2/5078 (0.0%)
1	E	0.50	0/3766	0.80	0/5078
1	F	0.51	0/3766	0.83	0/5078
1	G	0.43	0/3766	0.77	1/5078 (0.0%)
1	H	0.43	0/3766	0.81	4/5078 (0.1%)
1	I	0.39	0/104	1.07	0/141
1	J	0.30	0/104	0.95	0/141
1	K	0.39	0/104	1.25	0/141
1	L	0.30	0/104	0.99	0/141
1	M	0.39	0/104	1.05	0/141
1	N	0.29	0/104	0.90	0/141
1	O	0.36	0/104	1.23	0/141
1	P	0.30	0/104	0.98	0/141
All	All	0.47	1/30960 (0.0%)	0.82	8/41752 (0.0%)

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	C	0	3
1	D	0	2
1	E	0	1
1	F	0	1
1	G	0	2
1	H	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
1	K	0	1
1	L	0	1
1	N	0	1
1	O	0	1
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ILE	C-N	-5.04	1.24	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	67	SER	CA-C-N	14.43	140.28	120.65
1	D	67	SER	C-N-CA	14.43	140.28	120.65
1	H	67	SER	CA-C-N	11.17	136.35	120.49
1	H	67	SER	C-N-CA	11.17	136.35	120.49
1	G	172	ASP	N-CA-C	5.08	118.33	111.17
1	C	172	ASP	N-CA-C	5.01	118.24	111.17
1	H	116	THR	CA-C-N	5.01	134.03	121.80
1	H	116	THR	C-N-CA	5.01	134.03	121.80

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	ARG	Peptide
1	C	107	VAL	Peptide
1	C	364	ASP	Peptide
1	C	470	ASP	Peptide
1	D	117	ASP	Peptide
1	D	164	ASP	Peptide
1	E	407	ARG	Peptide
1	F	390	LEU	Peptide
1	G	107	VAL	Peptide
1	G	364	ASP	Peptide
1	H	117	ASP	Peptide
1	H	164	ASP	Peptide
1	J	11	SER	Peptide

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Mol	Chain	Res	Type	Group
1	K	9	GLY	Peptide
1	L	12	TYR	Peptide
1	N	11	SER	Peptide
1	O	9	GLY	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	3710	0	3766	126	0
1	B	3710	0	3766	113	0
1	C	3710	0	3764	115	0
1	D	3710	0	3764	124	0
1	E	3710	0	3766	125	0
1	F	3710	0	3766	120	0
1	G	3710	0	3763	115	0
1	H	3710	0	3764	118	0
1	I	102	0	99	2	0
1	J	102	0	99	0	0
1	K	102	0	99	2	0
1	L	102	0	99	1	0
1	M	102	0	99	2	0
1	N	102	0	99	1	0
1	O	102	0	99	4	0
1	P	102	0	99	1	0
2	A	64	0	24	10	0
2	B	64	0	22	5	0
2	E	64	0	24	7	0
2	F	64	0	22	4	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
3	C	93	0	36	4	0
3	D	31	0	12	1	0
3	E	31	0	12	2	0
3	F	31	0	12	0	0
3	G	93	0	35	3	0
3	H	31	0	12	2	0
4	A	23	0	11	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	23	0	11	1	0
4	C	23	0	11	4	0
4	D	23	0	10	4	0
4	E	23	0	11	2	0
4	F	23	0	11	3	0
4	G	23	0	11	3	0
4	H	23	0	10	3	0
5	A	44	0	24	2	0
5	B	44	0	24	1	0
5	C	44	0	24	1	0
5	D	44	0	24	2	0
5	E	44	0	24	2	0
5	F	44	0	24	0	0
5	G	44	0	24	1	0
5	H	44	0	24	2	0
All	All	31660	0	31424	896	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 14.

All (896) 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:G:375:LYS:O	1:G:379:LEU:HB2	1.62	0.99
1:C:375:LYS:O	1:C:379:LEU:HB2	1.62	0.99
1:B:56:THR:HG1	1:B:59:ILE:H	1.32	0.76
1:F:56:THR:HG1	1:F:59:ILE:H	1.32	0.76
1:E:112:GLN:HE22	2:E:601:GTP:H2'	1.52	0.74
1:B:104:VAL:HA	1:B:107:VAL:HG12	1.71	0.72
1:H:75:GLU:HG2	1:H:77:GLY:H	1.54	0.72
1:D:79:ALA:O	1:D:83:ALA:HB2	1.88	0.72
1:F:386:MET:HB3	1:F:390:LEU:HD21	1.71	0.72
1:F:104:VAL:HA	1:F:107:VAL:HG12	1.72	0.72
1:H:79:ALA:O	1:H:83:ALA:HB2	1.90	0.71
1:A:311:LYS:HE2	1:D:13:VAL:H	1.55	0.71
1:A:362:ILE:HG22	1:A:383:THR:HB	1.74	0.70
1:E:362:ILE:HG22	1:E:383:THR:HB	1.73	0.70
1:E:311:LYS:HE2	1:H:13:VAL:H	1.57	0.69
1:D:95:CYS:SG	1:D:100:GLN:NE2	2.65	0.69
1:B:18:LEU:H	1:B:489:LYS:HB3	1.57	0.69
1:B:104:VAL:HG21	1:B:268:VAL:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:VAL:HG21	1:F:268:VAL:HG22	1.74	0.68
1:D:75:GLU:HG2	1:D:77:GLY:H	1.58	0.68
1:H:482:MET:HG3	1:H:488:LEU:HB2	1.76	0.68
1:A:195:LYS:HD3	2:A:602:GTP:H4'	1.75	0.67
1:H:386:MET:HG3	1:H:390:LEU:HD22	1.76	0.67
1:B:280:SER:H	1:B:283:GLN:HE21	1.42	0.67
1:E:186:VAL:H	1:E:206:LYS:HZ1	1.41	0.66
1:H:95:CYS:SG	1:H:100:GLN:NE2	2.68	0.66
1:G:19:THR:H	1:G:22:GLN:HE21	1.44	0.66
1:D:58:LYS:HB2	1:D:298:GLN:HE22	1.59	0.66
1:A:112:GLN:HE22	2:A:601:GTP:H2'	1.61	0.66
1:F:280:SER:H	1:F:283:GLN:HE21	1.43	0.65
1:C:19:THR:H	1:C:22:GLN:HE21	1.44	0.65
1:C:13:VAL:H	1:D:311:LYS:HE2	1.61	0.65
1:H:58:LYS:HB2	1:H:298:GLN:HE22	1.61	0.65
1:B:75:GLU:HG2	1:B:77:GLY:H	1.62	0.65
1:G:323:VAL:HG21	1:G:350:VAL:HG21	1.78	0.65
1:D:412:ARG:HD2	1:D:418:ASP:HB3	1.78	0.64
1:F:94:ASN:ND2	1:F:414:MET:SD	2.70	0.64
1:H:412:ARG:HD2	1:H:418:ASP:HB3	1.78	0.64
1:B:478:GLN:O	1:B:482:MET:HB2	1.97	0.64
1:D:165:PHE:HB3	1:G:202:GLN:HG2	1.80	0.64
1:C:345:THR:OG1	1:C:349:LYS:NZ	2.31	0.64
1:C:323:VAL:HG21	1:C:350:VAL:HG21	1.78	0.64
1:D:283:GLN:HE22	1:D:302:GLY:H	1.44	0.64
1:H:68:SER:OG	1:H:70:MET:SD	2.56	0.64
1:B:143:PRO:HA	1:B:157:ILE:HA	1.79	0.64
1:G:345:THR:OG1	1:G:349:LYS:NZ	2.31	0.64
1:F:143:PRO:HA	1:F:157:ILE:HA	1.80	0.63
1:G:300:ILE:HG22	1:G:320:ALA:HB3	1.78	0.63
1:D:68:SER:OG	1:D:70:MET:SD	2.57	0.63
1:B:94:ASN:ND2	1:B:414:MET:SD	2.72	0.63
1:D:482:MET:HG3	1:D:488:LEU:HB2	1.81	0.63
1:F:321:LEU:HD12	1:F:361:VAL:HG12	1.81	0.63
1:C:72:THR:HG21	1:C:412:ARG:HB3	1.79	0.62
1:D:19:THR:HG22	1:D:22:GLN:HG2	1.79	0.62
1:D:386:MET:HG3	1:D:390:LEU:HD22	1.81	0.62
1:F:75:GLU:HG2	1:F:77:GLY:H	1.64	0.62
1:G:95:CYS:SG	1:G:100:GLN:NE2	2.72	0.62
1:A:478:GLN:O	1:A:482:MET:HB2	1.99	0.62
1:H:283:GLN:HE22	1:H:302:GLY:H	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:501:GLY:O	1:H:334:GLN:NE2	2.33	0.62
1:H:19:THR:HG22	1:H:22:GLN:HG2	1.79	0.62
1:E:110:TYR:O	1:E:229:LYS:NZ	2.32	0.61
1:F:512:ARG:HH22	1:G:417:LEU:HD11	1.65	0.61
1:E:80:ILE:O	1:E:84:LEU:HB2	2.00	0.61
1:C:300:ILE:HG22	1:C:320:ALA:HB3	1.82	0.61
1:D:323:VAL:HG21	1:D:350:VAL:HG21	1.82	0.61
1:D:201:LEU:HD11	1:D:224:ARG:HG3	1.80	0.61
1:D:211:ILE:HG23	1:D:219:VAL:HG23	1.82	0.61
1:E:208:LYS:NZ	3:E:603:ATP:O2B	2.34	0.61
1:F:52:THR:HA	1:F:62:LYS:HA	1.81	0.61
1:B:52:THR:HA	1:B:62:LYS:HA	1.82	0.61
1:C:501:GLY:O	1:D:334:GLN:NE2	2.34	0.60
1:A:110:TYR:O	1:A:229:LYS:NZ	2.34	0.60
1:A:241:LYS:HE3	1:A:243:GLN:HE22	1.65	0.60
1:H:323:VAL:HG21	1:H:350:VAL:HG21	1.81	0.60
1:B:369:ASN:ND2	1:C:335:GLU:O	2.34	0.60
1:B:321:LEU:HD12	1:B:361:VAL:HG12	1.83	0.60
1:E:246:CYS:SG	1:E:247:GLY:N	2.75	0.60
1:E:341:ARG:HH21	1:E:345:THR:HB	1.67	0.60
1:E:141:GLY:H	2:E:601:GTP:HN21	1.50	0.60
1:G:13:VAL:H	1:H:311:LYS:HE2	1.66	0.60
1:E:252:THR:O	5:E:605:NAD:N6A	2.35	0.60
1:E:228:LYS:HA	1:E:231:ARG:HG2	1.82	0.60
1:G:133:ALA:O	1:G:137:HIS:ND1	2.34	0.60
1:H:169:GLU:HG2	1:H:170:GLU:HG2	1.84	0.60
1:E:241:LYS:HE3	1:E:243:GLN:HE22	1.66	0.59
1:B:314:ILE:HA	1:B:318:VAL:HG12	1.84	0.59
1:D:261:ASP:O	1:D:265:GLN:NE2	2.36	0.59
1:F:76:ALA:O	1:F:80:ILE:HB	2.01	0.59
1:A:252:THR:O	5:A:605:NAD:N6A	2.34	0.59
1:D:32:TYR:HB3	1:D:375:LYS:HE3	1.83	0.59
1:A:302:GLY:HA2	1:A:304:VAL:HG12	1.83	0.59
1:C:414:MET:SD	1:C:414:MET:N	2.70	0.59
1:E:369:ASN:ND2	1:F:335:GLU:O	2.36	0.59
1:F:373:ILE:HD11	1:F:464:ILE:HG21	1.84	0.59
1:A:126:ARG:NH2	1:A:170:GLU:OE2	2.35	0.59
1:D:57:LYS:NZ	1:D:357:PHE:O	2.35	0.59
1:B:304:VAL:HG23	1:B:309:GLN:HG2	1.82	0.59
1:B:373:ILE:HD11	1:B:464:ILE:HG21	1.85	0.59
1:C:161:ARG:O	1:H:224:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:TYR:HB3	1:H:375:LYS:HE3	1.84	0.59
1:H:261:ASP:O	1:H:265:GLN:NE2	2.36	0.59
1:H:288:LYS:HD3	1:H:291:LYS:HZ3	1.68	0.59
1:H:480:ARG:NH2	1:K:5:LEU:O	2.35	0.59
1:A:369:ASN:ND2	1:B:335:GLU:O	2.36	0.59
1:D:328:GLY:N	1:D:331:CYS:SG	2.75	0.59
1:E:302:GLY:HA2	1:E:304:VAL:HG12	1.83	0.59
1:F:314:ILE:HA	1:F:318:VAL:HG12	1.84	0.59
1:H:57:LYS:NZ	1:H:357:PHE:O	2.36	0.59
1:A:368:GLN:HE22	1:D:505:SER:HB3	1.68	0.59
1:B:76:ALA:N	1:B:103:GLU:OE2	2.36	0.59
1:D:279:ASN:HD21	1:D:312:ASN:HD21	1.49	0.59
1:D:414:MET:SD	1:D:414:MET:N	2.76	0.59
1:D:480:ARG:NH2	1:O:5:LEU:O	2.35	0.59
1:H:279:ASN:HD21	1:H:312:ASN:HD21	1.49	0.59
1:D:288:LYS:HD3	1:D:291:LYS:HZ3	1.68	0.58
1:E:368:GLN:HE22	1:H:505:SER:HB3	1.68	0.58
1:F:304:VAL:HG23	1:F:309:GLN:HG2	1.83	0.58
1:H:478:GLN:O	1:H:482:MET:HB2	2.03	0.58
1:A:126:ARG:HG2	1:A:170:GLU:HG2	1.85	0.58
1:F:369:ASN:ND2	1:G:335:GLU:O	2.36	0.58
1:G:414:MET:SD	1:G:414:MET:N	2.71	0.58
1:C:147:THR:HG1	1:C:152:SER:HG	1.48	0.58
1:D:241:LYS:NZ	1:D:243:GLN:OE1	2.36	0.58
1:D:279:ASN:HD22	1:D:309:GLN:HG2	1.68	0.58
1:A:246:CYS:SG	1:A:247:GLY:N	2.77	0.58
1:B:115:ILE:HD11	1:B:118:PRO:HB3	1.86	0.58
1:C:412:ARG:HD2	1:C:418:ASP:HB3	1.84	0.58
1:E:347:VAL:HG23	1:E:379:LEU:HD12	1.85	0.58
1:E:367:ILE:HG23	1:E:372:HIS:HB2	1.85	0.58
1:H:70:MET:HB2	1:H:73:VAL:HG12	1.85	0.58
1:B:49:VAL:HG13	1:B:465:GLN:HB2	1.86	0.58
1:F:269:ASP:OD1	1:F:269:ASP:N	2.36	0.58
1:G:304:VAL:HG13	1:G:323:VAL:HG23	1.85	0.57
1:F:18:LEU:H	1:F:489:LYS:HB3	1.69	0.57
1:G:304:VAL:HG23	1:G:309:GLN:HB2	1.85	0.57
1:C:304:VAL:HG13	1:C:323:VAL:HG23	1.85	0.57
1:E:200:ILE:O	1:E:204:SER:HB3	2.04	0.57
2:A:601:GTP:O2B	2:A:601:GTP:N2	2.38	0.57
1:A:96:THR:O	1:A:100:GLN:NE2	2.38	0.57
1:A:275:SER:O	1:A:303:ASN:ND2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:PRO:HA	3:C:602:ATP:HN62	1.69	0.57
1:G:16:ASP:OD2	1:H:341:ARG:NH2	2.38	0.57
1:A:347:VAL:HG23	1:A:379:LEU:HD12	1.85	0.57
1:E:96:THR:O	1:E:100:GLN:NE2	2.38	0.57
1:F:82:MET:HE1	1:F:390:LEU:HD13	1.86	0.57
1:H:279:ASN:HD22	1:H:309:GLN:HG2	1.69	0.57
1:E:275:SER:O	1:E:303:ASN:ND2	2.38	0.57
1:C:186:VAL:H	3:C:601:ATP:HN62	1.53	0.57
1:G:412:ARG:HD2	1:G:418:ASP:HB3	1.85	0.57
1:C:16:ASP:OD2	1:D:341:ARG:NH2	2.38	0.57
1:G:18:LEU:H	1:G:489:LYS:HB3	1.70	0.57
1:G:72:THR:HG21	1:G:412:ARG:HB3	1.86	0.57
1:H:328:GLY:N	1:H:331:CYS:SG	2.77	0.57
1:A:412:ARG:HA	1:A:444:SER:HA	1.87	0.56
1:B:56:THR:HG1	1:B:59:ILE:N	2.01	0.56
1:E:21:GLN:O	1:E:25:ASN:ND2	2.38	0.56
1:E:43:ASP:OD1	1:E:43:ASP:N	2.38	0.56
1:G:57:LYS:NZ	1:G:357:PHE:O	2.38	0.56
1:C:304:VAL:HG23	1:C:309:GLN:HB2	1.86	0.56
1:C:306:THR:HG23	1:C:308:ALA:H	1.70	0.56
1:D:478:GLN:O	1:D:482:MET:HB2	2.04	0.56
1:F:56:THR:HG1	1:F:59:ILE:N	2.01	0.56
1:A:43:ASP:OD1	1:A:43:ASP:N	2.38	0.56
1:B:76:ALA:O	1:B:80:ILE:HB	2.05	0.56
1:H:73:VAL:HG23	1:H:78:MET:HE2	1.86	0.56
1:G:50:ASP:HB3	1:G:475:SER:HB3	1.88	0.56
1:H:414:MET:SD	1:H:414:MET:N	2.77	0.56
1:C:18:LEU:H	1:C:489:LYS:HB3	1.70	0.56
1:H:347:VAL:HG23	1:H:379:LEU:HD12	1.87	0.56
1:F:49:VAL:HG13	1:F:465:GLN:HB2	1.88	0.56
1:G:326:GLY:HA3	1:G:334:GLN:HE22	1.69	0.56
1:A:367:ILE:HG23	1:A:372:HIS:HB2	1.86	0.56
1:E:117:ASP:HA	1:E:150:MET:HG3	1.88	0.56
1:F:76:ALA:N	1:F:103:GLU:OE2	2.35	0.56
1:F:80:ILE:O	1:F:84:LEU:HB3	2.06	0.56
1:G:275:SER:O	1:G:303:ASN:ND2	2.39	0.56
1:A:80:ILE:O	1:A:84:LEU:HB2	2.06	0.56
1:C:57:LYS:NZ	1:C:357:PHE:O	2.39	0.56
1:F:85:THR:HG21	1:F:457:VAL:HG21	1.87	0.56
1:H:63:THR:HG23	1:H:65:LEU:H	1.69	0.56
1:A:15:ASP:O	1:A:489:LYS:NZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLN:O	1:A:25:ASN:ND2	2.39	0.56
1:D:273:LEU:HD11	1:D:283:GLN:HG3	1.87	0.56
1:E:15:ASP:O	1:E:489:LYS:NZ	2.39	0.56
1:F:392:ALA:HB1	1:F:449:ASP:HA	1.87	0.56
1:B:85:THR:HG21	1:B:457:VAL:HG21	1.88	0.55
1:B:504:HIS:ND1	1:B:505:SER:OG	2.33	0.55
1:A:412:ARG:NH1	1:A:416:SER:OG	2.39	0.55
1:D:91:ILE:H	1:D:248:ALA:HA	1.71	0.55
1:D:347:VAL:HG23	1:D:379:LEU:HD12	1.88	0.55
1:E:280:SER:OG	1:E:283:GLN:NE2	2.38	0.55
1:G:306:THR:HG23	1:G:308:ALA:H	1.71	0.55
1:H:241:LYS:NZ	1:H:243:GLN:OE1	2.37	0.55
1:C:97:PRO:HG3	1:C:259:ARG:HG2	1.88	0.55
1:D:182:ARG:NH2	1:D:185:LEU:O	2.39	0.55
1:C:95:CYS:SG	1:C:100:GLN:NE2	2.80	0.55
1:E:239:ASP:OD1	1:E:243:GLN:N	2.38	0.55
1:B:339:CYS:SG	1:B:340:GLY:N	2.79	0.55
1:E:18:LEU:O	1:E:490:PHE:N	2.37	0.55
1:H:393:THR:O	1:H:400:TYR:OH	2.24	0.55
1:A:239:ASP:OD1	1:A:243:GLN:N	2.38	0.55
1:C:275:SER:O	1:C:303:ASN:ND2	2.40	0.55
1:C:373:ILE:HD11	1:C:464:ILE:HG21	1.88	0.55
1:F:396:ALA:O	1:F:409:LYS:NZ	2.39	0.55
1:B:36:LEU:HD21	1:C:334:GLN:HE21	1.71	0.55
1:B:355:ARG:HH22	1:M:14:PRO:HG3	1.72	0.55
1:C:74:THR:HA	1:C:78:MET:HG3	1.89	0.55
1:G:339:CYS:SG	1:G:340:GLY:N	2.80	0.55
1:G:478:GLN:O	1:G:482:MET:HB2	2.06	0.55
1:H:453:ILE:HA	1:H:456:PHE:HB3	1.88	0.55
1:A:112:GLN:HA	1:A:243:GLN:HG3	1.88	0.55
1:C:356:ARG:NH2	1:P:11:SER:O	2.40	0.55
1:D:34:ASP:OD1	1:D:34:ASP:N	2.32	0.55
1:D:115:ILE:HG13	1:D:221:ILE:HG23	1.89	0.55
1:G:111:GLU:HB3	1:G:114:PHE:HB2	1.88	0.55
1:B:392:ALA:HB1	1:B:449:ASP:HA	1.89	0.55
1:C:339:CYS:SG	1:C:340:GLY:N	2.80	0.55
1:A:56:THR:HG23	1:A:58:LYS:H	1.72	0.55
1:A:208:LYS:NZ	3:A:603:ATP:O2A	2.39	0.55
1:C:326:GLY:HA3	1:C:334:GLN:HE22	1.71	0.55
1:D:33:ASN:O	1:D:493:ARG:NH1	2.40	0.55
1:D:117:ASP:O	3:D:601:ATP:N6	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:VAL:HG22	1:F:108:LYS:HD2	1.89	0.55
1:F:414:MET:HE1	1:F:419:ALA:HA	1.89	0.55
1:G:373:ILE:HD11	1:G:464:ILE:HG21	1.88	0.55
1:H:34:ASP:OD1	1:H:34:ASP:N	2.31	0.55
1:C:50:ASP:HB3	1:C:475:SER:HB3	1.88	0.54
1:D:393:THR:O	1:D:400:TYR:OH	2.24	0.54
1:A:280:SER:OG	1:A:283:GLN:NE2	2.40	0.54
1:E:112:GLN:HA	1:E:243:GLN:HG3	1.89	0.54
1:F:76:ALA:HA	1:F:79:ALA:HB3	1.89	0.54
1:H:153:ARG:NH2	1:H:154:LEU:O	2.40	0.54
1:A:275:SER:OG	1:A:303:ASN:N	2.39	0.54
1:H:182:ARG:NH2	1:H:185:LEU:O	2.40	0.54
1:B:224:ARG:NH2	1:E:164:ASP:OD2	2.38	0.54
1:E:275:SER:OG	1:E:303:ASN:N	2.39	0.54
1:H:273:LEU:HD11	1:H:283:GLN:HG3	1.88	0.54
1:B:42:ILE:HG22	1:B:472:GLY:HA2	1.89	0.54
1:E:412:ARG:NH1	1:E:416:SER:OG	2.40	0.54
1:A:453:ILE:HA	1:A:456:PHE:HB3	1.88	0.54
1:H:33:ASN:O	1:H:493:ARG:NH1	2.41	0.54
1:B:88:ILE:HD13	1:B:245:LEU:HB3	1.89	0.54
1:B:104:VAL:HG22	1:B:108:LYS:HD2	1.90	0.54
1:C:74:THR:HG23	1:C:91:ILE:HD12	1.90	0.54
1:E:478:GLN:O	1:E:482:MET:HB2	2.08	0.54
1:D:373:ILE:HG23	1:D:384:VAL:HG21	1.90	0.54
1:F:453:ILE:HA	1:F:456:PHE:HB3	1.89	0.54
1:H:91:ILE:H	1:H:248:ALA:HA	1.71	0.54
1:A:200:ILE:HA	1:A:203:ARG:HG2	1.89	0.54
1:B:76:ALA:HA	1:B:79:ALA:HB3	1.89	0.54
1:E:53:SER:O	1:E:60:THR:OG1	2.24	0.54
1:F:504:HIS:ND1	1:F:505:SER:OG	2.33	0.54
1:A:18:LEU:O	1:A:490:PHE:N	2.38	0.53
1:A:53:SER:O	1:A:60:THR:OG1	2.25	0.53
1:C:66:VAL:HB	1:C:88:ILE:HG23	1.90	0.53
1:C:369:ASN:ND2	1:D:335:GLU:O	2.40	0.53
1:D:412:ARG:NH2	1:D:418:ASP:O	2.41	0.53
1:F:42:ILE:HG22	1:F:472:GLY:HA2	1.89	0.53
1:F:300:ILE:HA	1:F:320:ALA:HB3	1.88	0.53
1:B:279:ASN:HD21	1:B:312:ASN:HD21	1.56	0.53
1:D:153:ARG:NH2	1:D:154:LEU:O	2.41	0.53
1:F:195:LYS:HD3	2:F:602:GTP:H4'	1.91	0.53
1:F:355:ARG:HH22	1:I:14:PRO:HG3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ALA:HA	1:A:409:LYS:HD2	1.90	0.53
1:C:104:VAL:HA	1:C:107:VAL:HG12	1.90	0.53
1:B:161:ARG:NH2	3:B:603:ATP:O1G	2.42	0.53
1:D:377:LEU:HA	1:D:381:ALA:HB3	1.90	0.53
1:E:200:ILE:HA	1:E:203:ARG:HG2	1.89	0.53
1:F:62:LYS:HE3	1:F:236:ALA:H	1.73	0.53
1:A:228:LYS:HA	1:A:231:ARG:HD3	1.91	0.53
3:C:601:ATP:O2A	1:H:161:ARG:NH2	2.42	0.53
1:E:453:ILE:HA	1:E:456:PHE:HB3	1.89	0.53
1:B:70:MET:HB3	1:B:73:VAL:HG22	1.90	0.53
1:C:279:ASN:OD1	1:C:312:ASN:ND2	2.40	0.53
1:E:126:ARG:NH2	1:E:170:GLU:OE2	2.42	0.53
1:E:367:ILE:HG21	1:E:373:ILE:HG23	1.91	0.53
1:F:339:CYS:SG	1:F:340:GLY:N	2.78	0.53
1:D:303:ASN:ND2	1:D:322:ARG:O	2.42	0.53
1:G:97:PRO:HG3	1:G:259:ARG:HG2	1.91	0.53
1:A:388:SER:OG	4:A:604:IMP:O3P	2.27	0.53
1:H:303:ASN:ND2	1:H:322:ARG:O	2.42	0.53
1:A:417:LEU:HD21	1:D:512:ARG:HD3	1.91	0.53
1:G:369:ASN:ND2	1:H:335:GLU:O	2.42	0.53
1:B:453:ILE:HA	1:B:456:PHE:HB3	1.90	0.52
1:E:475:SER:OG	1:E:478:GLN:OE1	2.23	0.52
1:A:209:LEU:HD23	1:A:222:ILE:HD11	1.91	0.52
1:D:453:ILE:HA	1:D:456:PHE:HB3	1.90	0.52
1:E:417:LEU:HD21	1:H:512:ARG:HD3	1.92	0.52
1:C:246:CYS:SG	1:C:247:GLY:N	2.82	0.52
1:F:36:LEU:HD21	1:G:334:GLN:HE21	1.74	0.52
1:B:91:ILE:H	1:B:248:ALA:HA	1.74	0.52
1:G:66:VAL:HB	1:G:88:ILE:HG23	1.92	0.52
1:E:95:CYS:O	1:E:100:GLN:NE2	2.43	0.52
1:H:373:ILE:HG23	1:H:384:VAL:HG21	1.92	0.52
1:H:412:ARG:NH2	1:H:418:ASP:O	2.42	0.52
1:A:97:PRO:HG3	1:A:259:ARG:HG2	1.91	0.52
1:E:18:LEU:HA	1:E:22:GLN:HE21	1.74	0.52
1:E:241:LYS:HB2	1:E:243:GLN:HE22	1.75	0.52
1:F:80:ILE:O	1:F:84:LEU:CB	2.57	0.52
1:G:279:ASN:OD1	1:G:312:ASN:ND2	2.40	0.52
1:G:453:ILE:HA	1:G:456:PHE:HB3	1.92	0.52
1:H:51:LEU:HA	1:H:476:LEU:HD23	1.92	0.52
1:B:71:ASP:OD1	1:B:71:ASP:N	2.43	0.52
1:B:133:ALA:O	1:B:137:HIS:ND1	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:504:HIS:O	1:F:329:SER:OG	2.24	0.52
1:A:241:LYS:HB2	1:A:243:GLN:HE22	1.75	0.52
1:A:323:VAL:HG21	1:A:350:VAL:HG21	1.92	0.52
1:B:300:ILE:HA	1:B:320:ALA:HB3	1.90	0.52
1:C:69:PRO:HD2	1:C:385:MET:HE2	1.90	0.52
1:C:478:GLN:O	1:C:482:MET:HB2	2.08	0.52
1:E:32:TYR:OH	1:E:343:GLN:NE2	2.43	0.52
1:E:51:LEU:HA	1:E:476:LEU:HD23	1.91	0.52
1:F:175:LEU:HD13	1:F:178:ILE:HD12	1.92	0.52
1:G:104:VAL:HA	1:G:107:VAL:HG12	1.92	0.52
1:E:512:ARG:NH2	1:E:514:PHE:OXT	2.43	0.52
1:G:82:MET:O	1:G:85:THR:OG1	2.28	0.52
1:B:164:ASP:HB2	1:E:227:LEU:HD21	1.92	0.51
1:C:228:LYS:NZ	1:H:164:ASP:OD2	2.42	0.51
1:C:453:ILE:HA	1:C:456:PHE:HB3	1.92	0.51
1:D:98:GLU:OE2	1:D:258:TYR:OH	2.26	0.51
1:D:275:SER:O	5:D:603:NAD:N7N	2.43	0.51
1:D:322:ARG:NH2	4:D:602:IMP:O3'	2.42	0.51
1:G:198:ASN:OD1	1:G:202:GLN:NE2	2.43	0.51
1:H:117:ASP:O	3:H:601:ATP:N6	2.43	0.51
1:H:377:LEU:HA	1:H:381:ALA:HB3	1.91	0.51
1:A:95:CYS:O	1:A:100:GLN:NE2	2.44	0.51
1:D:51:LEU:HA	1:D:476:LEU:HD23	1.93	0.51
1:E:323:VAL:HG21	1:E:350:VAL:HG21	1.92	0.51
1:F:88:ILE:HD13	1:F:245:LEU:HB3	1.90	0.51
1:G:69:PRO:HD2	1:G:385:MET:HE2	1.92	0.51
1:H:212:VAL:HG22	1:H:218:LEU:HA	1.92	0.51
1:D:224:ARG:NH2	1:G:161:ARG:O	2.43	0.51
1:F:373:ILE:HB	1:F:384:VAL:HG11	1.92	0.51
1:H:353:TYR:HA	1:H:356:ARG:HH11	1.76	0.51
1:A:18:LEU:HA	1:A:22:GLN:HE21	1.75	0.51
1:B:175:LEU:HD13	1:B:178:ILE:HD12	1.93	0.51
1:D:128:ARG:HH22	1:D:172:ASP:H	1.59	0.51
1:C:187:VAL:HG11	1:C:212:VAL:HG22	1.92	0.51
1:E:97:PRO:HG3	1:E:259:ARG:HG2	1.93	0.51
1:B:83:ALA:O	1:B:237:SER:OG	2.28	0.51
1:A:141:GLY:N	2:A:601:GTP:O2B	2.44	0.51
1:B:62:LYS:HE3	1:B:236:ALA:H	1.76	0.51
1:H:35:PHE:HA	1:H:492:LYS:HA	1.92	0.51
1:H:211:ILE:HG23	1:H:219:VAL:HG23	1.92	0.51
1:A:75:GLU:OE2	1:A:92:HIS:NE2	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:HA	1:A:185:LEU:HD13	1.93	0.51
1:B:80:ILE:O	1:B:84:LEU:HB3	2.11	0.51
1:C:121:LEU:HD11	1:C:130:VAL:HG12	1.92	0.51
1:D:63:THR:HG23	1:D:65:LEU:H	1.75	0.51
1:D:353:TYR:HA	1:D:356:ARG:HH11	1.76	0.51
1:D:403:SER:HB3	1:D:408:LEU:HD21	1.93	0.51
1:F:279:ASN:HD21	1:F:312:ASN:HD21	1.59	0.51
1:A:367:ILE:HG21	1:A:373:ILE:HG23	1.93	0.51
1:D:35:PHE:HA	1:D:492:LYS:HA	1.92	0.51
1:H:275:SER:O	5:H:603:NAD:N7N	2.44	0.51
1:H:403:SER:HB3	1:H:408:LEU:HD21	1.93	0.51
1:B:80:ILE:O	1:B:84:LEU:CB	2.59	0.50
1:C:200:ILE:HD13	1:C:203:ARG:HH21	1.77	0.50
1:D:227:LEU:O	1:D:231:ARG:NH1	2.44	0.50
1:E:388:SER:OG	4:E:604:IMP:O1P	2.27	0.50
1:E:392:ALA:HA	1:E:409:LYS:HD2	1.92	0.50
1:C:198:ASN:OD1	1:C:202:GLN:NE2	2.43	0.50
1:C:322:ARG:NH2	4:C:603:IMP:O2'	2.44	0.50
1:C:475:SER:OG	1:C:478:GLN:OE1	2.22	0.50
1:F:506:LEU:HA	1:G:447:VAL:HG23	1.93	0.50
1:B:328:GLY:N	1:B:331:CYS:SG	2.80	0.50
1:B:506:LEU:HA	1:C:447:VAL:HG23	1.93	0.50
2:B:602:GTP:H2'	2:B:602:GTP:PG	2.51	0.50
1:E:263:LEU:O	1:E:267:GLY:N	2.44	0.50
1:F:415:GLY:N	4:F:604:IMP:O6	2.39	0.50
1:C:334:GLN:HA	1:C:338:ALA:HA	1.93	0.50
1:M:2:ALA:HA	1:M:5:LEU:HD12	1.93	0.50
1:E:209:LEU:HD23	1:E:222:ILE:HD11	1.93	0.50
1:H:97:PRO:HB2	1:H:262:LEU:HD22	1.94	0.50
1:D:392:ALA:HB2	1:D:447:VAL:HG13	1.93	0.50
1:E:182:ARG:HA	1:E:185:LEU:HD13	1.94	0.50
1:F:92:HIS:ND1	1:F:94:ASN:OD1	2.42	0.50
1:D:329:SER:N	4:D:602:IMP:O3P	2.44	0.50
1:E:412:ARG:HA	1:E:444:SER:HA	1.93	0.50
1:H:274:ASP:OD1	1:H:322:ARG:NH1	2.44	0.50
1:B:306:THR:OG1	1:B:307:ALA:N	2.45	0.50
1:D:45:THR:O	1:D:469:GLN:NE2	2.45	0.50
1:G:187:VAL:HG11	1:G:212:VAL:HG22	1.94	0.50
1:G:322:ARG:NH2	4:G:604:IMP:O2'	2.44	0.50
1:A:328:GLY:N	1:A:331:CYS:SG	2.85	0.50
1:G:84:LEU:HD23	1:G:454:HIS:HE1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:322:ARG:NH2	4:H:602:IMP:O3'	2.45	0.50
1:G:334:GLN:HA	1:G:338:ALA:HA	1.94	0.49
1:C:84:LEU:HD23	1:C:454:HIS:HE1	1.77	0.49
1:C:388:SER:OG	4:C:603:IMP:O3P	2.29	0.49
1:G:200:ILE:HD13	1:G:203:ARG:HH21	1.77	0.49
1:H:392:ALA:HB2	1:H:447:VAL:HG13	1.92	0.49
1:A:200:ILE:O	1:A:204:SER:HB3	2.12	0.49
1:A:475:SER:OG	1:A:478:GLN:OE1	2.24	0.49
1:A:504:HIS:O	1:B:329:SER:OG	2.19	0.49
1:E:140:CYS:N	2:E:601:GTP:O2B	2.35	0.49
1:A:341:ARG:HH21	1:A:345:THR:HB	1.76	0.49
1:B:386:MET:HE1	1:B:389:LEU:H	1.76	0.49
1:E:363:ALA:H	1:E:384:VAL:HA	1.76	0.49
1:F:306:THR:OG1	1:F:307:ALA:N	2.45	0.49
1:B:386:MET:HE1	1:B:389:LEU:HG	1.92	0.49
1:B:396:ALA:O	1:B:409:LYS:NZ	2.46	0.49
1:G:108:LYS:NZ	1:G:269:ASP:OD2	2.45	0.49
1:G:475:SER:OG	1:G:478:GLN:OE1	2.22	0.49
1:A:133:ALA:O	1:A:137:HIS:ND1	2.38	0.49
1:A:227:LEU:HD11	1:F:165:PHE:HB3	1.95	0.49
1:E:239:ASP:N	1:E:243:GLN:O	2.39	0.49
1:B:159:SER:OG	1:B:160:SER:N	2.40	0.49
1:E:195:LYS:HD3	2:E:602:GTP:H4'	1.93	0.49
1:F:32:TYR:O	1:F:375:LYS:NZ	2.43	0.49
1:G:414:MET:HE2	5:G:605:NAD:H2N	1.94	0.49
1:H:45:THR:O	1:H:469:GLN:NE2	2.46	0.49
1:B:288:LYS:NZ	1:B:316:ALA:O	2.38	0.49
1:D:69:PRO:HB3	1:D:90:PHE:HB2	1.95	0.49
1:E:444:SER:OG	1:H:510:GLU:OE2	2.31	0.49
1:G:31:THR:OG1	1:G:32:TYR:N	2.45	0.49
1:G:388:SER:OG	4:G:604:IMP:O3P	2.29	0.49
1:H:352:GLU:O	1:H:356:ARG:NE	2.46	0.49
1:A:480:ARG:HH21	1:N:6:ILE:HA	1.78	0.49
1:D:304:VAL:HG13	1:D:323:VAL:HG23	1.95	0.49
1:F:115:ILE:HD11	1:F:118:PRO:HB3	1.95	0.49
1:I:2:ALA:HA	1:I:5:LEU:HD12	1.93	0.49
1:A:444:SER:OG	1:D:510:GLU:OE2	2.31	0.49
1:B:373:ILE:HB	1:B:384:VAL:HG11	1.94	0.49
1:B:414:MET:N	4:B:604:IMP:O6	2.46	0.49
1:F:133:ALA:O	1:F:137:HIS:ND1	2.36	0.49
1:A:117:ASP:HA	1:A:150:MET:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ILE:HG23	1:B:158:ILE:HB	1.95	0.48
1:C:288:LYS:HD3	1:C:291:LYS:HZ3	1.78	0.48
1:E:369:ASN:OD1	1:E:369:ASN:N	2.44	0.48
1:G:158:ILE:HD13	1:G:179:MET:HB3	1.95	0.48
1:A:239:ASP:N	1:A:243:GLN:O	2.39	0.48
1:D:79:ALA:O	1:D:83:ALA:CB	2.57	0.48
1:D:352:GLU:O	1:D:356:ARG:NE	2.46	0.48
1:G:246:CYS:SG	1:G:247:GLY:N	2.85	0.48
1:A:141:GLY:H	2:A:601:GTP:HN21	1.60	0.48
1:A:161:ARG:HA	1:F:224:ARG:HH12	1.78	0.48
1:A:311:LYS:HE2	1:D:12:TYR:HB3	1.96	0.48
1:A:496:SER:HA	1:A:499:VAL:HG22	1.94	0.48
1:E:388:SER:HG	1:E:411:TYR:HH	1.61	0.48
1:F:93:HIS:O	1:F:259:ARG:NH2	2.47	0.48
1:G:68:SER:HA	1:G:385:MET:HE2	1.94	0.48
1:F:450:LYS:O	1:F:455:LYS:NZ	2.46	0.48
1:G:356:ARG:NH2	1:L:11:SER:O	2.46	0.48
1:H:79:ALA:O	1:H:83:ALA:CB	2.58	0.48
1:K:3:ASP:N	1:K:3:ASP:OD1	2.45	0.48
1:A:369:ASN:N	1:A:369:ASN:OD1	2.44	0.48
1:F:142:ILE:HG23	1:F:158:ILE:HB	1.96	0.48
1:B:195:LYS:HD3	2:B:602:GTP:H4'	1.95	0.48
1:E:56:THR:HG23	1:E:58:LYS:H	1.79	0.48
1:G:74:THR:HG23	1:G:91:ILE:HD12	1.95	0.48
1:F:91:ILE:H	1:F:248:ALA:HA	1.78	0.48
1:F:288:LYS:NZ	1:F:316:ALA:O	2.39	0.48
1:C:457:VAL:HA	1:C:460:LEU:HB2	1.96	0.48
1:G:118:PRO:HA	3:G:603:ATP:HN62	1.79	0.48
1:G:492:LYS:HE3	1:H:28:ASP:HA	1.96	0.48
1:H:227:LEU:O	1:H:231:ARG:NH1	2.47	0.48
1:E:154:LEU:HD23	1:E:218:LEU:HD21	1.96	0.48
1:F:207:GLY:HA2	1:F:224:ARG:HB2	1.95	0.48
1:G:369:ASN:ND2	1:H:335:GLU:OE2	2.44	0.48
1:G:372:HIS:HA	1:G:375:LYS:HZ3	1.77	0.48
1:A:104:VAL:HA	1:A:107:VAL:HG22	1.96	0.47
1:D:145:THR:HG23	1:D:148:GLY:H	1.79	0.47
1:E:496:SER:HA	1:E:499:VAL:HG22	1.95	0.47
1:F:305:VAL:H	1:F:309:GLN:HE21	1.62	0.47
1:H:66:VAL:HG23	1:H:88:ILE:HG23	1.96	0.47
1:D:68:SER:HB2	1:D:385:MET:HE2	1.96	0.47
1:O:3:ASP:OD1	1:O:3:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:VAL:HA	1:E:107:VAL:HG22	1.96	0.47
1:D:104:VAL:HA	1:D:107:VAL:HG22	1.95	0.47
1:E:36:LEU:HB2	1:E:493:ARG:HD2	1.96	0.47
1:G:458:PRO:HA	1:G:461:ILE:HG12	1.97	0.47
1:E:57:LYS:N	1:E:319:ASP:OD2	2.43	0.47
1:F:54:ALA:HA	1:F:60:THR:HA	1.96	0.47
1:G:457:VAL:HA	1:G:460:LEU:HB2	1.96	0.47
1:H:201:LEU:HD11	1:H:224:ARG:HG3	1.95	0.47
1:H:260:LEU:HD22	1:H:290:ILE:HG22	1.97	0.47
1:H:329:SER:N	4:H:602:IMP:O3P	2.47	0.47
1:A:36:LEU:HB2	1:A:493:ARG:HD2	1.97	0.47
1:A:261:ASP:O	1:A:265:GLN:NE2	2.47	0.47
1:A:263:LEU:O	1:A:267:GLY:N	2.48	0.47
1:B:382:SER:O	1:B:480:ARG:NH2	2.47	0.47
1:C:133:ALA:O	1:C:137:HIS:ND1	2.30	0.47
1:E:133:ALA:O	1:E:137:HIS:ND1	2.39	0.47
1:H:197:ALA:O	1:H:201:LEU:CB	2.62	0.47
1:B:242:LYS:HE3	2:B:602:GTP:C6	2.49	0.47
1:C:145:THR:HG21	1:C:218:LEU:HD22	1.96	0.47
1:C:458:PRO:HA	1:C:461:ILE:HG12	1.97	0.47
1:D:47:ASP:OD1	1:D:47:ASP:N	2.47	0.47
1:E:159:SER:OG	3:E:603:ATP:O2B	2.33	0.47
1:F:417:LEU:H	1:F:417:LEU:HG	1.51	0.47
1:H:115:ILE:HG13	1:H:221:ILE:HG23	1.96	0.47
1:A:91:ILE:H	1:A:248:ALA:HA	1.80	0.47
1:A:225:THR:OG1	2:A:601:GTP:O3'	2.29	0.47
1:B:54:ALA:HA	1:B:60:THR:HA	1.95	0.47
1:B:207:GLY:HA2	1:B:224:ARG:HB2	1.97	0.47
1:B:505:SER:OG	1:C:368:GLN:NE2	2.40	0.47
1:C:272:VAL:HG22	1:C:300:ILE:HD11	1.97	0.47
1:C:362:ILE:HG22	1:C:383:THR:HB	1.97	0.47
1:A:406:ILE:HG13	1:F:406:ILE:HG13	1.96	0.47
1:C:80:ILE:O	1:C:84:LEU:HB2	2.15	0.47
1:G:115:ILE:HG13	1:G:221:ILE:HG23	1.97	0.47
1:G:288:LYS:HD3	1:G:291:LYS:HZ3	1.80	0.47
1:A:114:PHE:HB3	1:A:220:ALA:HB1	1.97	0.47
1:A:375:LYS:O	1:A:379:LEU:N	2.48	0.47
1:C:373:ILE:HB	1:C:384:VAL:HG11	1.97	0.47
1:C:495:SER:HG	1:D:495:SER:HG	1.63	0.47
1:E:113:GLY:HA2	1:E:242:LYS:HE3	1.97	0.47
1:G:66:VAL:HG13	1:G:385:MET:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLY:HA2	1:A:159:SER:HA	1.96	0.47
1:B:72:THR:HG21	1:B:411:TYR:HA	1.96	0.47
1:E:328:GLY:N	1:E:331:CYS:SG	2.88	0.47
1:F:242:LYS:HE3	2:F:602:GTP:C6	2.50	0.47
1:G:19:THR:OG1	1:G:20:ALA:N	2.47	0.47
1:H:476:LEU:HA	1:H:479:VAL:HG22	1.97	0.47
1:C:19:THR:OG1	1:C:20:ALA:N	2.48	0.46
1:C:314:ILE:HD11	1:C:359:VAL:HG11	1.97	0.46
1:G:314:ILE:HD11	1:G:359:VAL:HG11	1.97	0.46
1:G:373:ILE:HB	1:G:384:VAL:HG11	1.97	0.46
1:A:19:THR:H	1:A:22:GLN:HE21	1.62	0.46
1:D:476:LEU:HA	1:D:479:VAL:HG22	1.97	0.46
1:E:261:ASP:O	1:E:265:GLN:NE2	2.48	0.46
1:E:352:GLU:HG2	1:E:355:ARG:HE	1.80	0.46
1:A:154:LEU:HD23	1:A:218:LEU:HD21	1.97	0.46
1:B:93:HIS:O	1:B:259:ARG:NH2	2.49	0.46
1:D:402:PHE:HA	1:D:407:ARG:HA	1.96	0.46
1:H:47:ASP:OD1	1:H:47:ASP:N	2.48	0.46
1:H:506:LEU:HD11	1:H:509:TYR:HB3	1.97	0.46
1:A:363:ALA:H	1:A:384:VAL:HA	1.80	0.46
1:B:82:MET:HA	1:B:85:THR:HG22	1.96	0.46
1:D:506:LEU:HD11	1:D:509:TYR:HB3	1.97	0.46
1:B:164:ASP:O	1:E:231:ARG:NH1	2.48	0.46
1:B:66:VAL:HG13	1:B:385:MET:HA	1.98	0.46
1:B:319:ASP:OD1	1:B:319:ASP:N	2.38	0.46
1:C:31:THR:OG1	1:C:32:TYR:N	2.48	0.46
1:G:201:LEU:HB2	1:G:209:LEU:HD11	1.97	0.46
1:H:145:THR:HG23	1:H:148:GLY:H	1.81	0.46
1:A:341:ARG:HA	1:D:36:LEU:HD21	1.96	0.46
1:A:342:PRO:O	1:A:345:THR:OG1	2.32	0.46
1:B:97:PRO:HG3	1:B:259:ARG:HG2	1.96	0.46
1:E:311:LYS:HE2	1:H:12:TYR:HB3	1.98	0.46
1:G:134:LYS:HE3	1:G:140:CYS:HA	1.98	0.46
1:H:274:ASP:OD2	5:H:603:NAD:O2D	2.33	0.46
1:B:363:ALA:HB3	1:B:384:VAL:HG23	1.98	0.46
1:B:406:ILE:HG13	1:E:406:ILE:HG13	1.97	0.46
1:C:372:HIS:HA	1:C:375:LYS:HZ3	1.79	0.46
1:D:301:GLY:O	1:D:322:ARG:N	2.39	0.46
1:F:319:ASP:OD1	1:F:319:ASP:N	2.39	0.46
1:G:145:THR:HG21	1:G:218:LEU:HD22	1.98	0.46
1:A:56:THR:OG1	1:A:319:ASP:OD2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:MET:O	1:C:85:THR:OG1	2.27	0.46
1:E:375:LYS:O	1:E:379:LEU:N	2.48	0.46
1:G:509:TYR:HA	1:H:445:GLY:HA2	1.98	0.46
1:B:73:VAL:HG12	1:B:391:ALA:HB2	1.97	0.45
1:B:323:VAL:HG21	1:B:350:VAL:HG21	1.97	0.45
1:C:349:LYS:HB2	1:C:349:LYS:HE2	1.76	0.45
1:C:509:TYR:HA	1:D:445:GLY:HA2	1.98	0.45
1:D:55:LEU:HG	1:D:56:THR:HG23	1.97	0.45
1:F:323:VAL:HG21	1:F:350:VAL:HG21	1.97	0.45
1:H:402:PHE:HA	1:H:407:ARG:HA	1.97	0.45
1:A:276:SER:N	5:A:605:NAD:O1A	2.49	0.45
1:C:66:VAL:HG13	1:C:385:MET:HA	1.97	0.45
1:C:414:MET:HE2	5:C:604:NAD:H2N	1.98	0.45
1:D:159:SER:OG	3:G:601:ATP:O5'	2.27	0.45
1:D:365:GLY:HA2	4:D:602:IMP:H5'1	1.98	0.45
1:H:104:VAL:HA	1:H:107:VAL:HG22	1.97	0.45
1:H:269:ASP:OD1	1:H:269:ASP:N	2.49	0.45
1:C:14:PRO:HD3	1:D:311:LYS:HD3	1.98	0.45
1:C:68:SER:HA	1:C:385:MET:HE2	1.97	0.45
1:E:80:ILE:O	1:E:84:LEU:CB	2.64	0.45
1:E:112:GLN:O	1:E:242:LYS:NZ	2.43	0.45
1:F:82:MET:HA	1:F:85:THR:HG22	1.97	0.45
1:G:188:ALA:HB3	1:G:211:ILE:HB	1.99	0.45
1:A:412:ARG:NH2	1:A:418:ASP:O	2.39	0.45
1:B:305:VAL:H	1:B:309:GLN:HE21	1.64	0.45
1:C:201:LEU:HB2	1:C:209:LEU:HD11	1.97	0.45
1:G:209:LEU:HB2	1:G:222:ILE:HB	1.99	0.45
1:H:98:GLU:OE2	1:H:258:TYR:OH	2.28	0.45
1:G:281:ILE:H	1:G:281:ILE:HG13	1.65	0.45
1:G:362:ILE:HG22	1:G:383:THR:HB	1.99	0.45
1:B:141:GLY:N	2:B:601:GTP:O1B	2.48	0.45
1:B:361:VAL:O	1:B:382:SER:N	2.48	0.45
1:D:73:VAL:HG23	1:D:78:MET:HE2	1.97	0.45
1:E:200:ILE:O	1:E:204:SER:CB	2.65	0.45
1:A:117:ASP:H	1:A:150:MET:HE3	1.82	0.45
1:A:159:SER:OG	2:A:601:GTP:O3G	2.32	0.45
1:E:19:THR:H	1:E:22:GLN:HE21	1.64	0.45
1:G:14:PRO:HD3	1:H:311:LYS:HD3	1.97	0.45
1:H:31:THR:OG1	1:H:32:TYR:N	2.48	0.45
1:B:348:TYR:HB2	1:B:379:LEU:HD21	1.99	0.45
1:D:131:PHE:HE2	1:D:169:GLU:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:PHE:HD1	1:F:247:GLY:HA3	1.82	0.45
1:F:97:PRO:HG3	1:F:259:ARG:HG2	1.97	0.45
1:F:328:GLY:HA2	1:F:365:GLY:HA3	1.99	0.45
1:A:51:LEU:HA	1:A:476:LEU:HD23	1.98	0.44
1:A:211:ILE:HB	1:A:220:ALA:HB3	1.99	0.44
1:G:42:ILE:HG13	1:H:280:SER:HA	1.99	0.44
1:G:272:VAL:HG22	1:G:300:ILE:HD11	1.99	0.44
1:A:238:LYS:HB3	1:A:242:LYS:HA	1.99	0.44
1:C:257:LYS:HA	1:C:260:LEU:HD12	1.99	0.44
1:C:209:LEU:HB2	1:C:222:ILE:HB	1.99	0.44
1:E:211:ILE:HB	1:E:220:ALA:HB3	1.99	0.44
1:E:276:SER:N	5:E:605:NAD:O1A	2.50	0.44
1:G:392:ALA:HA	1:G:409:LYS:HD2	2.00	0.44
1:G:495:SER:OG	1:H:495:SER:OG	2.35	0.44
1:H:197:ALA:O	1:H:201:LEU:HB2	2.17	0.44
1:C:493:ARG:HB3	1:C:497:ALA:HB3	1.99	0.44
1:D:31:THR:OG1	1:D:32:TYR:N	2.49	0.44
1:D:197:ALA:O	1:D:201:LEU:HB2	2.16	0.44
1:E:31:THR:OG1	1:E:32:TYR:N	2.48	0.44
1:G:352:GLU:HA	1:G:355:ARG:HG2	1.98	0.44
1:H:331:CYS:SG	1:H:334:GLN:NE2	2.81	0.44
1:A:492:LYS:HE3	1:A:492:LYS:HB2	1.83	0.44
2:A:602:GTP:O1B	2:A:602:GTP:H3'	2.17	0.44
1:B:199:GLU:HB3	1:B:203:ARG:HH22	1.83	0.44
1:C:366:GLY:N	4:C:603:IMP:O1P	2.42	0.44
1:D:145:THR:OG1	1:D:146:ASP:N	2.51	0.44
1:E:134:LYS:NZ	1:E:138:GLY:O	2.48	0.44
1:A:158:ILE:HD11	1:A:179:MET:HA	2.00	0.44
1:B:90:PHE:HD1	1:B:247:GLY:HA3	1.83	0.44
1:C:69:PRO:HA	1:C:74:THR:HG21	1.98	0.44
1:C:105:ARG:O	1:C:109:LYS:NZ	2.43	0.44
1:F:305:VAL:H	1:F:309:GLN:NE2	2.15	0.44
1:F:415:GLY:O	1:F:441:GLN:N	2.41	0.44
1:G:123:PRO:HA	1:G:175:LEU:HD12	1.99	0.44
1:H:55:LEU:HG	1:H:56:THR:HG23	1.99	0.44
1:A:127:VAL:HG23	1:A:173:CYS:HB3	1.98	0.44
1:A:343:GLN:H	1:A:343:GLN:HG3	1.59	0.44
1:D:274:ASP:OD2	5:D:603:NAD:O2D	2.36	0.44
1:D:385:MET:HE3	1:D:386:MET:HG2	1.99	0.44
1:D:453:ILE:O	1:D:457:VAL:N	2.46	0.44
1:E:238:LYS:HB3	1:E:242:LYS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:388:SER:N	4:E:604:IMP:O3P	2.50	0.44
1:F:505:SER:OG	1:G:368:GLN:NE2	2.42	0.44
1:B:39:PRO:HG2	1:C:309:GLN:NE2	2.33	0.44
1:C:280:SER:OG	1:C:282:PHE:N	2.48	0.44
1:D:97:PRO:HB2	1:D:262:LEU:HD22	1.98	0.44
1:D:152:SER:O	1:D:218:LEU:N	2.44	0.44
1:F:348:TYR:HB2	1:F:379:LEU:HD21	2.00	0.44
1:G:213:ASN:N	1:G:217:GLU:O	2.49	0.44
1:G:257:LYS:HA	1:G:260:LEU:HD12	1.99	0.44
1:G:493:ARG:HB3	1:G:497:ALA:HB3	1.99	0.44
1:B:305:VAL:H	1:B:309:GLN:NE2	2.16	0.44
1:E:492:LYS:HE3	1:E:492:LYS:HB2	1.84	0.44
1:F:361:VAL:O	1:F:382:SER:N	2.42	0.44
1:A:186:VAL:HG13	1:A:206:LYS:HZ1	1.83	0.43
1:D:322:ARG:HA	1:D:362:ILE:HG23	1.99	0.43
1:E:476:LEU:HA	1:E:479:VAL:HG13	2.00	0.43
1:F:482:MET:HG2	1:F:487:GLU:HG3	1.99	0.43
1:H:158:ILE:HG12	1:H:179:MET:HG2	2.00	0.43
1:A:82:MET:HE2	1:A:82:MET:HB3	1.75	0.43
1:A:388:SER:N	4:A:604:IMP:O2P	2.51	0.43
2:A:601:GTP:N2	2:A:601:GTP:O1A	2.41	0.43
1:D:158:ILE:HD11	1:D:175:LEU:HD11	1.99	0.43
1:F:263:LEU:O	1:F:267:GLY:N	2.43	0.43
1:A:460:LEU:O	1:A:464:ILE:HD12	2.18	0.43
1:E:460:LEU:O	1:E:464:ILE:HD12	2.18	0.43
1:F:159:SER:OG	1:F:160:SER:N	2.44	0.43
1:H:494:THR:OG1	1:H:497:ALA:N	2.50	0.43
1:A:304:VAL:HG23	1:A:309:GLN:HG3	1.99	0.43
1:D:260:LEU:HD22	1:D:290:ILE:HG22	2.00	0.43
1:D:388:SER:OG	4:D:602:IMP:O2P	2.37	0.43
1:B:466:HIS:HD2	1:B:469:GLN:HE21	1.66	0.43
1:C:392:ALA:HA	1:C:409:LYS:HD2	2.01	0.43
1:E:82:MET:HE2	1:E:82:MET:HB3	1.74	0.43
1:F:71:ASP:OD1	1:F:71:ASP:N	2.49	0.43
1:G:100:GLN:OE1	1:G:259:ARG:NH2	2.52	0.43
1:G:347:VAL:HG13	1:G:379:LEU:HD12	2.00	0.43
1:A:57:LYS:N	1:A:319:ASP:OD2	2.42	0.43
1:B:228:LYS:HD2	1:B:228:LYS:HA	1.80	0.43
1:D:269:ASP:OD1	1:D:269:ASP:N	2.47	0.43
1:D:306:THR:OG1	1:D:307:ALA:N	2.52	0.43
1:O:2:ALA:HA	1:O:5:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:PHE:O	1:E:469:GLN:NE2	2.33	0.43
1:E:249:ALA:HA	1:E:272:VAL:HG13	2.01	0.43
1:F:72:THR:OG1	1:F:412:ARG:N	2.50	0.43
1:E:56:THR:OG1	1:E:319:ASP:OD2	2.30	0.43
1:E:103:GLU:HA	1:E:106:LYS:HG2	2.01	0.43
1:B:492:LYS:O	1:C:29:GLY:N	2.51	0.43
1:B:493:ARG:HA	1:C:29:GLY:HA3	2.00	0.43
1:C:42:ILE:HG13	1:D:280:SER:HA	2.01	0.43
1:E:314:ILE:HA	1:E:318:VAL:HG12	2.01	0.43
1:E:512:ARG:HH11	1:F:417:LEU:HD13	1.84	0.43
1:G:314:ILE:HD13	1:G:314:ILE:HA	1.85	0.43
1:G:368:GLN:H	1:G:372:HIS:HD1	1.66	0.43
1:A:103:GLU:HA	1:A:106:LYS:HG2	2.01	0.43
1:C:350:VAL:O	1:C:354:ALA:HB2	2.18	0.43
1:F:239:ASP:OD1	1:F:243:GLN:N	2.36	0.43
1:A:314:ILE:HA	1:A:318:VAL:HG12	2.01	0.43
1:C:314:ILE:HA	1:C:314:ILE:HD13	1.85	0.43
1:D:56:THR:OG1	1:D:59:ILE:N	2.49	0.43
1:H:139:PHE:HB3	3:H:601:ATP:C4	2.54	0.43
1:C:69:PRO:HD3	1:C:90:PHE:HB2	2.01	0.42
1:E:341:ARG:HH12	1:E:349:LYS:HD2	1.83	0.42
1:F:280:SER:H	1:F:283:GLN:NE2	2.14	0.42
1:F:466:HIS:HD2	1:F:469:GLN:HE21	1.67	0.42
1:G:350:VAL:O	1:G:354:ALA:HB2	2.19	0.42
1:H:238:LYS:HZ3	1:H:242:LYS:HA	1.83	0.42
1:A:67:SER:HB3	1:A:82:MET:HE1	2.01	0.42
1:C:492:LYS:HE3	1:D:28:ASP:HA	2.00	0.42
1:D:197:ALA:O	1:D:201:LEU:CB	2.67	0.42
1:E:75:GLU:HB3	1:E:76:ALA:H	1.63	0.42
1:F:39:PRO:HG2	1:G:309:GLN:NE2	2.34	0.42
1:G:116:THR:HG22	1:G:117:ASP:H	1.83	0.42
1:H:306:THR:OG1	1:H:307:ALA:N	2.52	0.42
1:H:464:ILE:O	1:H:467:SER:OG	2.32	0.42
1:A:367:ILE:HA	1:A:372:HIS:HD1	1.84	0.42
1:B:108:LYS:O	1:B:243:GLN:NE2	2.52	0.42
1:B:269:ASP:OD1	1:B:269:ASP:N	2.40	0.42
1:E:66:VAL:HG22	1:E:385:MET:HG3	2.00	0.42
1:E:67:SER:HB3	1:E:82:MET:HE1	2.01	0.42
1:A:71:ASP:HA	1:A:92:HIS:CD2	2.55	0.42
1:B:82:MET:O	1:B:87:GLY:N	2.52	0.42
1:B:253:HIS:HE2	5:B:605:NAD:PA	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:ARG:HB3	1:C:172:ASP:HA	2.01	0.42
1:F:493:ARG:NH1	1:F:498:GLN:OE1	2.52	0.42
1:G:280:SER:OG	1:G:282:PHE:N	2.50	0.42
1:D:93:HIS:ND1	1:D:249:ALA:O	2.53	0.42
1:D:321:LEU:HD13	1:D:321:LEU:HA	1.79	0.42
1:G:80:ILE:O	1:G:84:LEU:HB2	2.19	0.42
1:A:112:GLN:HE21	1:A:115:ILE:HG12	1.85	0.42
1:A:341:ARG:HH12	1:A:349:LYS:HD2	1.84	0.42
1:B:306:THR:H	1:B:309:GLN:NE2	2.17	0.42
1:C:471:ILE:HD11	1:C:479:VAL:HG22	2.01	0.42
1:D:494:THR:OG1	1:D:497:ALA:N	2.52	0.42
1:E:304:VAL:HG23	1:E:309:GLN:HG3	2.00	0.42
1:F:82:MET:O	1:F:87:GLY:N	2.52	0.42
1:F:292:ASP:N	1:F:292:ASP:OD1	2.52	0.42
1:G:162:ASP:OD2	3:G:602:ATP:O2'	2.35	0.42
1:G:366:GLY:N	4:G:604:IMP:O1P	2.41	0.42
1:H:453:ILE:O	1:H:457:VAL:N	2.47	0.42
1:H:494:THR:H	1:H:497:ALA:HB3	1.85	0.42
1:B:239:ASP:OD1	1:B:243:GLN:N	2.36	0.42
1:C:186:VAL:O	3:C:601:ATP:N6	2.52	0.42
1:C:368:GLN:H	1:C:372:HIS:HD1	1.67	0.42
1:D:38:LEU:HD13	1:D:38:LEU:HA	1.88	0.42
1:D:494:THR:H	1:D:497:ALA:HB3	1.85	0.42
1:H:38:LEU:HD13	1:H:38:LEU:HA	1.87	0.42
1:H:257:LYS:HA	1:H:260:LEU:HG	2.02	0.42
1:B:161:ARG:HH11	1:E:224:ARG:HE	1.66	0.42
1:B:450:LYS:O	1:B:455:LYS:NZ	2.53	0.42
1:C:134:LYS:HE2	1:C:134:LYS:HB3	1.88	0.42
1:C:213:ASN:N	1:C:217:GLU:O	2.48	0.42
1:D:210:PRO:HA	1:D:221:ILE:HD12	2.02	0.42
1:E:91:ILE:H	1:E:248:ALA:HA	1.85	0.42
2:E:602:GTP:PB	2:E:602:GTP:H3'	2.59	0.42
1:F:283:GLN:H	1:F:283:GLN:HG3	1.69	0.42
1:F:322:ARG:HA	1:F:362:ILE:HG13	2.01	0.42
1:A:113:GLY:HA2	1:A:242:LYS:HE3	2.02	0.42
1:A:187:VAL:HG21	1:A:212:VAL:HG22	2.01	0.42
1:C:120:VAL:HG22	1:C:148:GLY:HA2	2.02	0.42
1:F:199:GLU:HB3	1:F:203:ARG:HH22	1.85	0.42
1:G:504:HIS:NE2	1:H:329:SER:HA	2.34	0.42
1:H:475:SER:OG	1:H:477:THR:OG1	2.28	0.42
1:A:142:ILE:HD12	1:A:143:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:H	1:B:332:ILE:HG13	1.68	0.42
1:C:441:GLN:O	4:C:603:IMP:N1	2.52	0.42
1:D:369:ASN:OD1	1:D:369:ASN:N	2.50	0.42
1:E:389:LEU:HD11	1:E:460:LEU:HD21	2.02	0.42
1:F:392:ALA:HB2	1:F:447:VAL:HG13	2.01	0.42
1:H:210:PRO:HA	1:H:221:ILE:HD12	2.00	0.42
1:C:352:GLU:HA	1:C:355:ARG:HG2	2.01	0.41
1:E:12:TYR:HB3	1:F:311:LYS:HE3	2.01	0.41
1:H:321:LEU:HD13	1:H:321:LEU:HA	1.79	0.41
1:A:249:ALA:HA	1:A:272:VAL:HG13	2.02	0.41
1:A:273:LEU:HD21	1:A:283:GLN:HG3	2.00	0.41
1:C:158:ILE:HD13	1:C:179:MET:HB3	2.02	0.41
1:F:332:ILE:H	1:F:332:ILE:HG13	1.68	0.41
1:G:390:LEU:O	1:G:393:THR:OG1	2.32	0.41
1:A:146:ASP:OD1	1:A:146:ASP:N	2.50	0.41
1:A:164:ASP:OD2	1:F:224:ARG:NH1	2.53	0.41
1:B:140:CYS:N	2:B:601:GTP:O1B	2.49	0.41
1:B:500:GLU:OE1	1:B:500:GLU:N	2.53	0.41
1:C:190:ALA:HA	1:C:211:ILE:HD11	2.00	0.41
1:C:297:LEU:HD22	1:C:298:GLN:H	1.85	0.41
1:D:292:ASP:OD1	1:D:292:ASP:N	2.53	0.41
1:D:464:ILE:O	1:D:467:SER:OG	2.32	0.41
1:E:71:ASP:HA	1:E:92:HIS:CG	2.56	0.41
1:E:370:VAL:HG21	1:E:463:GLY:HA3	2.03	0.41
1:F:301:GLY:HA3	1:F:318:VAL:HG21	2.02	0.41
1:F:386:MET:SD	1:F:387:GLY:N	2.94	0.41
1:G:35:PHE:HA	1:G:492:LYS:HA	2.02	0.41
1:A:125:ASP:OD1	1:A:125:ASP:N	2.54	0.41
1:B:71:ASP:OD2	1:B:94:ASN:ND2	2.42	0.41
1:C:369:ASN:ND2	1:D:335:GLU:OE2	2.44	0.41
1:E:103:GLU:HA	1:E:106:LYS:HZ3	1.85	0.41
2:F:602:GTP:O3B	2:F:602:GTP:H3'	2.21	0.41
1:F:483:MET:HB2	1:F:488:LEU:HD21	2.03	0.41
1:G:126:ARG:HB3	1:G:172:ASP:HA	2.03	0.41
1:H:145:THR:OG1	1:H:146:ASP:N	2.54	0.41
1:H:369:ASN:OD1	1:H:369:ASN:N	2.50	0.41
1:C:128:ARG:HD3	1:C:170:GLU:HB3	2.03	0.41
1:C:347:VAL:HG13	1:C:379:LEU:HD12	2.01	0.41
1:D:70:MET:HB2	1:D:73:VAL:HG12	2.03	0.41
1:D:71:ASP:OD1	1:D:92:HIS:ND1	2.53	0.41
1:D:88:ILE:HD12	1:D:88:ILE:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:THR:H	1:F:309:GLN:NE2	2.19	0.41
1:F:322:ARG:NH2	4:F:604:IMP:O2'	2.54	0.41
1:G:449:ASP:OD1	1:G:449:ASP:N	2.41	0.41
1:H:68:SER:HB2	1:H:385:MET:HE2	2.03	0.41
1:H:322:ARG:HA	1:H:362:ILE:HG23	2.02	0.41
1:B:61:LEU:HD13	1:B:61:LEU:HA	1.92	0.41
1:B:104:VAL:O	1:B:107:VAL:N	2.53	0.41
1:B:193:THR:OG1	1:B:194:LEU:N	2.53	0.41
1:C:82:MET:HG3	1:C:87:GLY:HA3	2.03	0.41
1:E:66:VAL:HB	1:E:88:ILE:HG23	2.03	0.41
1:E:100:GLN:NE2	1:E:259:ARG:HH22	2.19	0.41
1:E:504:HIS:NE2	1:F:329:SER:HA	2.36	0.41
1:H:144:ILE:HG21	1:H:175:LEU:HG	2.02	0.41
1:A:134:LYS:NZ	1:A:138:GLY:O	2.51	0.41
1:C:44:PHE:O	1:C:469:GLN:NE2	2.54	0.41
1:C:473:ALA:HB1	1:C:478:GLN:HG2	2.02	0.41
1:D:257:LYS:HA	1:D:260:LEU:HG	2.03	0.41
1:E:71:ASP:HA	1:E:92:HIS:CD2	2.56	0.41
1:E:112:GLN:NE2	2:E:601:GTP:H2'	2.28	0.41
1:E:146:ASP:OD1	1:E:146:ASP:N	2.52	0.41
1:G:354:ALA:O	1:G:358:GLY:N	2.53	0.41
1:A:44:PHE:O	1:A:469:GLN:NE2	2.33	0.41
1:A:66:VAL:HG13	1:A:385:MET:HA	2.02	0.41
1:A:71:ASP:HA	1:A:92:HIS:CG	2.56	0.41
1:A:80:ILE:O	1:A:84:LEU:CB	2.69	0.41
1:A:272:VAL:HG23	1:A:300:ILE:HD11	2.03	0.41
1:B:263:LEU:O	1:B:267:GLY:N	2.45	0.41
1:B:292:ASP:OD1	1:B:292:ASP:N	2.54	0.41
1:B:504:HIS:CE1	1:C:329:SER:HA	2.56	0.41
1:C:18:LEU:HD12	1:C:23:LEU:HD23	2.01	0.41
1:C:70:MET:HE1	1:C:414:MET:HB3	2.02	0.41
1:C:504:HIS:NE2	1:D:329:SER:HA	2.35	0.41
1:D:175:LEU:HD13	1:D:178:ILE:HB	2.03	0.41
1:D:212:VAL:HG22	1:D:218:LEU:HA	2.03	0.41
1:D:355:ARG:HH22	1:O:10:THR:HG23	1.86	0.41
1:D:392:ALA:HB1	1:D:449:ASP:HA	2.03	0.41
1:E:114:PHE:HB3	1:E:220:ALA:HB1	2.01	0.41
1:E:272:VAL:HG23	1:E:300:ILE:HD11	2.02	0.41
1:E:415:GLY:HA3	1:E:441:GLN:HE21	1.86	0.41
1:F:71:ASP:OD2	1:F:94:ASN:ND2	2.50	0.41
1:F:83:ALA:O	1:F:237:SER:OG	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:THR:OG1	1:F:194:LEU:N	2.53	0.41
1:F:363:ALA:HB3	1:F:384:VAL:HG23	2.02	0.41
1:F:388:SER:N	4:F:604:IMP:O1P	2.54	0.41
1:F:478:GLN:O	1:F:482:MET:CB	2.69	0.41
1:F:493:ARG:HA	1:G:29:GLY:HA3	2.02	0.41
1:F:500:GLU:OE1	1:F:500:GLU:N	2.54	0.41
1:F:504:HIS:CE1	1:G:329:SER:HA	2.56	0.41
1:G:18:LEU:HD12	1:G:23:LEU:HD23	2.01	0.41
1:G:69:PRO:HD3	1:G:90:PHE:HB2	2.03	0.41
1:G:453:ILE:O	1:G:456:PHE:N	2.51	0.41
1:B:199:GLU:HB3	1:B:203:ARG:NH2	2.36	0.41
1:C:70:MET:HB3	1:C:73:VAL:HG12	2.03	0.41
1:E:476:LEU:HB3	1:E:480:ARG:NH1	2.35	0.41
1:F:37:ILE:HG23	1:F:490:PHE:HE1	1.86	0.41
1:F:303:ASN:ND2	1:F:324:GLY:O	2.28	0.41
1:G:292:ASP:OD1	1:G:292:ASP:N	2.53	0.41
1:G:473:ALA:HB1	1:G:478:GLN:HG2	2.03	0.41
1:H:33:ASN:O	1:H:498:GLN:NE2	2.54	0.41
1:H:392:ALA:HB1	1:H:449:ASP:HA	2.03	0.41
1:A:112:GLN:O	1:A:242:LYS:NZ	2.43	0.40
1:A:411:TYR:N	1:A:445:GLY:O	2.53	0.40
1:A:509:TYR:HA	1:B:445:GLY:HA2	2.03	0.40
1:B:82:MET:HE1	1:B:390:LEU:HD12	2.03	0.40
1:E:466:HIS:HB3	1:F:337:LEU:HD11	2.03	0.40
1:H:100:GLN:CD	1:H:259:ARG:HH22	2.29	0.40
4:H:602:IMP:H8	4:H:602:IMP:H2'	1.80	0.40
1:A:389:LEU:HD11	1:A:460:LEU:HD21	2.03	0.40
1:C:292:ASP:OD1	1:C:292:ASP:N	2.54	0.40
1:E:273:LEU:HD21	1:E:283:GLN:HG3	2.02	0.40
1:E:341:ARG:HA	1:H:36:LEU:HD21	2.02	0.40
1:F:100:GLN:OE1	1:F:259:ARG:NH2	2.54	0.40
1:F:141:GLY:N	2:F:601:GTP:O1B	2.53	0.40
1:F:369:ASN:OD1	1:F:369:ASN:N	2.53	0.40
1:G:121:LEU:HD11	1:G:130:VAL:HG12	2.03	0.40
1:D:407:ARG:NH1	1:D:449:ASP:OD2	2.55	0.40
1:G:69:PRO:HA	1:G:74:THR:HG21	2.02	0.40
1:G:137:HIS:HB3	1:G:139:PHE:CE1	2.57	0.40
1:H:78:MET:O	1:H:82:MET:HG3	2.22	0.40
1:A:228:LYS:O	1:A:232:ASP:HB2	2.21	0.40
1:B:42:ILE:HD12	1:B:44:PHE:H	1.86	0.40
1:B:301:GLY:HA3	1:B:318:VAL:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ILE:H	1:C:163:ILE:HG13	1.82	0.40
1:D:208:LYS:HG3	1:D:221:ILE:HD11	2.02	0.40
1:E:286:MET:HE2	1:E:286:MET:HB2	1.97	0.40
1:F:13:VAL:H	1:G:311:LYS:NZ	2.20	0.40
1:F:61:LEU:HD13	1:F:61:LEU:HA	1.90	0.40
1:H:292:ASP:OD1	1:H:292:ASP:N	2.55	0.40
1:A:140:CYS:N	2:A:601:GTP:O2B	2.49	0.40
1:A:207:GLY:HA2	1:A:224:ARG:NE	2.37	0.40
1:A:321:LEU:HB3	1:A:361:VAL:HG23	2.02	0.40
1:B:51:LEU:HA	1:B:476:LEU:HD23	2.03	0.40
1:B:146:ASP:OD1	1:B:146:ASP:N	2.54	0.40
1:B:395:GLU:OE2	1:B:453:ILE:N	2.52	0.40
1:D:24:PHE:HD1	1:D:24:PHE:HA	1.77	0.40
2:E:602:GTP:H2'	2:E:602:GTP:PG	2.61	0.40
1:F:386:MET:HE1	1:F:388:SER:OG	2.22	0.40
1:G:229:LYS:HE3	1:G:229:LYS:HB3	1.85	0.40
1:H:24:PHE:HD1	1:H:24:PHE:HA	1.78	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 PDB entries followed by that with respect to all EM entries.

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	484/519 (93%)	430 (89%)	54 (11%)	0	100	100
1	B	484/519 (93%)	430 (89%)	54 (11%)	0	100	100
1	C	484/519 (93%)	438 (90%)	46 (10%)	0	100	100
1	D	484/519 (93%)	438 (90%)	45 (9%)	1 (0%)	44	77
1	E	484/519 (93%)	430 (89%)	54 (11%)	0	100	100
1	F	484/519 (93%)	434 (90%)	50 (10%)	0	100	100
1	G	484/519 (93%)	436 (90%)	48 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	484/519 (93%)	437 (90%)	46 (10%)	1 (0%)	44 77
1	I	12/519 (2%)	6 (50%)	6 (50%)	0	100 100
1	J	12/519 (2%)	6 (50%)	6 (50%)	0	100 100
1	K	12/519 (2%)	6 (50%)	6 (50%)	0	100 100
1	L	12/519 (2%)	5 (42%)	7 (58%)	0	100 100
1	M	12/519 (2%)	6 (50%)	6 (50%)	0	100 100
1	N	12/519 (2%)	5 (42%)	7 (58%)	0	100 100
1	O	12/519 (2%)	6 (50%)	6 (50%)	0	100 100
1	P	12/519 (2%)	6 (50%)	6 (50%)	0	100 100
All	All	3968/8304 (48%)	3519 (89%)	447 (11%)	2 (0%)	50 82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	110	TYR
1	H	110	TYR

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 PDB entries followed by that with respect to all EM entries.

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	398/425 (94%)	376 (94%)	22 (6%)	18 42
1	B	398/425 (94%)	381 (96%)	17 (4%)	25 48
1	C	398/425 (94%)	386 (97%)	12 (3%)	36 57
1	D	398/425 (94%)	384 (96%)	14 (4%)	31 53
1	E	398/425 (94%)	376 (94%)	22 (6%)	18 42
1	F	398/425 (94%)	380 (96%)	18 (4%)	23 47
1	G	398/425 (94%)	386 (97%)	12 (3%)	36 57
1	H	398/425 (94%)	385 (97%)	13 (3%)	33 54
1	I	11/425 (3%)	11 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	11/425 (3%)	10 (91%)	1 (9%)	7 26
1	K	11/425 (3%)	10 (91%)	1 (9%)	7 26
1	L	11/425 (3%)	11 (100%)	0	100 100
1	M	11/425 (3%)	11 (100%)	0	100 100
1	N	11/425 (3%)	10 (91%)	1 (9%)	7 26
1	O	11/425 (3%)	10 (91%)	1 (9%)	7 26
1	P	11/425 (3%)	11 (100%)	0	100 100
All	All	3272/6800 (48%)	3138 (96%)	134 (4%)	28 49

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	178	ILE
1	A	222	ILE
1	A	228	LYS
1	A	231	ARG
1	A	250	ILE
1	A	272	VAL
1	A	273	LEU
1	A	281	ILE
1	A	297	LEU
1	A	300	ILE
1	A	304	VAL
1	A	321	LEU
1	A	332	ILE
1	A	359	VAL
1	A	373	ILE
1	A	377	LEU
1	A	379	LEU
1	A	389	LEU
1	A	406	ILE
1	A	455	LYS
1	A	479	VAL
1	B	18	LEU
1	B	49	VAL
1	B	66	VAL
1	B	71	ASP
1	B	80	ILE
1	B	115	ILE

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Mol	Chain	Res	Type
1	B	178	ILE
1	B	260	LEU
1	B	300	ILE
1	B	313	LEU
1	B	321	LEU
1	B	332	ILE
1	B	370	VAL
1	B	373	ILE
1	B	383	THR
1	B	417	LEU
1	B	465	GLN
1	C	18	LEU
1	C	36	LEU
1	C	37	ILE
1	C	51	LEU
1	C	229	LYS
1	C	281	ILE
1	C	287	ILE
1	C	304	VAL
1	C	321	LEU
1	C	373	ILE
1	C	379	LEU
1	C	465	GLN
1	D	38	LEU
1	D	51	LEU
1	D	65	LEU
1	D	199	GLU
1	D	201	LEU
1	D	250	ILE
1	D	321	LEU
1	D	332	ILE
1	D	359	VAL
1	D	367	ILE
1	D	377	LEU
1	D	379	LEU
1	D	447	VAL
1	D	461	ILE
1	N	10	THR
1	O	10	THR
1	E	66	VAL
1	E	109	LYS
1	E	178	ILE

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Mol	Chain	Res	Type
1	E	222	ILE
1	E	228	LYS
1	E	250	ILE
1	E	272	VAL
1	E	273	LEU
1	E	281	ILE
1	E	297	LEU
1	E	300	ILE
1	E	304	VAL
1	E	321	LEU
1	E	332	ILE
1	E	359	VAL
1	E	373	ILE
1	E	377	LEU
1	E	379	LEU
1	E	389	LEU
1	E	406	ILE
1	E	455	LYS
1	E	479	VAL
1	F	18	LEU
1	F	49	VAL
1	F	66	VAL
1	F	71	ASP
1	F	80	ILE
1	F	115	ILE
1	F	178	ILE
1	F	260	LEU
1	F	300	ILE
1	F	313	LEU
1	F	321	LEU
1	F	332	ILE
1	F	370	VAL
1	F	373	ILE
1	F	383	THR
1	F	390	LEU
1	F	417	LEU
1	F	465	GLN
1	G	18	LEU
1	G	36	LEU
1	G	37	ILE
1	G	51	LEU
1	G	229	LYS

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Mol	Chain	Res	Type
1	G	281	ILE
1	G	287	ILE
1	G	304	VAL
1	G	321	LEU
1	G	373	ILE
1	G	379	LEU
1	G	465	GLN
1	H	38	LEU
1	H	65	LEU
1	H	199	GLU
1	H	201	LEU
1	H	250	ILE
1	H	321	LEU
1	H	332	ILE
1	H	359	VAL
1	H	367	ILE
1	H	377	LEU
1	H	379	LEU
1	H	447	VAL
1	H	461	ILE
1	J	10	THR
1	K	10	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	112	GLN
1	A	243	GLN
1	A	265	GLN
1	A	283	GLN
1	A	368	GLN
1	A	454	HIS
1	B	25	ASN
1	B	198	ASN
1	B	279	ASN
1	B	283	GLN
1	B	469	GLN
1	C	22	GLN
1	C	102	ASN
1	C	334	GLN
1	C	454	HIS

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Mol	Chain	Res	Type
1	D	94	ASN
1	D	265	GLN
1	D	279	ASN
1	D	285	ASN
1	D	298	GLN
1	D	309	GLN
1	D	368	GLN
1	E	22	GLN
1	E	33	ASN
1	E	112	GLN
1	E	243	GLN
1	E	265	GLN
1	E	283	GLN
1	E	343	GLN
1	E	368	GLN
1	E	454	HIS
1	F	25	ASN
1	F	198	ASN
1	F	279	ASN
1	F	283	GLN
1	F	441	GLN
1	F	469	GLN
1	G	22	GLN
1	G	102	ASN
1	G	334	GLN
1	G	454	HIS
1	G	469	GLN
1	H	94	ASN
1	H	112	GLN
1	H	230	ASN
1	H	265	GLN
1	H	279	ASN
1	H	285	ASN
1	H	298	GLN
1	H	309	GLN
1	H	368	GLN

5.3.3 RNA

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

36 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	ATP	C	602	-	28,33,33	3.39	14 (50%)	34,52,52	3.72	5 (14%)
5	NAD	F	605	-	42,48,48	3.71	18 (42%)	50,73,73	2.92	6 (12%)
2	GTP	F	601	-	29,34,34	4.13	17 (58%)	35,54,54	2.50	6 (17%)
3	ATP	B	603	-	28,33,33	3.43	13 (46%)	34,52,52	4.04	5 (14%)
2	GTP	B	601	-	29,34,34	4.18	17 (58%)	35,54,54	1.60	6 (17%)
5	NAD	C	604	-	42,48,48	3.66	16 (38%)	50,73,73	2.95	9 (18%)
2	GTP	A	602	-	29,34,34	4.21	17 (58%)	35,54,54	2.24	5 (14%)
5	NAD	H	603	-	42,48,48	3.72	18 (42%)	50,73,73	2.79	7 (14%)
4	IMP	F	604	-	21,25,25	2.78	6 (28%)	22,38,38	1.90	6 (27%)
5	NAD	A	605	-	42,48,48	3.67	17 (40%)	50,73,73	2.88	8 (16%)
2	GTP	E	601	-	29,34,34	4.23	17 (58%)	35,54,54	1.55	8 (22%)
4	IMP	B	604	-	21,25,25	2.74	6 (28%)	22,38,38	1.91	5 (22%)
3	ATP	E	603	-	28,33,33	3.39	14 (50%)	34,52,52	4.21	6 (17%)
5	NAD	D	603	-	42,48,48	3.71	17 (40%)	50,73,73	2.80	7 (14%)
2	GTP	A	601	-	29,34,34	4.25	17 (58%)	35,54,54	1.62	6 (17%)
5	NAD	G	605	-	42,48,48	3.68	16 (38%)	50,73,73	3.04	10 (20%)
3	ATP	A	603	-	28,33,33	3.30	14 (50%)	34,52,52	3.89	5 (14%)
4	IMP	A	604	-	21,25,25	2.75	7 (33%)	22,38,38	1.62	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	IMP	E	604	-	21,25,25	2.74	7 (33%)	22,38,38	1.72	5 (22%)
3	ATP	G	603	-	28,33,33	3.39	14 (50%)	34,52,52	3.72	5 (14%)
2	GTP	E	602	-	29,34,34	4.28	18 (62%)	35,54,54	1.84	5 (14%)
3	ATP	H	601	-	28,33,33	3.45	14 (50%)	34,52,52	3.93	5 (14%)
3	ATP	F	603	-	28,33,33	3.40	13 (46%)	34,52,52	4.04	5 (14%)
3	ATP	G	602	-	28,33,33	3.47	14 (50%)	34,52,52	3.68	6 (17%)
3	ATP	D	601	-	28,33,33	3.56	14 (50%)	34,52,52	3.80	5 (14%)
4	IMP	G	604	-	21,25,25	2.82	8 (38%)	22,38,38	1.72	5 (22%)
4	IMP	D	602	-	21,25,25	2.80	7 (33%)	22,38,38	1.58	5 (22%)
4	IMP	C	603	-	21,25,25	2.80	7 (33%)	22,38,38	1.74	5 (22%)
2	GTP	F	602	-	29,34,34	4.28	17 (58%)	35,54,54	2.10	6 (17%)
3	ATP	C	601	-	28,33,33	3.44	14 (50%)	34,52,52	3.68	5 (14%)
4	IMP	H	602	-	21,25,25	2.78	7 (33%)	22,38,38	1.60	5 (22%)
3	ATP	C	605	-	28,33,33	3.32	13 (46%)	34,52,52	3.74	5 (14%)
5	NAD	E	605	-	42,48,48	3.68	17 (40%)	50,73,73	2.94	8 (16%)
2	GTP	B	602	-	29,34,34	4.25	18 (62%)	35,54,54	2.25	7 (20%)
3	ATP	G	601	-	28,33,33	3.40	14 (50%)	34,52,52	3.71	5 (14%)
5	NAD	B	605	-	42,48,48	3.73	18 (42%)	50,73,73	3.05	7 (14%)

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
3	ATP	C	602	-	-	3/18/38/38	0/3/3/3
5	NAD	F	605	-	-	10/26/62/62	0/5/5/5
2	GTP	F	601	-	-	6/18/38/38	0/3/3/3
3	ATP	B	603	-	-	6/18/38/38	0/3/3/3
2	GTP	B	601	-	-	5/18/38/38	0/3/3/3
5	NAD	C	604	-	-	18/26/62/62	0/5/5/5
2	GTP	A	602	-	-	3/18/38/38	0/3/3/3
5	NAD	H	603	-	-	14/26/62/62	0/5/5/5
4	IMP	F	604	-	-	6/6/26/26	0/3/3/3
5	NAD	A	605	-	-	2/26/62/62	0/5/5/5
2	GTP	E	601	-	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IMP	B	604	-	-	5/6/26/26	0/3/3/3
3	ATP	E	603	-	-	3/18/38/38	0/3/3/3
5	NAD	D	603	-	-	14/26/62/62	0/5/5/5
2	GTP	A	601	-	-	5/18/38/38	0/3/3/3
5	NAD	G	605	-	-	13/26/62/62	0/5/5/5
3	ATP	A	603	-	-	1/18/38/38	0/3/3/3
4	IMP	A	604	-	-	5/6/26/26	0/3/3/3
4	IMP	E	604	-	-	5/6/26/26	0/3/3/3
3	ATP	G	603	-	-	3/18/38/38	0/3/3/3
2	GTP	E	602	-	-	8/18/38/38	0/3/3/3
3	ATP	H	601	-	-	7/18/38/38	0/3/3/3
3	ATP	F	603	-	-	4/18/38/38	0/3/3/3
3	ATP	G	602	-	-	3/18/38/38	0/3/3/3
3	ATP	D	601	-	-	13/18/38/38	0/3/3/3
4	IMP	G	604	-	-	5/6/26/26	0/3/3/3
4	IMP	D	602	-	-	5/6/26/26	0/3/3/3
4	IMP	C	603	-	-	5/6/26/26	0/3/3/3
2	GTP	F	602	-	-	5/18/38/38	0/3/3/3
3	ATP	C	601	-	-	3/18/38/38	0/3/3/3
4	IMP	H	602	-	-	2/6/26/26	0/3/3/3
3	ATP	C	605	-	-	5/18/38/38	0/3/3/3
5	NAD	E	605	-	-	2/26/62/62	0/5/5/5
2	GTP	B	602	-	-	5/18/38/38	0/3/3/3
3	ATP	G	601	-	-	5/18/38/38	0/3/3/3
5	NAD	B	605	-	-	10/26/62/62	0/5/5/5

All (495) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	GTP	C2'-C3'	-11.12	1.23	1.53
2	A	601	GTP	C2'-C3'	-11.11	1.23	1.53
2	B	601	GTP	C2'-C3'	-11.06	1.23	1.53
2	E	602	GTP	C2'-C3'	-10.77	1.24	1.53
2	F	602	GTP	C2'-C3'	-10.75	1.24	1.53
2	B	602	GTP	C2'-C3'	-10.73	1.24	1.53
3	F	603	ATP	C2'-C3'	-10.69	1.24	1.53
2	F	601	GTP	C2'-C3'	-10.66	1.24	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	ATP	C2'-C3'	-10.65	1.24	1.53
2	A	602	GTP	C2'-C3'	-10.53	1.24	1.53
3	G	601	ATP	C2'-C3'	-10.49	1.24	1.53
3	A	603	ATP	C2'-C3'	-10.46	1.25	1.53
3	C	601	ATP	C2'-C3'	-10.42	1.25	1.53
3	E	603	ATP	C2'-C3'	-10.36	1.25	1.53
3	C	605	ATP	C2'-C3'	-10.34	1.25	1.53
3	G	602	ATP	C2'-C3'	-10.13	1.25	1.53
3	D	601	ATP	C2'-C3'	-10.10	1.26	1.53
3	G	603	ATP	C2'-C3'	-10.09	1.26	1.53
3	C	602	ATP	C2'-C3'	-10.06	1.26	1.53
3	H	601	ATP	C2'-C3'	-10.05	1.26	1.53
4	G	604	IMP	C2-N3	9.95	1.46	1.29
4	C	603	IMP	C2-N3	9.82	1.46	1.29
4	F	604	IMP	C2-N3	9.82	1.46	1.29
4	D	602	IMP	C2-N3	9.77	1.46	1.29
4	H	602	IMP	C2-N3	9.75	1.45	1.29
4	B	604	IMP	C2-N3	9.71	1.45	1.29
4	E	604	IMP	C2-N3	9.65	1.45	1.29
4	A	604	IMP	C2-N3	9.60	1.45	1.29
5	B	605	NAD	C3B-C4B	-9.45	1.29	1.53
5	G	605	NAD	C3D-C4D	-9.14	1.29	1.53
5	C	604	NAD	C3D-C4D	-9.13	1.29	1.53
5	F	605	NAD	C3B-C4B	-9.08	1.30	1.53
5	D	603	NAD	C3D-C4D	-8.95	1.30	1.53
5	B	605	NAD	C3D-C4D	-8.91	1.30	1.53
5	H	603	NAD	C3D-C4D	-8.89	1.30	1.53
5	E	605	NAD	C3D-C4D	-8.85	1.30	1.53
5	F	605	NAD	C3D-C4D	-8.84	1.30	1.53
5	C	604	NAD	C3B-C4B	-8.80	1.30	1.53
5	E	605	NAD	C3B-C4B	-8.78	1.30	1.53
5	G	605	NAD	C3B-C4B	-8.78	1.30	1.53
5	A	605	NAD	C3D-C4D	-8.77	1.30	1.53
5	B	605	NAD	O4D-C1D	-8.76	1.29	1.40
5	A	605	NAD	C3B-C4B	-8.76	1.30	1.53
5	E	605	NAD	O4D-C1D	-8.71	1.29	1.40
5	A	605	NAD	O4D-C1D	-8.60	1.29	1.40
5	D	603	NAD	C3B-C4B	-8.59	1.31	1.53
5	H	603	NAD	C3B-C4B	-8.55	1.31	1.53
5	F	605	NAD	O4D-C1D	-8.55	1.29	1.40
5	H	603	NAD	O4B-C1B	-8.27	1.30	1.40
5	D	603	NAD	O4B-C1B	-8.18	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	605	NAD	O4B-C1B	-8.18	1.30	1.40
2	E	602	GTP	O4'-C1'	8.03	1.51	1.40
5	G	605	NAD	O4D-C1D	-7.99	1.30	1.40
5	B	605	NAD	O4B-C1B	-7.97	1.30	1.40
5	H	603	NAD	O4D-C1D	-7.93	1.30	1.40
5	C	604	NAD	O4D-C1D	-7.91	1.30	1.40
5	D	603	NAD	O4D-C1D	-7.90	1.30	1.40
2	E	601	GTP	O4'-C1'	7.89	1.51	1.40
5	E	605	NAD	O4B-C1B	-7.84	1.30	1.40
2	A	601	GTP	O4'-C1'	7.82	1.51	1.40
5	A	605	NAD	O4B-C1B	-7.82	1.30	1.40
5	G	605	NAD	O4B-C4B	7.80	1.62	1.45
5	C	604	NAD	O4B-C4B	7.76	1.62	1.45
5	E	605	NAD	O4B-C4B	7.68	1.62	1.45
5	A	605	NAD	O4B-C4B	7.67	1.62	1.45
5	G	605	NAD	O4B-C1B	-7.64	1.30	1.40
2	F	602	GTP	O4'-C1'	7.63	1.50	1.40
5	H	603	NAD	O4B-C4B	7.62	1.61	1.45
5	C	604	NAD	O4B-C1B	-7.59	1.30	1.40
2	A	602	GTP	O4'-C1'	7.57	1.50	1.40
5	H	603	NAD	O4D-C4D	7.57	1.61	1.45
5	D	603	NAD	O4B-C4B	7.54	1.61	1.45
5	D	603	NAD	O4D-C4D	7.54	1.61	1.45
5	A	605	NAD	O4D-C4D	7.43	1.61	1.45
5	F	605	NAD	O4B-C4B	7.39	1.61	1.45
5	E	605	NAD	O4D-C4D	7.38	1.61	1.45
3	E	603	ATP	O4'-C1'	-7.36	1.31	1.40
2	B	602	GTP	O4'-C1'	7.30	1.50	1.40
5	G	605	NAD	O4D-C4D	7.26	1.61	1.45
5	B	605	NAD	O4B-C4B	7.22	1.61	1.45
5	C	604	NAD	O4D-C4D	7.19	1.61	1.45
5	F	605	NAD	O4D-C4D	7.18	1.60	1.45
5	B	605	NAD	O4D-C4D	7.07	1.60	1.45
3	D	601	ATP	PB-O3A	7.05	1.67	1.59
3	D	601	ATP	PA-O3A	7.03	1.67	1.59
2	B	601	GTP	O4'-C1'	6.94	1.50	1.40
5	B	605	NAD	C7N-N7N	6.89	1.45	1.33
3	D	601	ATP	O4'-C1'	-6.86	1.31	1.40
2	F	601	GTP	O4'-C1'	6.83	1.49	1.40
2	F	601	GTP	O4'-C4'	-6.82	1.29	1.45
5	F	605	NAD	C7N-N7N	6.82	1.45	1.33
3	C	605	ATP	O4'-C1'	-6.75	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	ATP	O4'-C1'	-6.75	1.32	1.40
3	C	602	ATP	O4'-C1'	-6.74	1.32	1.40
3	G	603	ATP	O4'-C1'	-6.71	1.32	1.40
3	H	601	ATP	O4'-C1'	-6.70	1.32	1.40
3	A	603	ATP	O4'-C1'	-6.68	1.32	1.40
5	C	604	NAD	C7N-N7N	6.66	1.45	1.33
3	G	601	ATP	O4'-C1'	-6.62	1.32	1.40
3	H	601	ATP	PA-O3A	6.62	1.66	1.59
2	B	601	GTP	C1'-N9	-6.61	1.32	1.50
2	F	602	GTP	O4'-C4'	-6.61	1.30	1.45
5	H	603	NAD	C7N-N7N	6.60	1.45	1.33
2	A	601	GTP	O4'-C4'	-6.60	1.30	1.45
5	G	605	NAD	C7N-N7N	6.59	1.45	1.33
2	B	602	GTP	C1'-N9	-6.59	1.32	1.50
3	F	603	ATP	O4'-C1'	-6.58	1.32	1.40
2	A	601	GTP	C1'-N9	-6.58	1.32	1.50
5	A	605	NAD	C7N-N7N	6.57	1.45	1.33
3	G	602	ATP	O4'-C1'	-6.57	1.32	1.40
2	F	602	GTP	C1'-N9	-6.55	1.32	1.50
5	D	603	NAD	C7N-N7N	6.54	1.45	1.33
5	E	605	NAD	C7N-N7N	6.54	1.45	1.33
2	F	601	GTP	C1'-N9	-6.52	1.32	1.50
2	E	601	GTP	O4'-C4'	-6.52	1.30	1.45
2	B	602	GTP	O4'-C4'	-6.49	1.30	1.45
2	E	602	GTP	O4'-C4'	-6.43	1.30	1.45
2	B	601	GTP	O4'-C4'	-6.42	1.30	1.45
2	A	602	GTP	O4'-C4'	-6.40	1.30	1.45
3	C	601	ATP	O4'-C1'	-6.38	1.32	1.40
3	B	603	ATP	PA-O3A	6.37	1.66	1.59
2	E	601	GTP	C1'-N9	-6.36	1.32	1.50
3	H	601	ATP	PB-O3A	6.34	1.66	1.59
3	G	602	ATP	PB-O3A	6.32	1.66	1.59
2	E	602	GTP	C1'-N9	-6.31	1.33	1.50
2	A	602	GTP	C1'-N9	-6.27	1.33	1.50
3	C	601	ATP	PB-O3A	6.24	1.66	1.59
3	C	602	ATP	PA-O3A	6.19	1.66	1.59
3	F	603	ATP	PA-O3A	6.11	1.66	1.59
3	E	603	ATP	PA-O3A	6.05	1.66	1.59
3	G	603	ATP	PB-O3A	5.97	1.65	1.59
3	G	603	ATP	PA-O3A	5.97	1.65	1.59
3	G	601	ATP	PA-O3A	5.96	1.65	1.59
3	C	601	ATP	PA-O3A	5.95	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	ATP	PA-O3A	5.91	1.65	1.59
2	E	602	GTP	PB-O3A	5.91	1.65	1.59
3	B	603	ATP	PB-O3A	5.90	1.65	1.59
3	G	601	ATP	PB-O3A	5.90	1.65	1.59
2	F	601	GTP	C2-N3	5.87	1.47	1.33
2	E	602	GTP	PA-O3A	5.85	1.65	1.59
2	B	602	GTP	C3'-C4'	5.79	1.67	1.53
3	F	603	ATP	PB-O3A	5.79	1.65	1.59
3	C	602	ATP	PB-O3A	5.76	1.65	1.59
2	F	602	GTP	PB-O3B	5.75	1.65	1.59
2	B	601	GTP	C2-N3	5.73	1.47	1.33
2	B	602	GTP	PB-O3B	5.71	1.65	1.59
2	F	602	GTP	PB-O3A	5.68	1.65	1.59
2	A	602	GTP	PB-O3A	5.65	1.65	1.59
2	B	602	GTP	PB-O3A	5.63	1.65	1.59
2	A	602	GTP	PA-O3A	5.57	1.65	1.59
2	A	602	GTP	C3'-C4'	5.53	1.67	1.53
3	C	605	ATP	PA-O3A	5.51	1.65	1.59
2	F	602	GTP	C3'-C4'	5.50	1.66	1.53
2	F	602	GTP	C2-N3	5.47	1.46	1.33
2	F	602	GTP	PA-O3A	5.45	1.65	1.59
2	B	602	GTP	C2-N3	5.43	1.46	1.33
2	F	601	GTP	C2-N2	5.42	1.46	1.34
2	E	602	GTP	C2-N3	5.40	1.46	1.33
2	A	601	GTP	PB-O3B	5.39	1.65	1.59
3	A	603	ATP	PA-O3A	5.39	1.65	1.59
2	B	601	GTP	C2-N2	5.38	1.46	1.34
2	A	602	GTP	PB-O3B	5.37	1.65	1.59
2	E	601	GTP	PA-O3A	5.35	1.65	1.59
2	E	602	GTP	PB-O3B	5.34	1.65	1.59
2	A	602	GTP	C2-N3	5.33	1.46	1.33
2	F	601	GTP	C3'-C4'	5.31	1.66	1.53
2	E	601	GTP	PB-O3A	5.31	1.65	1.59
2	B	601	GTP	C3'-C4'	5.29	1.66	1.53
2	A	601	GTP	C2-N3	5.26	1.46	1.33
2	F	601	GTP	C4-N3	5.26	1.49	1.37
2	E	602	GTP	C3'-C4'	5.24	1.66	1.53
2	B	602	GTP	PA-O3A	5.23	1.65	1.59
2	A	601	GTP	C2-N2	5.23	1.46	1.34
3	C	605	ATP	PB-O3A	5.20	1.65	1.59
2	E	601	GTP	C2-N2	5.13	1.46	1.34
2	E	602	GTP	C2-N2	5.11	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	GTP	C4-N3	5.10	1.49	1.37
2	A	601	GTP	PA-O3A	5.10	1.65	1.59
2	B	601	GTP	PB-O3A	5.08	1.65	1.59
2	A	602	GTP	C2-N2	5.08	1.46	1.34
5	H	603	NAD	PN-O3	5.06	1.65	1.59
5	D	603	NAD	PN-O3	5.06	1.65	1.59
2	E	601	GTP	C3'-C4'	5.06	1.65	1.53
2	F	602	GTP	C2-N2	5.05	1.46	1.34
2	B	602	GTP	C2-N2	5.05	1.46	1.34
2	A	601	GTP	C4-N3	5.05	1.49	1.37
2	A	601	GTP	C3'-C4'	5.04	1.65	1.53
3	A	603	ATP	PB-O3A	5.04	1.64	1.59
2	E	601	GTP	C2-N3	5.00	1.45	1.33
5	H	603	NAD	PA-O3	4.98	1.64	1.59
5	D	603	NAD	PA-O3	4.98	1.64	1.59
3	E	603	ATP	PB-O3A	4.98	1.64	1.59
2	F	602	GTP	C4-N3	4.95	1.49	1.37
2	F	601	GTP	PB-O3B	4.95	1.64	1.59
2	A	601	GTP	PB-O3A	4.92	1.64	1.59
2	B	601	GTP	PB-O3B	4.89	1.64	1.59
2	B	601	GTP	PA-O3A	4.88	1.64	1.59
2	E	601	GTP	PB-O3B	4.88	1.64	1.59
2	A	602	GTP	C4-N3	4.87	1.49	1.37
2	B	602	GTP	C4-N3	4.87	1.49	1.37
2	E	602	GTP	C4-N3	4.87	1.49	1.37
2	E	601	GTP	C4-N3	4.84	1.48	1.37
4	H	602	IMP	C2-N1	4.84	1.43	1.35
4	D	602	IMP	C2-N1	4.80	1.43	1.35
4	G	604	IMP	C2-N1	4.79	1.43	1.35
3	G	602	ATP	PB-O3B	4.76	1.64	1.59
4	C	603	IMP	C2-N1	4.72	1.43	1.35
5	G	605	NAD	PN-O3	4.69	1.64	1.59
5	C	604	NAD	PN-O3	4.51	1.64	1.59
2	F	601	GTP	PA-O3A	4.49	1.64	1.59
2	F	601	GTP	PB-O3A	4.48	1.64	1.59
5	G	605	NAD	PA-O3	4.47	1.64	1.59
4	A	604	IMP	C2-N1	4.41	1.43	1.35
5	C	604	NAD	PA-O3	4.40	1.64	1.59
5	B	605	NAD	PA-O3	4.30	1.64	1.59
4	E	604	IMP	C2-N1	4.28	1.43	1.35
4	F	604	IMP	C2-N1	4.26	1.42	1.35
3	B	603	ATP	C1'-N9	-4.17	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	603	ATP	C1'-N9	-4.12	1.39	1.49
2	E	601	GTP	C6-N1	4.11	1.44	1.37
3	B	603	ATP	C5'-C4'	-4.06	1.39	1.51
3	F	603	ATP	C5'-C4'	-3.99	1.39	1.51
5	A	605	NAD	PN-O3	3.95	1.63	1.59
3	C	601	ATP	C1'-N9	-3.94	1.40	1.49
5	E	605	NAD	PN-O3	3.94	1.63	1.59
3	C	601	ATP	PB-O3B	3.93	1.63	1.59
2	A	601	GTP	C6-N1	3.93	1.43	1.37
3	G	602	ATP	C1'-N9	-3.87	1.40	1.49
5	F	605	NAD	PN-O3	3.86	1.63	1.59
3	C	602	ATP	C1'-N9	-3.84	1.40	1.49
4	B	604	IMP	C2-N1	3.83	1.42	1.35
3	C	602	ATP	C5'-C4'	-3.82	1.40	1.51
5	F	605	NAD	PA-O3	3.79	1.63	1.59
3	G	601	ATP	C1'-N9	-3.79	1.40	1.49
3	C	605	ATP	C1'-N9	-3.77	1.40	1.49
5	A	605	NAD	PA-O3	3.76	1.63	1.59
3	A	603	ATP	C5'-C4'	-3.75	1.40	1.51
3	G	603	ATP	C1'-N9	-3.74	1.40	1.49
2	B	602	GTP	C6-N1	3.73	1.43	1.37
3	E	603	ATP	C5'-C4'	-3.73	1.40	1.51
4	F	604	IMP	C4-N3	3.72	1.48	1.37
3	D	601	ATP	PB-O3B	3.71	1.63	1.59
3	E	603	ATP	C1'-N9	-3.71	1.40	1.49
2	F	602	GTP	C6-N1	3.70	1.43	1.37
3	D	601	ATP	C1'-N9	-3.67	1.40	1.49
5	B	605	NAD	PN-O3	3.66	1.63	1.59
5	E	605	NAD	PA-O3	3.65	1.63	1.59
3	G	603	ATP	C5'-C4'	-3.63	1.40	1.51
4	D	602	IMP	C4-N3	3.59	1.48	1.37
3	G	601	ATP	C5'-C4'	-3.58	1.40	1.51
3	H	601	ATP	C1'-N9	-3.56	1.41	1.49
4	H	602	IMP	C4-N3	3.55	1.48	1.37
3	C	605	ATP	C5'-C4'	-3.53	1.40	1.51
3	G	602	ATP	C5'-C4'	-3.51	1.41	1.51
4	B	604	IMP	C4-N3	3.50	1.48	1.37
3	D	601	ATP	C5'-C4'	-3.48	1.41	1.51
2	A	602	GTP	C6-N1	3.47	1.43	1.37
4	G	604	IMP	C4-N3	3.47	1.48	1.37
3	A	603	ATP	C1'-N9	-3.46	1.41	1.49
2	F	601	GTP	C6-N1	3.46	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	GTP	C6-N1	3.45	1.43	1.37
3	H	601	ATP	C3'-C4'	3.44	1.61	1.53
4	A	604	IMP	C4-N3	3.43	1.48	1.37
5	F	605	NAD	C4N-C3N	-3.43	1.34	1.39
4	E	604	IMP	C4-N3	3.42	1.47	1.37
4	C	603	IMP	C4-N3	3.41	1.47	1.37
5	A	605	NAD	O7N-C7N	-3.40	1.17	1.24
3	H	601	ATP	C5'-C4'	-3.39	1.41	1.51
2	A	602	GTP	C5-C6	3.38	1.54	1.47
2	E	602	GTP	C6-N1	3.37	1.42	1.37
4	F	604	IMP	C5-C4	-3.36	1.34	1.43
5	E	605	NAD	O7N-C7N	-3.35	1.17	1.24
3	D	601	ATP	C3'-C4'	3.35	1.61	1.53
3	C	602	ATP	PB-O3B	3.33	1.63	1.59
2	A	602	GTP	O2'-C2'	3.32	1.51	1.43
3	C	601	ATP	C5'-C4'	-3.32	1.41	1.51
2	A	601	GTP	O2'-C2'	3.30	1.51	1.43
2	E	602	GTP	C5-C6	3.28	1.53	1.47
4	E	604	IMP	C5-C4	-3.28	1.35	1.43
2	E	602	GTP	O2'-C2'	3.27	1.51	1.43
5	C	604	NAD	O7N-C7N	-3.24	1.18	1.24
2	E	601	GTP	O2'-C2'	3.24	1.51	1.43
5	B	605	NAD	C4N-C3N	-3.24	1.34	1.39
2	F	602	GTP	O2'-C2'	3.23	1.51	1.43
2	B	602	GTP	O2'-C2'	3.23	1.51	1.43
4	B	604	IMP	C5-C4	-3.23	1.35	1.43
4	A	604	IMP	C5-C4	-3.22	1.35	1.43
3	H	601	ATP	O3'-C3'	3.21	1.50	1.43
3	G	603	ATP	PB-O3B	3.21	1.63	1.59
3	C	605	ATP	O3'-C3'	3.21	1.50	1.43
5	G	605	NAD	O7N-C7N	-3.20	1.18	1.24
4	C	603	IMP	C5-C4	-3.20	1.35	1.43
5	E	605	NAD	O2D-C2D	-3.19	1.35	1.43
3	D	601	ATP	O3'-C3'	3.19	1.50	1.43
4	G	604	IMP	C5-C4	-3.17	1.35	1.43
5	F	605	NAD	O2D-C2D	-3.17	1.35	1.43
5	H	603	NAD	O7N-C7N	-3.16	1.18	1.24
5	D	603	NAD	O7N-C7N	-3.16	1.18	1.24
4	H	602	IMP	C5-C4	-3.16	1.35	1.43
3	G	603	ATP	O3'-C3'	3.15	1.50	1.43
2	B	601	GTP	O2'-C2'	3.15	1.50	1.43
2	F	602	GTP	C5-C6	3.14	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	603	ATP	C3'-C4'	3.14	1.61	1.53
5	B	605	NAD	O7N-C7N	-3.14	1.18	1.24
5	B	605	NAD	O2D-C2D	-3.14	1.35	1.43
3	C	605	ATP	C3'-C4'	3.14	1.60	1.53
2	B	602	GTP	C5-C6	3.14	1.53	1.47
5	F	605	NAD	O7N-C7N	-3.13	1.18	1.24
3	H	601	ATP	PB-O3B	3.13	1.62	1.59
3	D	601	ATP	PA-O5'	3.12	1.71	1.59
4	D	602	IMP	C5-C4	-3.12	1.35	1.43
3	C	601	ATP	O3'-C3'	3.12	1.50	1.43
3	H	601	ATP	PA-O5'	3.12	1.71	1.59
3	G	602	ATP	O3'-C3'	3.12	1.50	1.43
3	G	601	ATP	O3'-C3'	3.12	1.50	1.43
2	E	601	GTP	C5-C6	3.12	1.53	1.47
5	H	603	NAD	C4N-C3N	-3.11	1.34	1.39
3	G	601	ATP	C3'-C4'	3.09	1.60	1.53
3	G	602	ATP	C3'-C4'	3.09	1.60	1.53
3	C	602	ATP	O3'-C3'	3.09	1.50	1.43
2	F	601	GTP	O2'-C2'	3.09	1.50	1.43
5	H	603	NAD	C6A-N6A	3.08	1.45	1.34
5	A	605	NAD	O2D-C2D	-3.08	1.35	1.43
5	C	604	NAD	O2D-C2D	-3.07	1.35	1.43
5	D	603	NAD	C4N-C3N	-3.07	1.34	1.39
3	C	601	ATP	C3'-C4'	3.06	1.60	1.53
2	F	601	GTP	C5-C6	3.06	1.53	1.47
3	A	603	ATP	O3'-C3'	3.06	1.50	1.43
5	G	605	NAD	O2D-C2D	-3.06	1.35	1.43
5	D	603	NAD	C6A-N6A	3.05	1.45	1.34
3	E	603	ATP	O3'-C3'	3.03	1.50	1.43
5	F	605	NAD	O2B-C2B	-3.03	1.35	1.43
5	C	604	NAD	C6A-N6A	3.03	1.44	1.34
3	G	601	ATP	PB-O3B	3.02	1.62	1.59
5	G	605	NAD	C6A-N6A	3.01	1.44	1.34
3	C	602	ATP	C3'-C4'	3.01	1.60	1.53
2	B	601	GTP	C5-C6	3.01	1.53	1.47
3	A	603	ATP	C3'-C4'	3.00	1.60	1.53
3	G	603	ATP	C3'-C4'	3.00	1.60	1.53
3	G	603	ATP	PA-O5'	3.00	1.71	1.59
4	B	604	IMP	O6-C6	-2.99	1.16	1.23
2	F	601	GTP	C2-N1	2.97	1.44	1.37
5	D	603	NAD	O2B-C2B	-2.97	1.35	1.43
5	F	605	NAD	C6A-N6A	2.97	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	ATP	PA-O5'	2.97	1.71	1.59
5	E	605	NAD	C6A-N6A	2.96	1.44	1.34
3	E	603	ATP	PA-O5'	2.96	1.71	1.59
5	B	605	NAD	C6A-N6A	2.96	1.44	1.34
3	C	601	ATP	PA-O5'	2.95	1.70	1.59
5	B	605	NAD	O2B-C2B	-2.95	1.35	1.43
3	C	605	ATP	PA-O5'	2.95	1.70	1.59
2	B	601	GTP	C2-N1	2.95	1.44	1.37
5	A	605	NAD	C6A-N6A	2.95	1.44	1.34
2	E	601	GTP	C2-N1	2.94	1.44	1.37
5	D	603	NAD	O2D-C2D	-2.94	1.35	1.43
2	A	601	GTP	C2-N1	2.93	1.44	1.37
5	H	603	NAD	O2D-C2D	-2.92	1.35	1.43
2	A	601	GTP	C5-C6	2.92	1.53	1.47
2	A	602	GTP	C2-N1	2.92	1.44	1.37
5	H	603	NAD	O2B-C2B	-2.91	1.35	1.43
2	E	602	GTP	C2-N1	2.91	1.44	1.37
3	F	603	ATP	O3'-C3'	2.90	1.50	1.43
3	B	603	ATP	O3'-C3'	2.90	1.50	1.43
5	A	605	NAD	C4N-C3N	-2.89	1.35	1.39
3	G	601	ATP	PA-O5'	2.88	1.70	1.59
5	C	604	NAD	C4N-C3N	-2.87	1.35	1.39
3	G	602	ATP	PA-O5'	2.87	1.70	1.59
5	C	604	NAD	O2B-C2B	-2.86	1.35	1.43
5	E	605	NAD	O2B-C2B	-2.86	1.35	1.43
5	G	605	NAD	C4N-C3N	-2.85	1.35	1.39
5	E	605	NAD	C4N-C3N	-2.85	1.35	1.39
5	G	605	NAD	O2B-C2B	-2.85	1.35	1.43
2	E	601	GTP	C5-C4	-2.82	1.36	1.43
3	A	603	ATP	O4'-C4'	2.81	1.51	1.45
5	A	605	NAD	O2B-C2B	-2.81	1.36	1.43
3	F	603	ATP	PA-O5'	2.80	1.70	1.59
3	B	603	ATP	PA-O5'	2.80	1.70	1.59
2	F	602	GTP	C2-N1	2.78	1.44	1.37
3	H	601	ATP	C6-N6	2.78	1.44	1.34
3	C	601	ATP	O4'-C4'	2.78	1.51	1.45
3	A	603	ATP	PA-O5'	2.77	1.70	1.59
3	E	603	ATP	C6-N6	2.77	1.44	1.34
5	E	605	NAD	O3B-C3B	2.77	1.49	1.43
3	H	601	ATP	O4'-C4'	2.77	1.51	1.45
2	B	602	GTP	C2-N1	2.76	1.44	1.37
3	A	603	ATP	C6-N6	2.76	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	602	ATP	O4'-C4'	2.74	1.51	1.45
3	G	601	ATP	C6-N6	2.74	1.43	1.34
3	D	601	ATP	C6-N6	2.74	1.43	1.34
2	A	601	GTP	C5-C4	-2.73	1.36	1.43
3	C	601	ATP	C6-N6	2.73	1.43	1.34
3	G	602	ATP	C6-N6	2.73	1.43	1.34
5	A	605	NAD	O3B-C3B	2.73	1.49	1.43
2	B	602	GTP	C5-C4	-2.72	1.36	1.43
3	E	603	ATP	PB-O3B	2.72	1.62	1.59
3	C	605	ATP	C6-N6	2.72	1.43	1.34
3	C	605	ATP	PB-O3B	2.71	1.62	1.59
5	G	605	NAD	O3B-C3B	2.70	1.49	1.43
5	C	604	NAD	O3B-C3B	2.70	1.49	1.43
5	H	603	NAD	O3B-C3B	2.69	1.49	1.43
5	D	603	NAD	O3B-C3B	2.69	1.49	1.43
2	F	602	GTP	C5-C4	-2.68	1.36	1.43
4	F	604	IMP	O6-C6	-2.68	1.17	1.23
3	G	603	ATP	C6-N6	2.67	1.43	1.34
3	D	601	ATP	O4'-C4'	2.67	1.50	1.45
3	F	603	ATP	C6-N6	2.66	1.43	1.34
3	A	603	ATP	PB-O3B	2.65	1.62	1.59
3	B	603	ATP	C6-N6	2.63	1.43	1.34
5	D	603	NAD	O3D-C3D	2.62	1.49	1.43
3	G	603	ATP	O4'-C4'	2.62	1.50	1.45
5	F	605	NAD	O3B-C3B	2.61	1.49	1.43
5	H	603	NAD	O3D-C3D	2.60	1.49	1.43
3	F	603	ATP	C3'-C4'	2.60	1.59	1.53
4	D	602	IMP	C6-N1	2.60	1.42	1.38
5	B	605	NAD	C5N-C4N	-2.60	1.34	1.38
3	B	603	ATP	C3'-C4'	2.58	1.59	1.53
3	C	602	ATP	O4'-C4'	2.58	1.50	1.45
5	G	605	NAD	O3D-C3D	2.57	1.49	1.43
3	E	603	ATP	O4'-C4'	2.57	1.50	1.45
5	C	604	NAD	O3D-C3D	2.56	1.49	1.43
5	B	605	NAD	O3B-C3B	2.56	1.49	1.43
3	C	602	ATP	C6-N6	2.55	1.43	1.34
5	F	605	NAD	C5N-C4N	-2.55	1.34	1.38
2	E	602	GTP	C5-C4	-2.55	1.36	1.43
3	G	601	ATP	O4'-C4'	2.55	1.50	1.45
5	A	605	NAD	O3D-C3D	2.54	1.49	1.43
5	F	605	NAD	O3D-C3D	2.54	1.49	1.43
2	B	601	GTP	C5-C4	-2.53	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	605	NAD	O3D-C3D	2.53	1.49	1.43
5	B	605	NAD	O3D-C3D	2.52	1.49	1.43
2	A	602	GTP	C5-C4	-2.51	1.36	1.43
4	H	602	IMP	C6-N1	2.51	1.42	1.38
3	F	603	ATP	PB-O3B	2.46	1.62	1.59
2	F	601	GTP	C5-C4	-2.46	1.37	1.43
3	C	605	ATP	O4'-C4'	2.44	1.50	1.45
4	D	602	IMP	C5-C6	2.44	1.52	1.47
4	A	604	IMP	C5-C6	2.43	1.52	1.47
3	G	603	ATP	C2-N3	2.43	1.35	1.32
3	G	602	ATP	O2'-C2'	2.41	1.48	1.43
3	B	603	ATP	PB-O3B	2.40	1.62	1.59
3	C	602	ATP	C2-N3	2.38	1.35	1.32
3	G	601	ATP	O2'-C2'	2.37	1.48	1.43
3	C	602	ATP	O2'-C2'	2.36	1.48	1.43
3	H	601	ATP	C2-N3	2.36	1.35	1.32
4	H	602	IMP	C5-C6	2.36	1.52	1.47
3	G	603	ATP	O2'-C2'	2.35	1.48	1.43
3	C	605	ATP	O2'-C2'	2.35	1.48	1.43
3	G	602	ATP	C2-N3	2.33	1.35	1.32
3	C	601	ATP	O2'-C2'	2.33	1.48	1.43
4	A	604	IMP	C6-N1	2.32	1.42	1.38
3	A	603	ATP	O2'-C2'	2.31	1.48	1.43
3	F	603	ATP	O4'-C4'	2.31	1.50	1.45
3	D	601	ATP	O2'-C2'	2.31	1.48	1.43
4	C	603	IMP	O6-C6	-2.31	1.18	1.23
3	D	601	ATP	C2-N3	2.31	1.35	1.32
4	E	604	IMP	O6-C6	-2.31	1.18	1.23
3	H	601	ATP	O2'-C2'	2.30	1.48	1.43
3	C	601	ATP	C2-N3	2.30	1.35	1.32
4	C	603	IMP	C6-N1	2.30	1.42	1.38
2	A	602	GTP	O3'-C3'	2.29	1.48	1.43
4	G	604	IMP	C6-N1	2.27	1.42	1.38
2	B	602	GTP	O3'-C3'	2.27	1.48	1.43
2	E	602	GTP	O3'-C3'	2.25	1.48	1.43
5	H	603	NAD	C5N-C4N	-2.24	1.35	1.38
2	F	602	GTP	O3'-C3'	2.22	1.48	1.43
4	G	604	IMP	O6-C6	-2.22	1.18	1.23
4	E	604	IMP	C5-C6	2.21	1.51	1.47
3	E	603	ATP	O2'-C2'	2.20	1.48	1.43
5	D	603	NAD	C5N-C4N	-2.20	1.35	1.38
4	E	604	IMP	C6-N1	2.20	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	IMP	O6-C6	-2.19	1.18	1.23
2	E	601	GTP	O3'-C3'	2.19	1.48	1.43
3	F	603	ATP	O2'-C2'	2.16	1.48	1.43
3	B	603	ATP	O4'-C4'	2.15	1.49	1.45
3	B	603	ATP	O2'-C2'	2.15	1.48	1.43
4	C	603	IMP	C5-C6	2.14	1.51	1.47
5	F	605	NAD	C2A-N3A	2.13	1.35	1.32
2	A	601	GTP	O3'-C3'	2.13	1.48	1.43
4	B	604	IMP	C5-C6	2.12	1.51	1.47
2	F	601	GTP	O3'-C3'	2.12	1.48	1.43
4	G	604	IMP	C1'-N9	-2.06	1.44	1.50
3	G	601	ATP	C2-N3	2.06	1.35	1.32
5	B	605	NAD	C2A-N3A	2.06	1.35	1.32
4	H	602	IMP	O6-C6	-2.06	1.18	1.23
4	G	604	IMP	C5-C6	2.06	1.51	1.47
5	A	605	NAD	C5N-C4N	-2.05	1.35	1.38
3	E	603	ATP	C2-N3	2.05	1.35	1.32
5	H	603	NAD	C2A-N3A	2.04	1.35	1.32
4	F	604	IMP	C6-N1	2.04	1.41	1.38
2	B	601	GTP	O3'-C3'	2.04	1.48	1.43
4	D	602	IMP	O6-C6	-2.03	1.18	1.23
2	E	602	GTP	O6-C6	-2.02	1.18	1.23
3	A	603	ATP	C2-N3	2.02	1.35	1.32
2	B	602	GTP	O6-C6	-2.01	1.18	1.23
5	E	605	NAD	C5N-C4N	-2.01	1.35	1.38

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	603	ATP	C5-C6-N6	14.99	143.14	120.31
3	F	603	ATP	C5-C6-N6	14.90	143.01	120.31
3	E	603	ATP	C5-C6-N6	14.83	142.90	120.31
3	B	603	ATP	C5-C6-N6	14.61	142.56	120.31
3	C	605	ATP	C5-C6-N6	14.26	142.04	120.31
3	G	601	ATP	C5-C6-N6	14.21	141.96	120.31
3	G	602	ATP	C5-C6-N6	14.18	141.91	120.31
3	H	601	ATP	C5-C6-N6	14.15	141.87	120.31
3	C	601	ATP	C5-C6-N6	14.15	141.86	120.31
3	D	601	ATP	C5-C6-N6	14.10	141.79	120.31
3	G	603	ATP	C5-C6-N6	13.99	141.62	120.31
3	C	602	ATP	C5-C6-N6	13.73	141.22	120.31
2	F	601	GTP	C4'-O4'-C1'	-12.12	98.82	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	605	NAD	C4D-O4D-C1D	-11.72	99.19	109.92
5	D	603	NAD	C5A-C6A-N6A	11.27	137.47	120.31
5	H	603	NAD	C5A-C6A-N6A	11.18	137.34	120.31
5	E	605	NAD	C5A-C6A-N6A	11.00	137.07	120.31
5	F	605	NAD	C5A-C6A-N6A	11.00	137.06	120.31
5	A	605	NAD	C5A-C6A-N6A	10.92	136.95	120.31
5	B	605	NAD	C5A-C6A-N6A	10.92	136.95	120.31
5	C	604	NAD	C4D-O4D-C1D	-10.92	99.93	109.92
3	E	603	ATP	C1'-N9-C4	-10.68	107.88	126.64
3	A	603	ATP	C1'-N9-C4	-10.65	107.92	126.64
2	B	602	GTP	C4'-O4'-C1'	-10.53	100.28	109.92
5	C	604	NAD	C5A-C6A-N6A	10.52	136.34	120.31
5	G	605	NAD	C5A-C6A-N6A	10.47	136.26	120.31
2	A	602	GTP	C4'-O4'-C1'	-10.46	100.35	109.92
5	B	605	NAD	C4D-O4D-C1D	-10.39	100.41	109.92
3	B	603	ATP	C1'-N9-C4	-10.37	108.42	126.64
5	F	605	NAD	C4D-O4D-C1D	-10.35	100.45	109.92
3	F	603	ATP	C1'-N9-C4	-10.22	108.69	126.64
3	C	605	ATP	C1'-N9-C4	-10.09	108.91	126.64
3	G	601	ATP	C1'-N9-C4	-10.07	108.95	126.64
3	E	603	ATP	C4'-O4'-C1'	-9.96	100.80	109.92
3	A	603	ATP	N6-C6-N1	-9.86	97.27	118.33
5	E	605	NAD	C4D-O4D-C1D	-9.83	100.92	109.92
3	E	603	ATP	N6-C6-N1	-9.82	97.34	118.33
2	F	602	GTP	C4'-O4'-C1'	-9.70	101.04	109.92
3	F	603	ATP	N6-C6-N1	-9.69	97.62	118.33
3	H	601	ATP	C1'-N9-C4	-9.66	109.67	126.64
3	D	601	ATP	C1'-N9-C4	-9.65	109.68	126.64
3	G	602	ATP	N6-C6-N1	-9.55	97.93	118.33
3	C	602	ATP	C1'-N9-C4	-9.54	109.87	126.64
3	C	601	ATP	C1'-N9-C4	-9.54	109.88	126.64
3	B	603	ATP	N6-C6-N1	-9.53	97.98	118.33
3	G	602	ATP	C1'-N9-C4	-9.50	109.96	126.64
3	G	603	ATP	C1'-N9-C4	-9.47	110.00	126.64
3	H	601	ATP	N6-C6-N1	-9.42	98.21	118.33
3	G	603	ATP	N6-C6-N1	-9.40	98.25	118.33
3	C	605	ATP	N6-C6-N1	-9.38	98.28	118.33
3	D	601	ATP	N6-C6-N1	-9.38	98.30	118.33
3	C	602	ATP	N6-C6-N1	-9.36	98.33	118.33
3	C	601	ATP	N6-C6-N1	-9.36	98.33	118.33
3	G	601	ATP	N6-C6-N1	-9.31	98.44	118.33
5	D	603	NAD	C1B-N9A-C4A	-9.19	110.50	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	603	NAD	C1B-N9A-C4A	-9.16	110.55	126.64
5	A	605	NAD	C4D-O4D-C1D	-9.13	101.56	109.92
3	H	601	ATP	C4'-O4'-C1'	-9.07	101.62	109.92
5	A	605	NAD	C1B-N9A-C4A	-8.54	111.64	126.64
3	B	603	ATP	C4'-O4'-C1'	-8.52	102.13	109.92
5	E	605	NAD	C1B-N9A-C4A	-8.52	111.68	126.64
5	C	604	NAD	C1B-N9A-C4A	-8.32	112.02	126.64
5	G	605	NAD	C1B-N9A-C4A	-8.20	112.24	126.64
5	B	605	NAD	C1B-N9A-C4A	-8.11	112.39	126.64
3	F	603	ATP	C4'-O4'-C1'	-8.04	102.56	109.92
5	F	605	NAD	C1B-N9A-C4A	-7.91	112.75	126.64
2	E	602	GTP	C4'-O4'-C1'	-7.82	102.76	109.92
5	D	603	NAD	N6A-C6A-N1A	-7.52	102.28	118.33
5	H	603	NAD	N6A-C6A-N1A	-7.43	102.45	118.33
5	E	605	NAD	N6A-C6A-N1A	-7.34	102.66	118.33
5	A	605	NAD	N6A-C6A-N1A	-7.30	102.73	118.33
5	F	605	NAD	N6A-C6A-N1A	-7.26	102.82	118.33
5	B	605	NAD	N6A-C6A-N1A	-7.18	102.99	118.33
3	D	601	ATP	C4'-O4'-C1'	-7.17	103.36	109.92
3	F	603	ATP	N3-C2-N1	-7.11	119.01	128.67
3	B	603	ATP	N3-C2-N1	-7.08	119.06	128.67
5	C	604	NAD	N6A-C6A-N1A	-7.00	103.37	118.33
3	A	603	ATP	N3-C2-N1	-6.98	119.19	128.67
5	G	605	NAD	N6A-C6A-N1A	-6.97	103.43	118.33
3	E	603	ATP	N3-C2-N1	-6.81	119.43	128.67
5	D	603	NAD	N3A-C2A-N1A	-6.79	119.46	128.67
5	H	603	NAD	N3A-C2A-N1A	-6.75	119.51	128.67
3	G	602	ATP	N3-C2-N1	-6.73	119.54	128.67
3	C	601	ATP	N3-C2-N1	-6.72	119.54	128.67
3	C	602	ATP	N3-C2-N1	-6.62	119.69	128.67
5	C	604	NAD	N3A-C2A-N1A	-6.61	119.69	128.67
5	G	605	NAD	N3A-C2A-N1A	-6.61	119.70	128.67
3	D	601	ATP	N3-C2-N1	-6.61	119.70	128.67
3	G	603	ATP	N3-C2-N1	-6.61	119.70	128.67
3	H	601	ATP	N3-C2-N1	-6.61	119.70	128.67
5	B	605	NAD	N3A-C2A-N1A	-6.46	119.91	128.67
3	G	601	ATP	N3-C2-N1	-6.45	119.91	128.67
5	F	605	NAD	N3A-C2A-N1A	-6.45	119.92	128.67
3	C	602	ATP	C4'-O4'-C1'	-6.39	104.07	109.92
3	C	605	ATP	N3-C2-N1	-6.39	120.00	128.67
5	E	605	NAD	N3A-C2A-N1A	-6.22	120.23	128.67
5	A	605	NAD	N3A-C2A-N1A	-6.17	120.30	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	603	NAD	C4B-O4B-C1B	-6.12	104.32	109.92
5	D	603	NAD	C4B-O4B-C1B	-6.10	104.34	109.92
3	G	603	ATP	C4'-O4'-C1'	-6.06	104.38	109.92
5	B	605	NAD	C4B-O4B-C1B	-5.98	104.45	109.92
4	B	604	IMP	C2-N1-C6	-5.68	116.59	123.42
2	A	601	GTP	C4'-O4'-C1'	-5.59	104.80	109.92
2	B	601	GTP	C4'-O4'-C1'	-5.48	104.91	109.92
3	C	605	ATP	C4'-O4'-C1'	-5.35	105.02	109.92
4	F	604	IMP	C2-N1-C6	-4.69	117.79	123.42
3	G	601	ATP	C4'-O4'-C1'	-4.67	105.65	109.92
4	C	603	IMP	C2-N1-C6	-4.32	118.23	123.42
4	G	604	IMP	C2-N1-C6	-4.32	118.23	123.42
3	A	603	ATP	C4'-O4'-C1'	-4.22	106.06	109.92
4	E	604	IMP	C2-N1-C6	-4.17	118.41	123.42
2	F	601	GTP	O4'-C1'-N9	4.16	114.26	108.75
4	B	604	IMP	C5-C6-N1	4.09	121.88	114.07
2	E	601	GTP	C4'-O4'-C1'	-4.07	106.20	109.92
3	C	601	ATP	C4'-O4'-C1'	-4.05	106.22	109.92
4	F	604	IMP	C5-C6-N1	4.02	121.74	114.07
4	A	604	IMP	C2-N1-C6	-4.02	118.59	123.42
4	H	602	IMP	C2-N1-C6	-3.67	119.02	123.42
2	A	602	GTP	O4'-C1'-N9	3.65	113.58	108.75
4	F	604	IMP	O6-C6-C5	-3.57	117.24	124.32
4	D	602	IMP	C8-N7-C5	3.53	108.56	102.55
2	A	602	GTP	C8-N7-C5	3.49	108.50	102.55
4	D	602	IMP	C2-N1-C6	-3.48	119.24	123.42
4	G	604	IMP	C8-N7-C5	3.43	108.38	102.55
4	E	604	IMP	C5-C6-N1	3.42	120.60	114.07
4	C	603	IMP	C8-N7-C5	3.41	108.35	102.55
3	G	602	ATP	C4'-O4'-C1'	-3.40	106.81	109.92
4	H	602	IMP	C8-N7-C5	3.36	108.27	102.55
2	E	602	GTP	C8-N7-C5	3.32	108.20	102.55
4	A	604	IMP	C5-C6-N1	3.31	120.39	114.07
2	F	602	GTP	C5-C6-N1	3.28	120.33	114.07
2	B	602	GTP	C5-C6-N1	3.25	120.28	114.07
4	C	603	IMP	C5-C6-N1	3.25	120.27	114.07
2	E	601	GTP	C5-C6-N1	3.25	120.27	114.07
2	B	602	GTP	C8-N7-C5	3.19	107.99	102.55
2	F	602	GTP	C2-N1-C6	-3.19	119.28	125.11
2	B	602	GTP	C2-N1-C6	-3.18	119.29	125.11
4	B	604	IMP	O6-C6-C5	-3.18	118.03	124.32
4	G	604	IMP	O6-C6-C5	-3.13	118.11	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	601	GTP	C8-N7-C5	3.13	107.88	102.55
4	C	603	IMP	O6-C6-C5	-3.13	118.12	124.32
2	E	602	GTP	C2-N1-C6	-3.11	119.41	125.11
2	F	602	GTP	C8-N7-C5	3.11	107.85	102.55
2	E	601	GTP	C8-N7-C5	3.11	107.84	102.55
2	A	601	GTP	C8-N7-C5	3.11	107.84	102.55
4	A	604	IMP	C8-N7-C5	3.08	107.80	102.55
4	H	602	IMP	C5-C6-N1	3.07	119.93	114.07
2	E	601	GTP	C2-N1-C6	-3.07	119.49	125.11
4	F	604	IMP	C8-N7-C5	3.07	107.77	102.55
2	A	602	GTP	C2-N1-C6	-3.07	119.50	125.11
2	A	601	GTP	C5-C6-N1	3.06	119.92	114.07
2	B	601	GTP	C8-N7-C5	3.06	107.76	102.55
4	E	604	IMP	C8-N7-C5	3.06	107.76	102.55
4	G	604	IMP	C5-C6-N1	3.05	119.89	114.07
4	B	604	IMP	C8-N7-C5	3.04	107.73	102.55
2	B	601	GTP	C2-N1-C6	-3.04	119.54	125.11
4	E	604	IMP	O6-C6-C5	-3.00	118.37	124.32
2	F	601	GTP	C2-N1-C6	-2.98	119.66	125.11
4	D	602	IMP	C5-C6-N1	2.97	119.75	114.07
2	F	601	GTP	C5-C6-N1	2.96	119.72	114.07
2	E	602	GTP	C5-C6-N1	2.95	119.70	114.07
2	A	602	GTP	C5-C6-N1	2.94	119.68	114.07
2	A	601	GTP	C2-N1-C6	-2.91	119.79	125.11
3	E	603	ATP	O4'-C1'-N9	2.90	112.59	108.75
2	B	601	GTP	C5-C6-N1	2.88	119.56	114.07
2	E	601	GTP	N2-C2-N1	2.87	122.82	116.76
5	B	605	NAD	C2N-C3N-C4N	2.86	121.58	118.26
2	E	602	GTP	O4'-C1'-N9	2.77	112.42	108.75
4	H	602	IMP	O6-C6-C5	-2.77	118.83	124.32
5	A	605	NAD	C4B-O4B-C1B	-2.75	107.41	109.92
5	H	603	NAD	C2N-C3N-C4N	2.75	121.45	118.26
4	A	604	IMP	O6-C6-C5	-2.73	118.90	124.32
5	D	603	NAD	C2N-C3N-C4N	2.71	121.42	118.26
5	E	605	NAD	C4B-O4B-C1B	-2.65	107.50	109.92
5	H	603	NAD	C4D-O4D-C1D	-2.65	107.50	109.92
5	D	603	NAD	C4D-O4D-C1D	-2.62	107.53	109.92
3	G	602	ATP	C2'-C3'-C4'	2.59	107.62	102.61
5	F	605	NAD	C2N-C3N-C4N	2.59	121.27	118.26
2	B	602	GTP	O4'-C1'-N9	2.57	112.16	108.75
2	E	601	GTP	O6-C6-C5	-2.52	119.32	124.32
4	D	602	IMP	O6-C6-C5	-2.47	119.42	124.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	GTP	O6-C6-C5	-2.46	119.45	124.32
5	G	605	NAD	C2N-C3N-C4N	2.41	121.06	118.26
5	C	604	NAD	O4D-C4D-C3D	-2.41	100.38	105.15
5	E	605	NAD	C3N-C7N-N7N	2.40	120.69	117.74
5	G	605	NAD	O4D-C4D-C3D	-2.40	100.39	105.15
5	C	604	NAD	C2N-C3N-C4N	2.38	121.02	118.26
5	G	605	NAD	C3N-C7N-N7N	2.37	120.66	117.74
4	F	604	IMP	O2P-P-O1P	2.37	120.06	110.83
2	B	602	GTP	O6-C6-C5	-2.36	119.63	124.32
4	G	604	IMP	O2P-P-O1P	2.36	120.01	110.83
2	F	602	GTP	O6-C6-C5	-2.35	119.66	124.32
2	E	601	GTP	N1-C2-N3	-2.32	119.06	123.32
5	C	604	NAD	C2B-C3B-C4B	2.30	107.05	102.61
2	B	601	GTP	O6-C6-C5	-2.29	119.78	124.32
5	A	605	NAD	C2N-C3N-C4N	2.27	120.90	118.26
2	B	602	GTP	C2'-C3'-C4'	2.26	106.98	102.61
2	B	601	GTP	O4'-C1'-N9	2.25	111.72	108.75
4	A	604	IMP	O2P-P-O1P	2.24	119.56	110.83
4	C	603	IMP	O2P-P-O1P	2.24	119.55	110.83
2	E	601	GTP	C5'-C4'-C3'	-2.23	107.18	115.21
5	G	605	NAD	C2B-C3B-C4B	2.23	106.92	102.61
5	G	605	NAD	C4B-O4B-C1B	-2.23	107.89	109.92
2	F	601	GTP	O6-C6-C5	-2.21	119.93	124.32
5	E	605	NAD	C2N-C3N-C4N	2.19	120.80	118.26
4	F	604	IMP	N1-C2-N3	-2.17	120.55	125.75
5	A	605	NAD	C3N-C7N-N7N	2.16	120.40	117.74
4	D	602	IMP	N1-C2-N3	-2.14	120.61	125.75
4	E	604	IMP	C4'-O4'-C1'	-2.14	107.97	109.92
4	H	602	IMP	N1-C2-N3	-2.13	120.64	125.75
5	C	604	NAD	C4B-O4B-C1B	-2.13	107.98	109.92
2	F	602	GTP	O4'-C1'-N9	2.08	111.50	108.75
4	B	604	IMP	O2P-P-O1P	2.08	118.93	110.83
2	A	601	GTP	N2-C2-N1	2.03	121.05	116.76

There are no chirality outliers.

All (217) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GTP	O4'-C4'-C5'-O5'
2	A	601	GTP	C3'-C4'-C5'-O5'
2	B	601	GTP	PB-O3B-PG-O2G
2	B	602	GTP	PB-O3A-PA-O5'

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Mol	Chain	Res	Type	Atoms
2	B	602	GTP	C5'-O5'-PA-O3A
2	B	602	GTP	C5'-O5'-PA-O1A
2	B	602	GTP	C5'-O5'-PA-O2A
2	E	601	GTP	PB-O3B-PG-O2G
2	E	602	GTP	C5'-O5'-PA-O3A
2	E	602	GTP	C5'-O5'-PA-O1A
2	E	602	GTP	C5'-O5'-PA-O2A
2	F	601	GTP	PB-O3B-PG-O2G
2	F	601	GTP	PB-O3B-PG-O3G
2	F	601	GTP	PB-O3A-PA-O5'
2	F	601	GTP	C5'-O5'-PA-O1A
2	F	602	GTP	C5'-O5'-PA-O3A
2	F	602	GTP	C5'-O5'-PA-O1A
2	F	602	GTP	C5'-O5'-PA-O2A
3	B	603	ATP	C5'-O5'-PA-O1A
3	B	603	ATP	C5'-O5'-PA-O3A
3	B	603	ATP	O4'-C4'-C5'-O5'
3	C	601	ATP	C5'-O5'-PA-O3A
3	D	601	ATP	C5'-O5'-PA-O1A
3	D	601	ATP	C5'-O5'-PA-O2A
3	D	601	ATP	C5'-O5'-PA-O3A
3	D	601	ATP	O4'-C4'-C5'-O5'
3	E	603	ATP	O4'-C4'-C5'-O5'
3	F	603	ATP	C5'-O5'-PA-O1A
3	F	603	ATP	O4'-C4'-C5'-O5'
3	H	601	ATP	C5'-O5'-PA-O1A
3	H	601	ATP	C5'-O5'-PA-O2A
3	H	601	ATP	C5'-O5'-PA-O3A
3	H	601	ATP	O4'-C4'-C5'-O5'
3	H	601	ATP	C3'-C4'-C5'-O5'
4	A	604	IMP	C5'-O5'-P-O2P
4	A	604	IMP	C5'-O5'-P-O3P
4	B	604	IMP	C5'-O5'-P-O1P
4	B	604	IMP	C5'-O5'-P-O2P
4	B	604	IMP	C5'-O5'-P-O3P
4	B	604	IMP	O4'-C4'-C5'-O5'
4	B	604	IMP	C3'-C4'-C5'-O5'
4	C	603	IMP	C5'-O5'-P-O1P
4	C	603	IMP	C5'-O5'-P-O2P
4	C	603	IMP	C5'-O5'-P-O3P
4	C	603	IMP	O4'-C4'-C5'-O5'
4	D	602	IMP	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
4	D	602	IMP	C5'-O5'-P-O2P
4	D	602	IMP	C5'-O5'-P-O3P
4	D	602	IMP	O4'-C4'-C5'-O5'
4	E	604	IMP	C5'-O5'-P-O1P
4	E	604	IMP	C5'-O5'-P-O2P
4	E	604	IMP	C5'-O5'-P-O3P
4	E	604	IMP	O4'-C4'-C5'-O5'
4	E	604	IMP	C3'-C4'-C5'-O5'
4	F	604	IMP	C5'-O5'-P-O1P
4	F	604	IMP	C5'-O5'-P-O2P
4	F	604	IMP	C3'-C4'-C5'-O5'
4	G	604	IMP	C5'-O5'-P-O1P
4	G	604	IMP	C5'-O5'-P-O2P
4	G	604	IMP	C5'-O5'-P-O3P
4	G	604	IMP	O4'-C4'-C5'-O5'
4	G	604	IMP	C3'-C4'-C5'-O5'
4	H	602	IMP	C3'-C4'-C5'-O5'
5	B	605	NAD	C5D-O5D-PN-O3
5	B	605	NAD	C5D-O5D-PN-O2N
5	B	605	NAD	O4D-C1D-N1N-C6N
5	B	605	NAD	C2D-C1D-N1N-C6N
5	C	604	NAD	C5B-O5B-PA-O2A
5	C	604	NAD	O4B-C4B-C5B-O5B
5	C	604	NAD	C5D-O5D-PN-O1N
5	C	604	NAD	C5D-O5D-PN-O2N
5	D	603	NAD	C5B-O5B-PA-O1A
5	D	603	NAD	C5B-O5B-PA-O2A
5	D	603	NAD	C5B-O5B-PA-O3
5	D	603	NAD	O4B-C4B-C5B-O5B
5	D	603	NAD	C5D-O5D-PN-O2N
5	D	603	NAD	C2D-C1D-N1N-C2N
5	D	603	NAD	C2D-C1D-N1N-C6N
5	F	605	NAD	C5B-O5B-PA-O2A
5	F	605	NAD	C2D-C1D-N1N-C2N
5	F	605	NAD	C2D-C1D-N1N-C6N
5	G	605	NAD	C5B-O5B-PA-O2A
5	G	605	NAD	O4B-C4B-C5B-O5B
5	G	605	NAD	C5D-O5D-PN-O1N
5	G	605	NAD	C5D-O5D-PN-O2N
5	H	603	NAD	C5B-O5B-PA-O1A
5	H	603	NAD	C5B-O5B-PA-O2A
5	H	603	NAD	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
5	H	603	NAD	O4B-C4B-C5B-O5B
5	H	603	NAD	C5D-O5D-PN-O3
5	H	603	NAD	C5D-O5D-PN-O2N
5	H	603	NAD	C2D-C1D-N1N-C2N
5	H	603	NAD	C2D-C1D-N1N-C6N
3	C	605	ATP	C3'-C4'-C5'-O5'
3	G	601	ATP	C3'-C4'-C5'-O5'
4	A	604	IMP	C3'-C4'-C5'-O5'
4	C	603	IMP	C3'-C4'-C5'-O5'
5	C	604	NAD	C3B-C4B-C5B-O5B
5	C	604	NAD	O4D-C4D-C5D-O5D
5	G	605	NAD	C3B-C4B-C5B-O5B
5	G	605	NAD	O4D-C4D-C5D-O5D
2	B	601	GTP	O4'-C4'-C5'-O5'
3	D	601	ATP	C3'-C4'-C5'-O5'
3	G	601	ATP	O4'-C4'-C5'-O5'
4	A	604	IMP	O4'-C4'-C5'-O5'
4	D	602	IMP	C3'-C4'-C5'-O5'
4	F	604	IMP	O4'-C4'-C5'-O5'
4	H	602	IMP	O4'-C4'-C5'-O5'
5	D	603	NAD	O4D-C4D-C5D-O5D
5	D	603	NAD	C3D-C4D-C5D-O5D
5	F	605	NAD	O4D-C4D-C5D-O5D
5	H	603	NAD	O4D-C4D-C5D-O5D
3	B	603	ATP	C3'-C4'-C5'-O5'
3	E	603	ATP	C3'-C4'-C5'-O5'
3	F	603	ATP	C3'-C4'-C5'-O5'
5	D	603	NAD	C3B-C4B-C5B-O5B
5	H	603	NAD	C3B-C4B-C5B-O5B
2	B	601	GTP	C3'-C4'-C5'-O5'
3	C	601	ATP	O4'-C4'-C5'-O5'
3	C	605	ATP	O4'-C4'-C5'-O5'
5	A	605	NAD	O4B-C4B-C5B-O5B
5	B	605	NAD	O4D-C4D-C5D-O5D
5	E	605	NAD	O4B-C4B-C5B-O5B
5	G	605	NAD	C3D-C4D-C5D-O5D
5	H	603	NAD	C3D-C4D-C5D-O5D
4	A	604	IMP	C5'-O5'-P-O1P
5	C	604	NAD	C2N-C3N-C7N-N7N
2	F	601	GTP	O4'-C4'-C5'-O5'
3	H	601	ATP	C4'-C5'-O5'-PA
5	F	605	NAD	C3D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
5	C	604	NAD	C2N-C3N-C7N-O7N
2	A	602	GTP	C4'-C5'-O5'-PA
5	B	605	NAD	O4B-C4B-C5B-O5B
2	E	602	GTP	PB-O3A-PA-O5'
2	F	602	GTP	PB-O3A-PA-O5'
3	D	601	ATP	PB-O3A-PA-O5'
3	H	601	ATP	PB-O3A-PA-O5'
4	F	604	IMP	C5'-O5'-P-O3P
2	E	601	GTP	PB-O3B-PG-O1G
2	A	602	GTP	PB-O3B-PG-O2G
3	B	603	ATP	PB-O3B-PG-O2G
3	B	603	ATP	PB-O3B-PG-O3G
5	H	603	NAD	C4B-C5B-O5B-PA
3	C	602	ATP	PG-O3B-PB-O2B
3	G	602	ATP	PB-O3A-PA-O1A
5	B	605	NAD	PN-O3-PA-O2A
5	C	604	NAD	PA-O3-PN-O1N
5	F	605	NAD	PN-O3-PA-O1A
5	G	605	NAD	PA-O3-PN-O1N
5	C	604	NAD	C4N-C3N-C7N-N7N
2	E	602	GTP	C4'-C5'-O5'-PA
2	F	602	GTP	C4'-C5'-O5'-PA
3	C	605	ATP	C4'-C5'-O5'-PA
4	F	604	IMP	C4'-C5'-O5'-P
5	D	603	NAD	C4D-C5D-O5D-PN
5	H	603	NAD	C4D-C5D-O5D-PN
2	A	601	GTP	C5'-O5'-PA-O1A
2	A	602	GTP	C5'-O5'-PA-O1A
3	A	603	ATP	C5'-O5'-PA-O1A
3	C	601	ATP	C5'-O5'-PA-O1A
3	C	605	ATP	C5'-O5'-PA-O1A
3	C	605	ATP	C5'-O5'-PA-O3A
3	F	603	ATP	C5'-O5'-PA-O3A
3	G	601	ATP	C5'-O5'-PA-O1A
3	G	601	ATP	C5'-O5'-PA-O3A
5	B	605	NAD	C5D-O5D-PN-O1N
5	C	604	NAD	C5B-O5B-PA-O1A
5	C	604	NAD	C5B-O5B-PA-O3
5	C	604	NAD	C5D-O5D-PN-O3
5	D	603	NAD	C5D-O5D-PN-O3
5	F	605	NAD	C5B-O5B-PA-O1A
5	F	605	NAD	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
5	F	605	NAD	C5D-O5D-PN-O1N
5	G	605	NAD	C5B-O5B-PA-O1A
5	G	605	NAD	C5B-O5B-PA-O3
5	G	605	NAD	C5D-O5D-PN-O3
2	B	602	GTP	C4'-C5'-O5'-PA
3	D	601	ATP	C4'-C5'-O5'-PA
5	D	603	NAD	C4B-C5B-O5B-PA
2	A	601	GTP	PG-O3B-PB-O2B
3	D	601	ATP	PA-O3A-PB-O2B
5	C	604	NAD	C4N-C3N-C7N-O7N
5	B	605	NAD	C2D-C1D-N1N-C2N
3	G	603	ATP	C4'-C5'-O5'-PA
3	G	601	ATP	C4'-C5'-O5'-PA
5	G	605	NAD	C4B-C5B-O5B-PA
5	B	605	NAD	O4D-C1D-N1N-C2N
5	C	604	NAD	C3D-C4D-C5D-O5D
5	C	604	NAD	O4D-C1D-N1N-C2N
2	E	602	GTP	PA-O3A-PB-O1B
3	C	602	ATP	PB-O3A-PA-O1A
3	C	602	ATP	PB-O3A-PA-O2A
3	D	601	ATP	PB-O3A-PA-O1A
2	B	601	GTP	C4'-C5'-O5'-PA
5	C	604	NAD	C4B-C5B-O5B-PA
2	E	602	GTP	C3'-C4'-C5'-O5'
2	B	601	GTP	PB-O3B-PG-O1G
2	F	601	GTP	PB-O3B-PG-O1G
3	D	601	ATP	PG-O3B-PB-O3A
2	A	601	GTP	PG-O3B-PB-O1B
3	D	601	ATP	PG-O3B-PB-O1B
3	D	601	ATP	PG-O3B-PB-O2B
3	D	601	ATP	PA-O3A-PB-O1B
3	E	603	ATP	PG-O3B-PB-O2B
5	A	605	NAD	PA-O3-PN-O2N
5	E	605	NAD	PA-O3-PN-O2N
5	F	605	NAD	PN-O3-PA-O2A
2	E	601	GTP	PA-O3A-PB-O2B
2	E	602	GTP	PA-O3A-PB-O2B
3	G	602	ATP	PG-O3B-PB-O2B
3	G	602	ATP	PB-O3A-PA-O2A
3	G	603	ATP	PG-O3B-PB-O2B
3	G	603	ATP	PA-O3A-PB-O2B
5	C	604	NAD	PA-O3-PN-O2N

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Mol	Chain	Res	Type	Atoms
5	D	603	NAD	PA-O3-PN-O2N
5	G	605	NAD	PA-O3-PN-O2N
5	H	603	NAD	PA-O3-PN-O2N

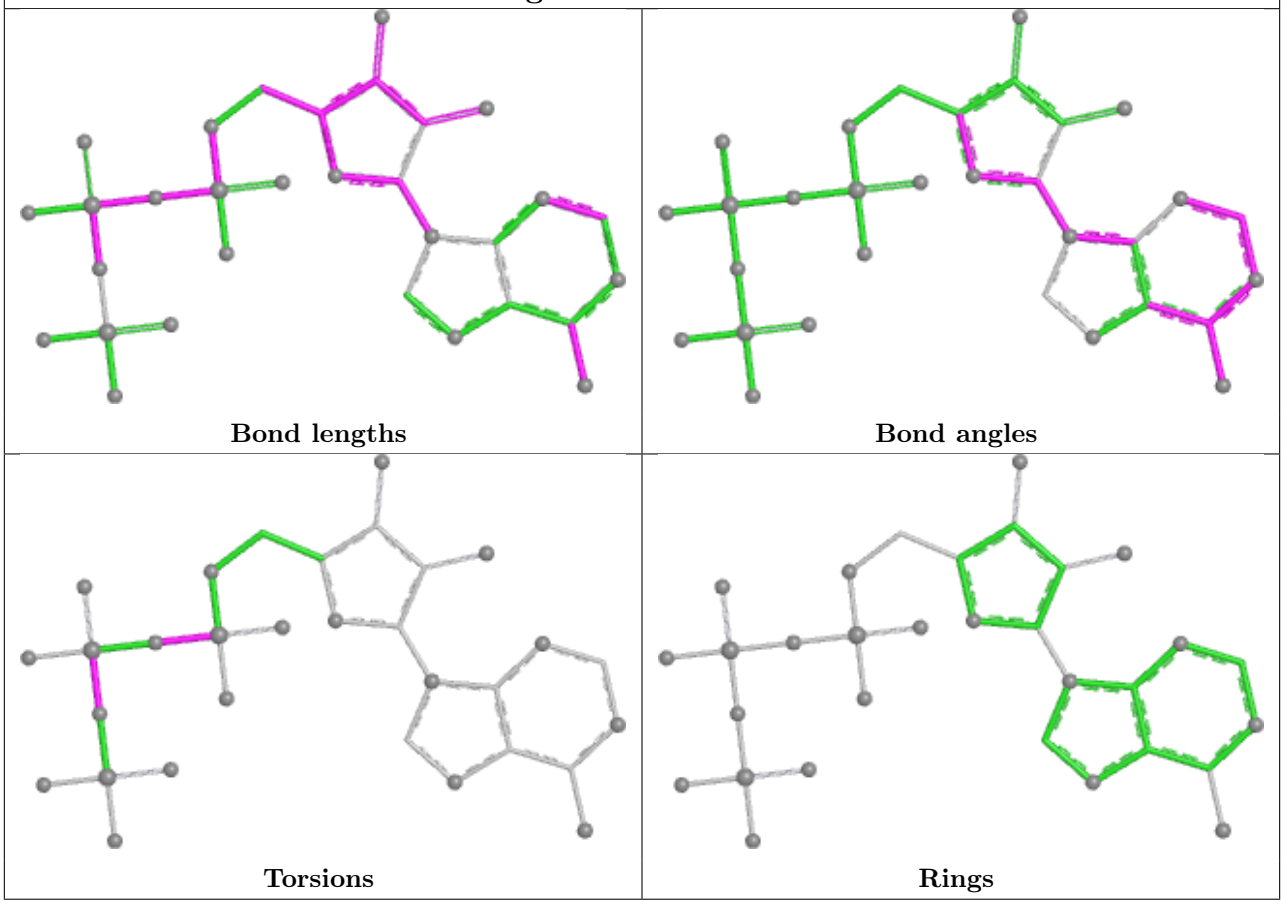
There are no ring outliers.

33 monomers are involved in 73 short contacts:

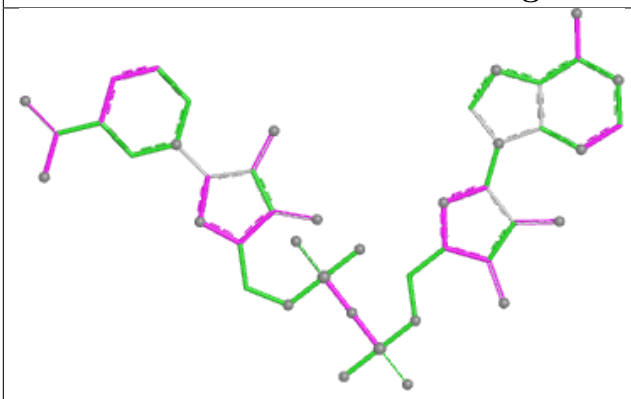
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	ATP	1	0
2	F	601	GTP	1	0
3	B	603	ATP	1	0
2	B	601	GTP	2	0
5	C	604	NAD	1	0
2	A	602	GTP	2	0
5	H	603	NAD	2	0
4	F	604	IMP	3	0
5	A	605	NAD	2	0
2	E	601	GTP	4	0
4	B	604	IMP	1	0
3	E	603	ATP	2	0
5	D	603	NAD	2	0
2	A	601	GTP	8	0
5	G	605	NAD	1	0
3	A	603	ATP	1	0
4	A	604	IMP	2	0
4	E	604	IMP	2	0
3	G	603	ATP	1	0
2	E	602	GTP	3	0
3	H	601	ATP	2	0
3	G	602	ATP	1	0
3	D	601	ATP	1	0
4	G	604	IMP	3	0
4	D	602	IMP	4	0
4	C	603	IMP	4	0
2	F	602	GTP	3	0
3	C	601	ATP	3	0
4	H	602	IMP	3	0
5	E	605	NAD	2	0
2	B	602	GTP	3	0
3	G	601	ATP	1	0
5	B	605	NAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

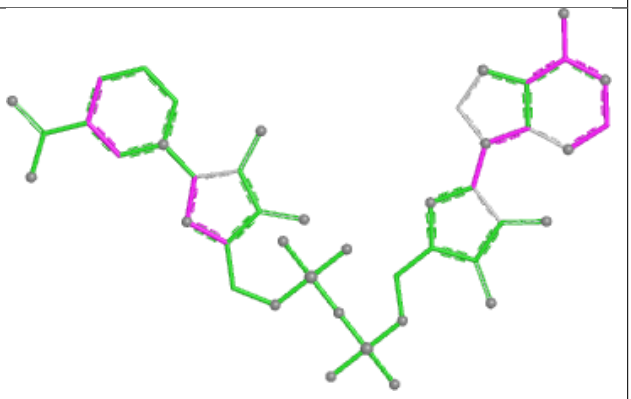
Ligand ATP C 602



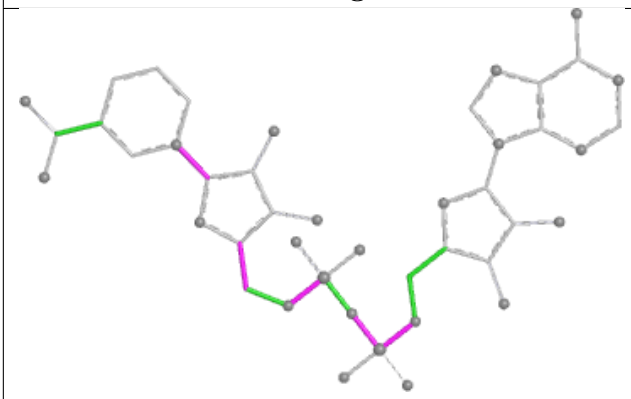
Ligand NAD F 605



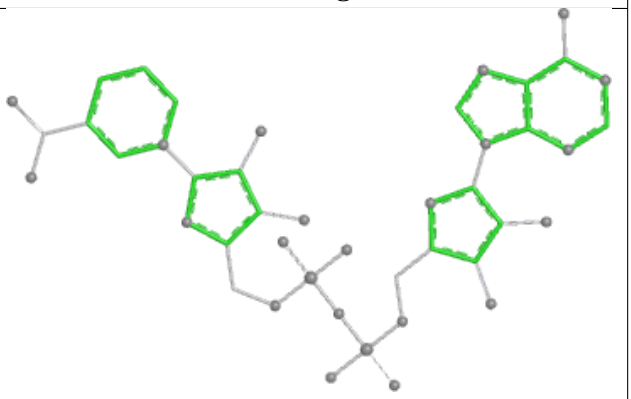
Bond lengths



Bond angles

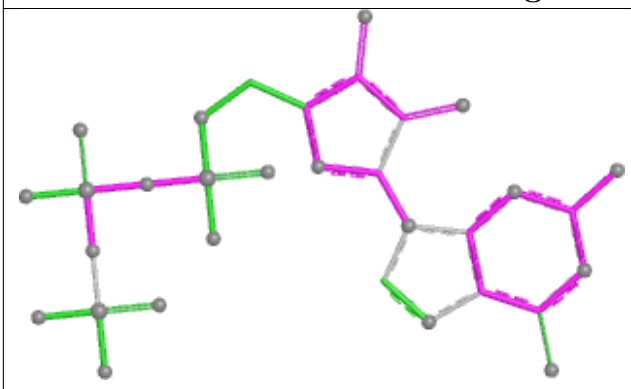


Torsions

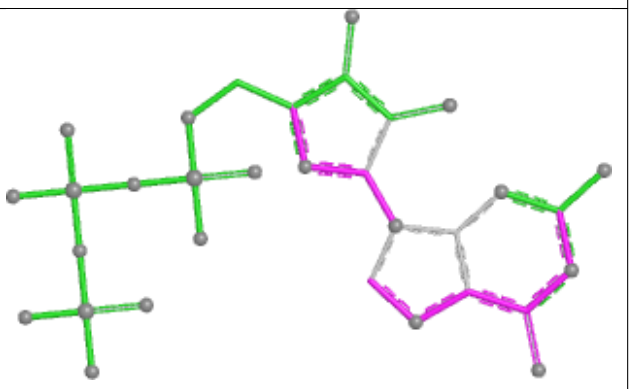


Rings

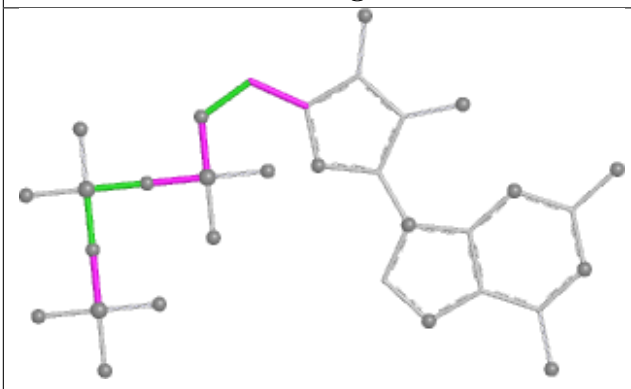
Ligand GTP F 601



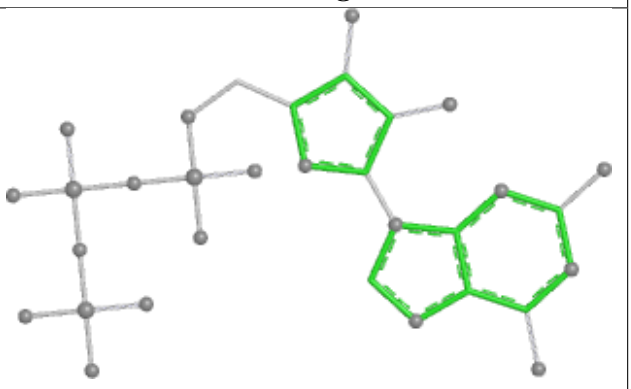
Bond lengths



Bond angles

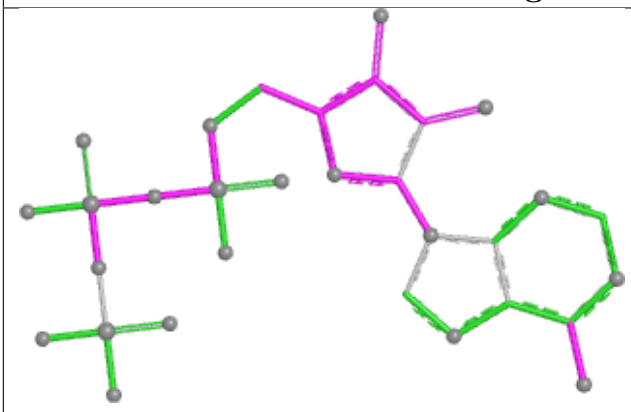


Torsions

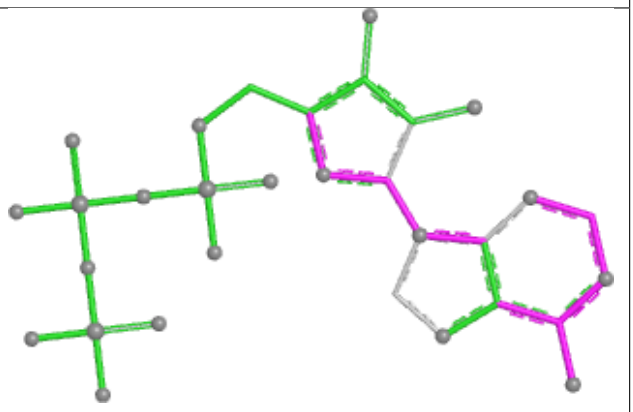


Rings

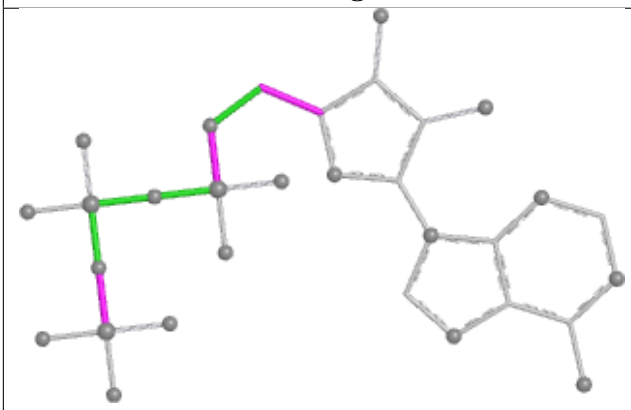
Ligand ATP B 603



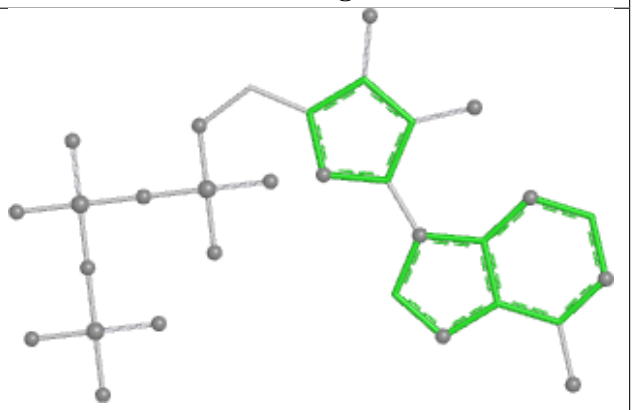
Bond lengths



Bond angles

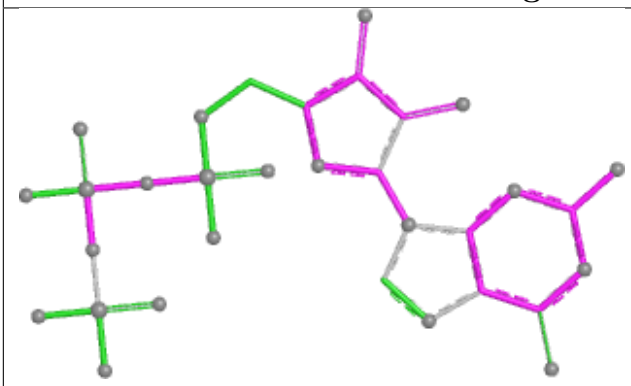


Torsions

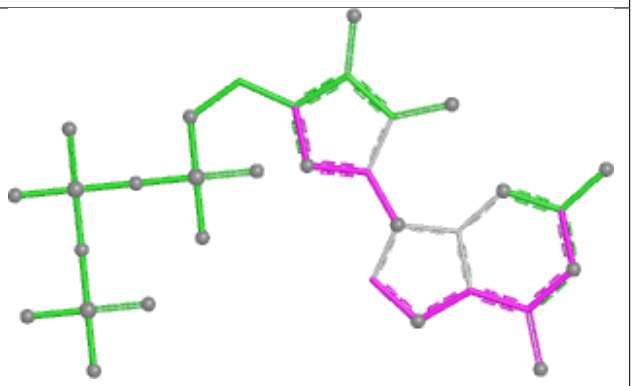


Rings

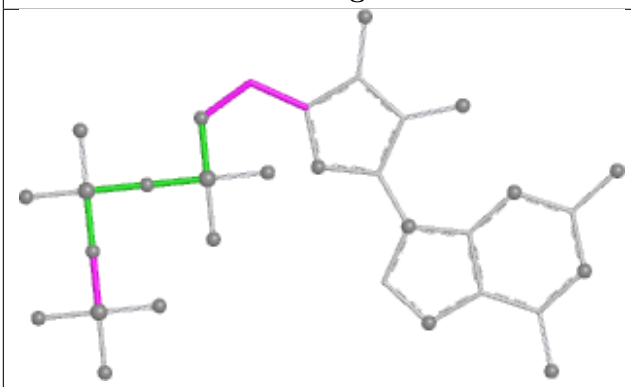
Ligand GTP B 601



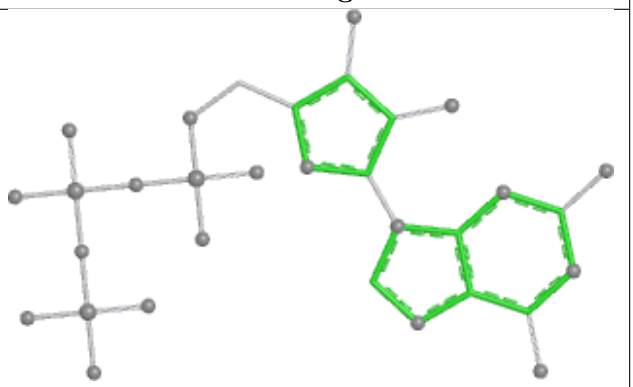
Bond lengths



Bond angles

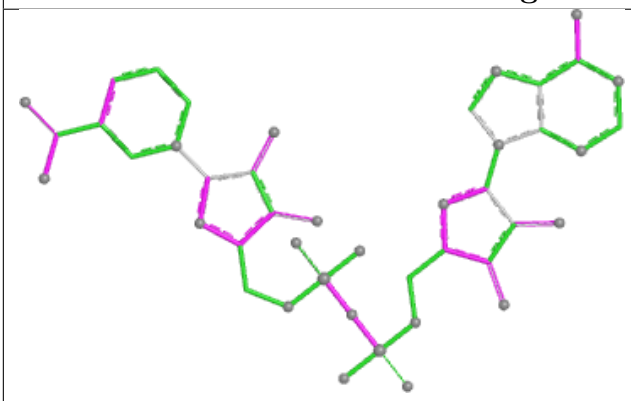


Torsions

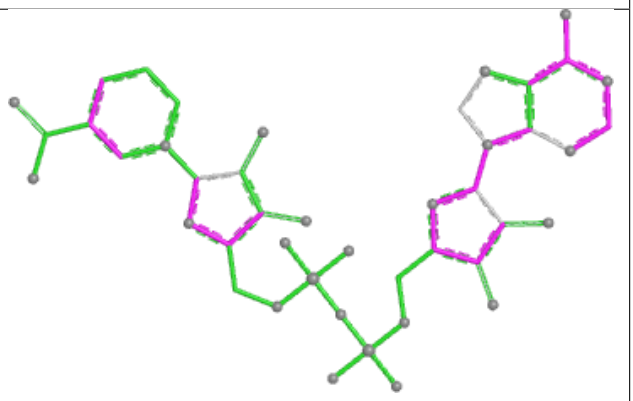


Rings

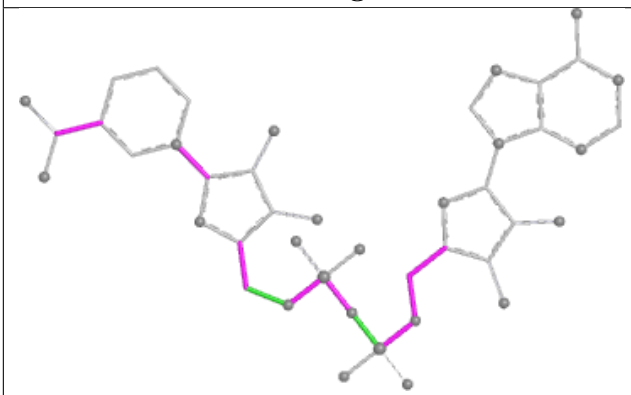
Ligand NAD C 604



Bond lengths



Bond angles



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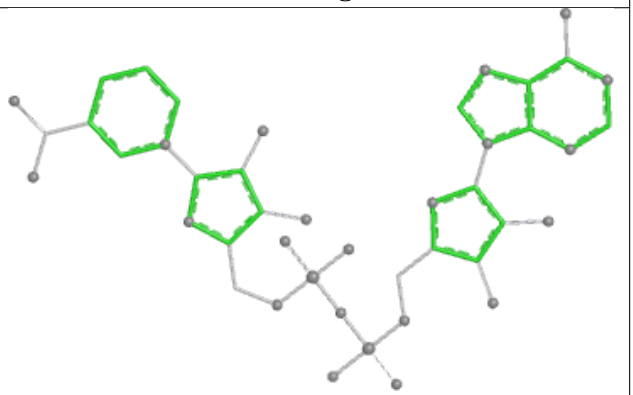

Rings

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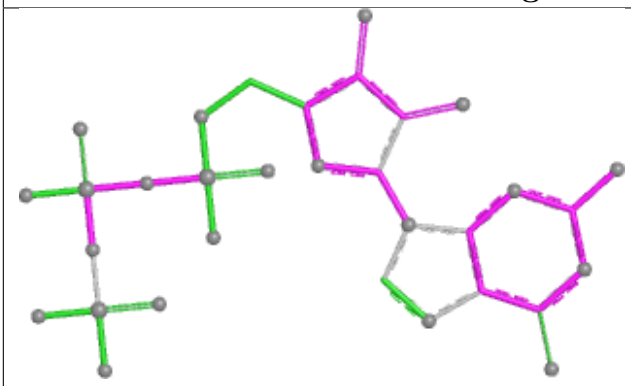

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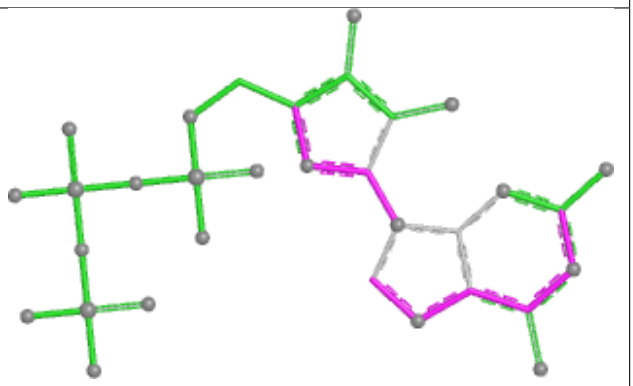
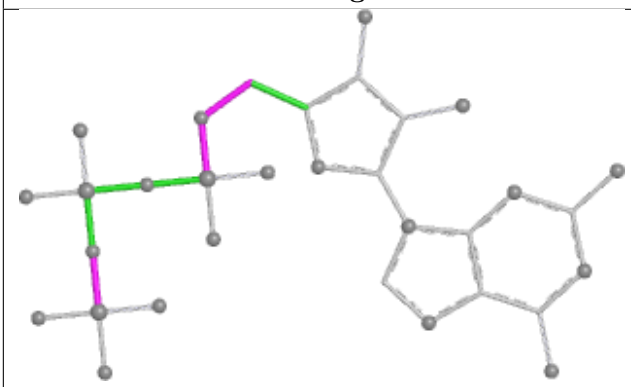


Bond angles



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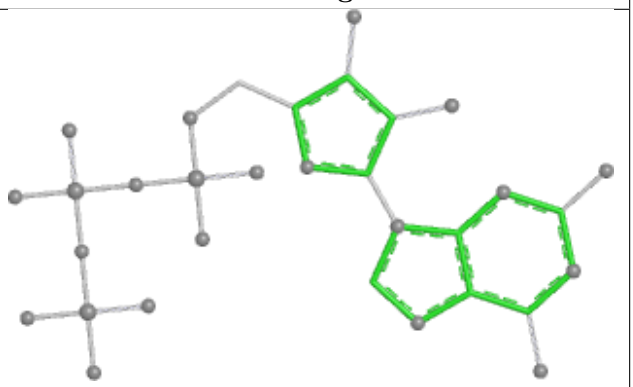
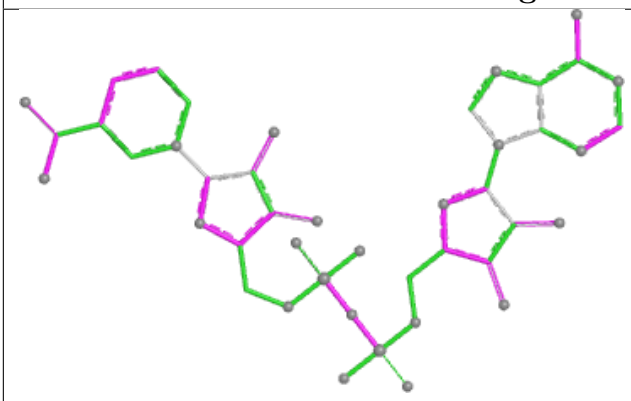


Rings

Ligand NAD H 603



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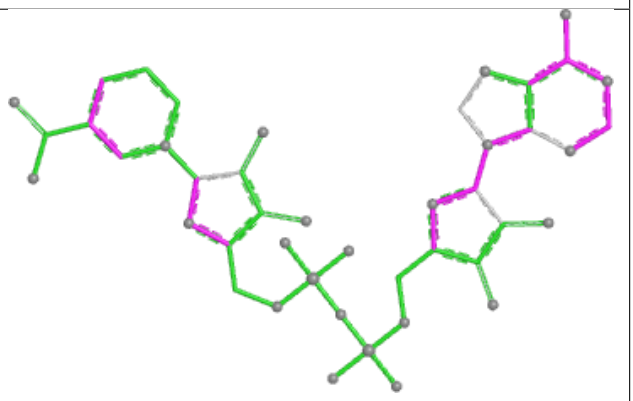

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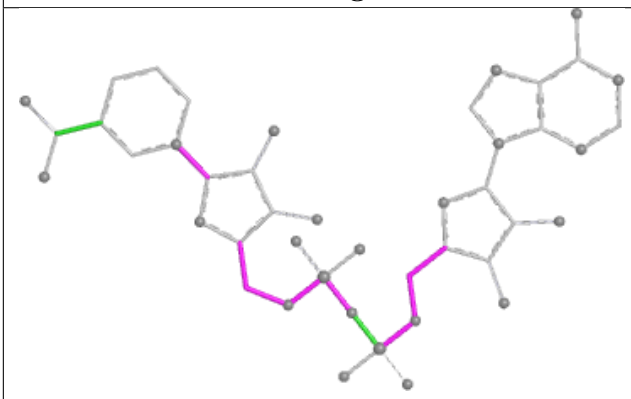

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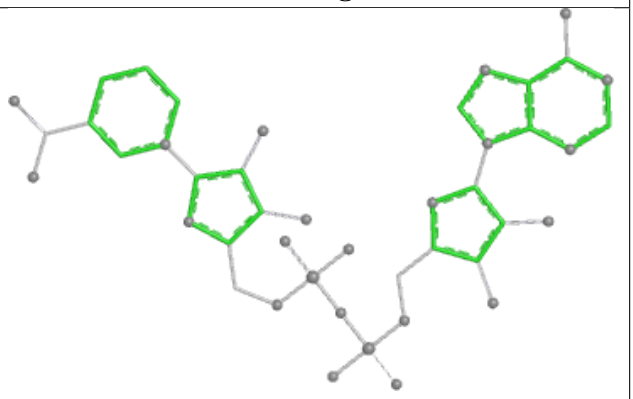
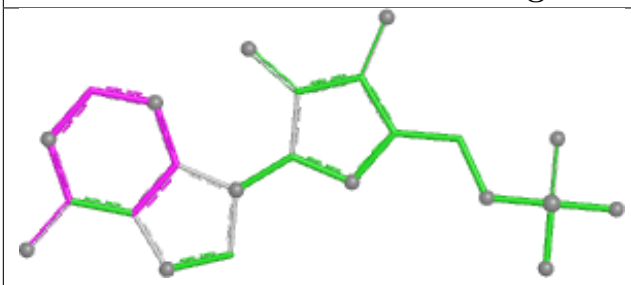


Rings

Ligand IMP F 604



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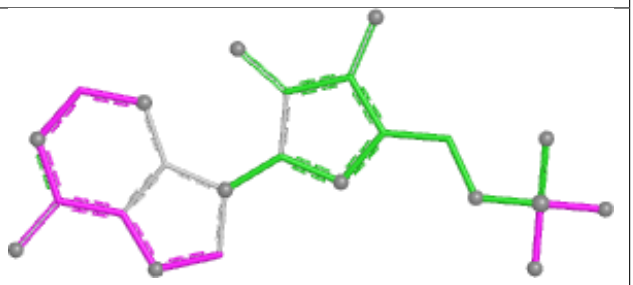
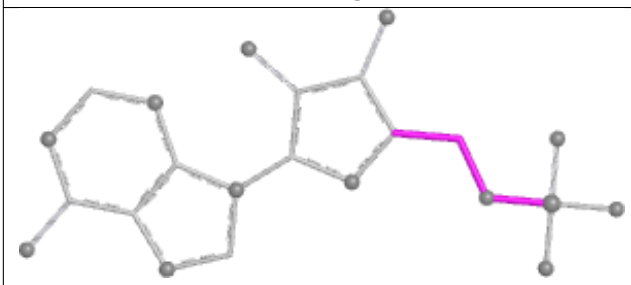


Bond angles



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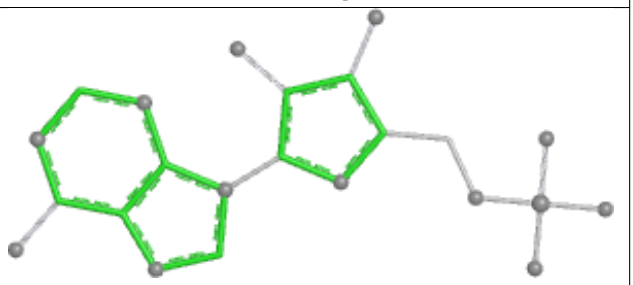
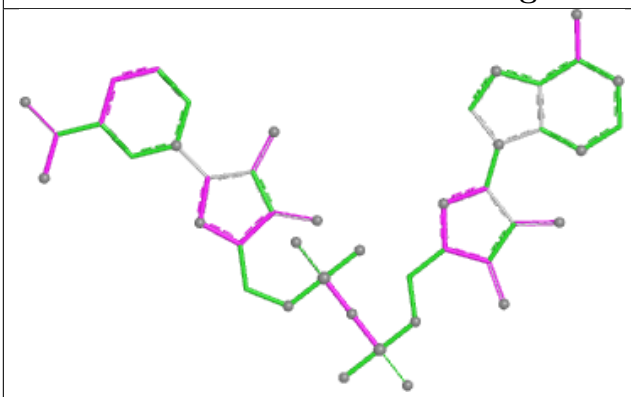


Rings

Ligand NAD A 605



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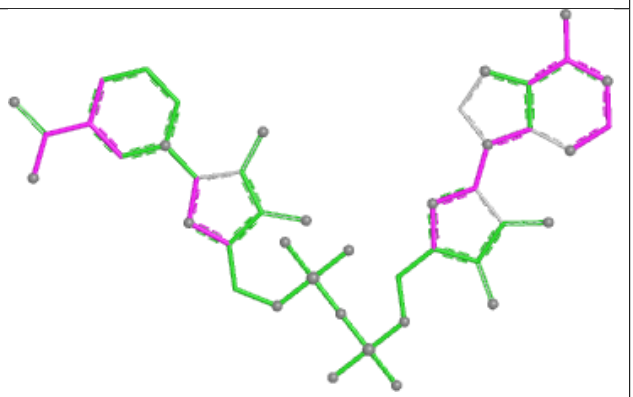
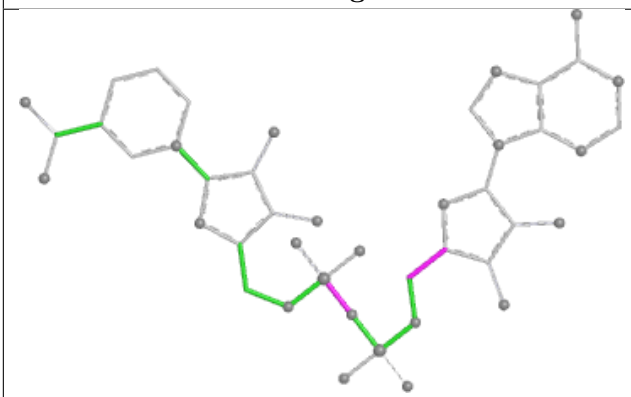
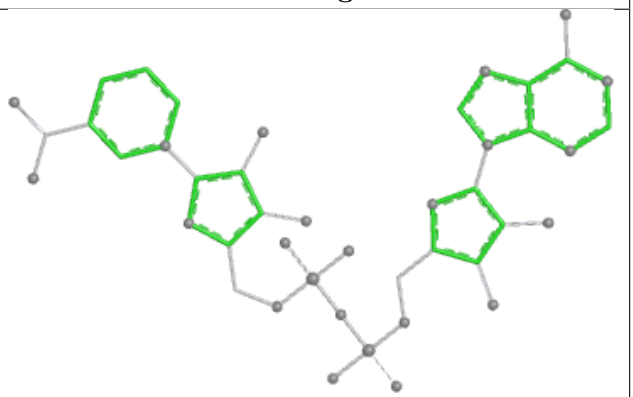


Bond angles

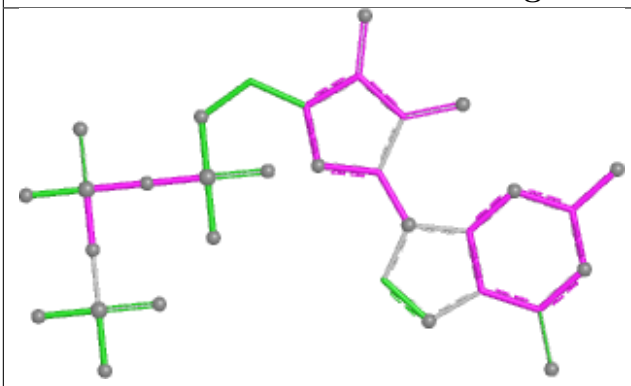


Torsions

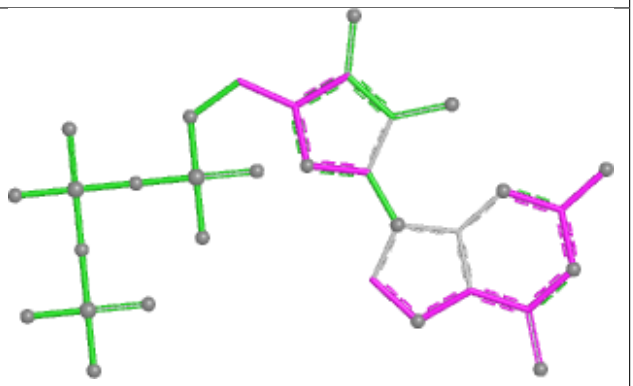


Rings

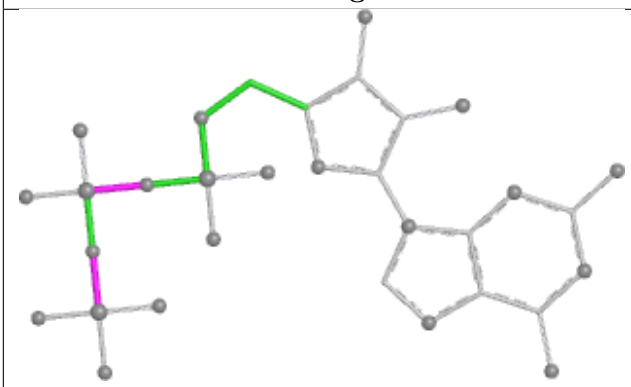
Ligand GTP E 601



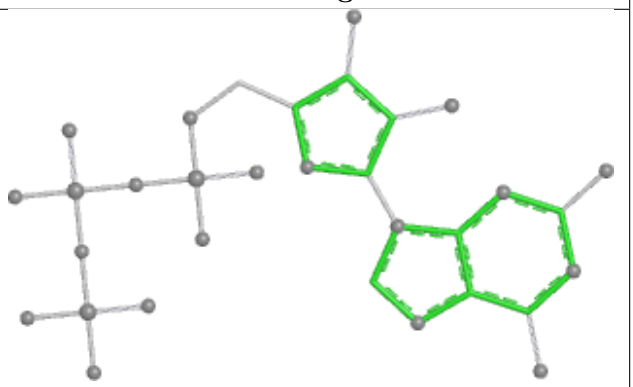
Bond lengths



Bond angles

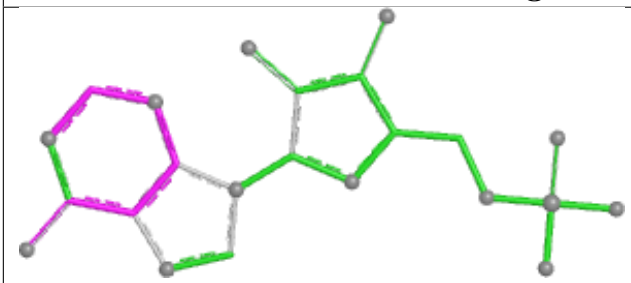


Torsions

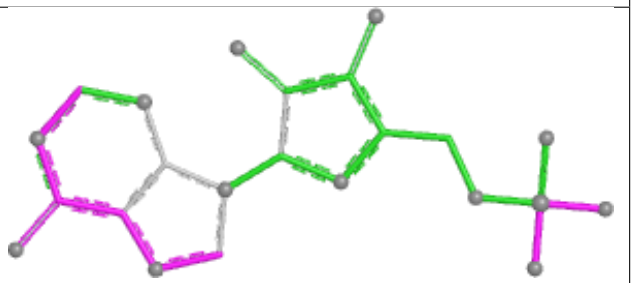


Rings

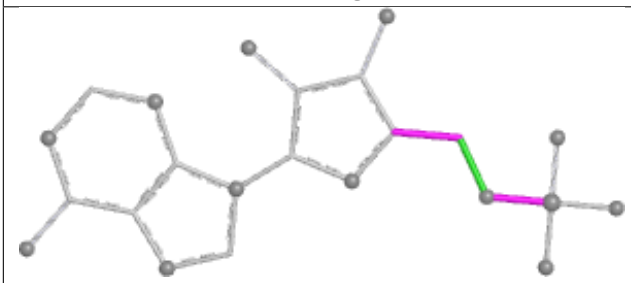
Ligand IMP B 604



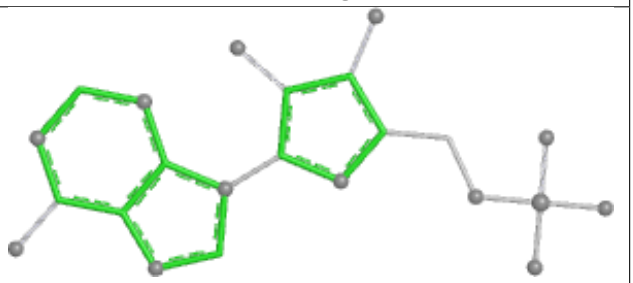
Bond lengths



Bond angles

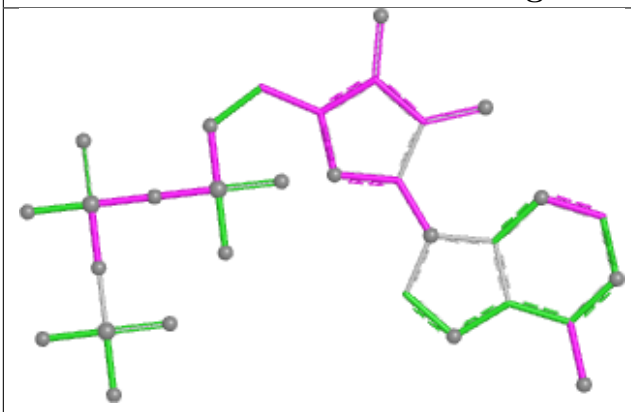


Torsions



Rings

Ligand ATP E 603



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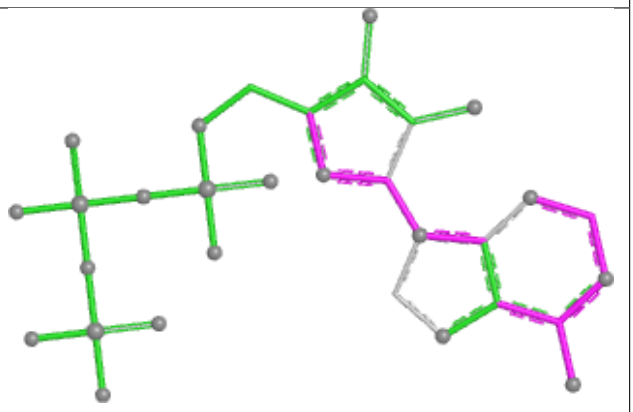
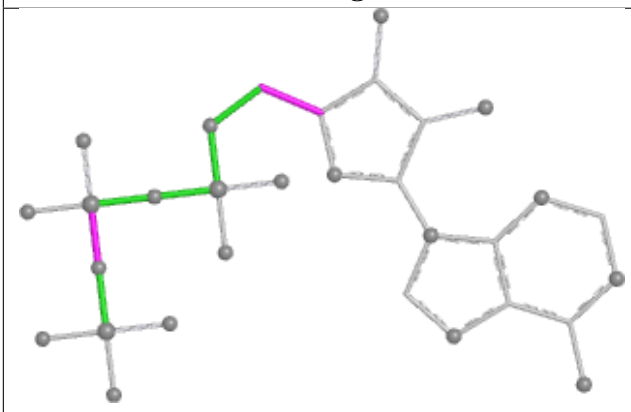


Bond angles



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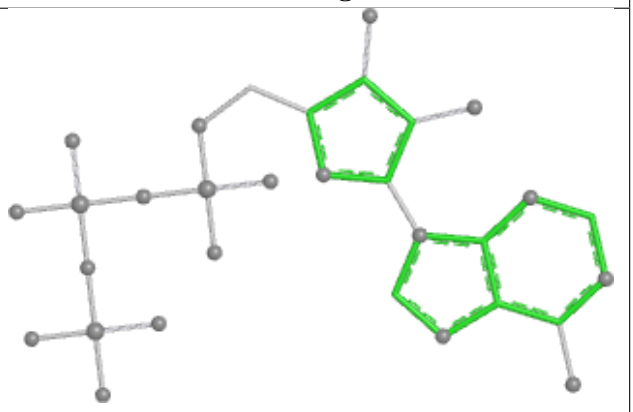
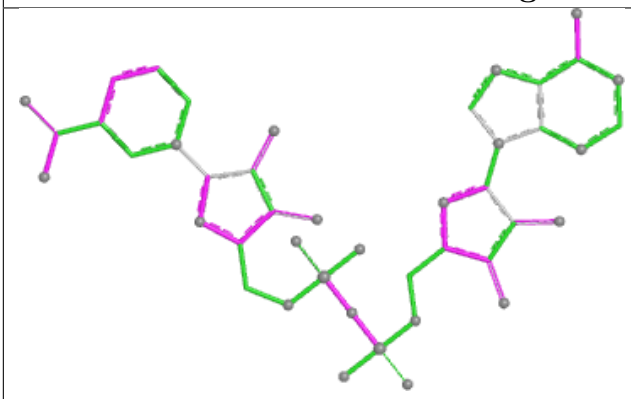


Rings

Ligand NAD D 603



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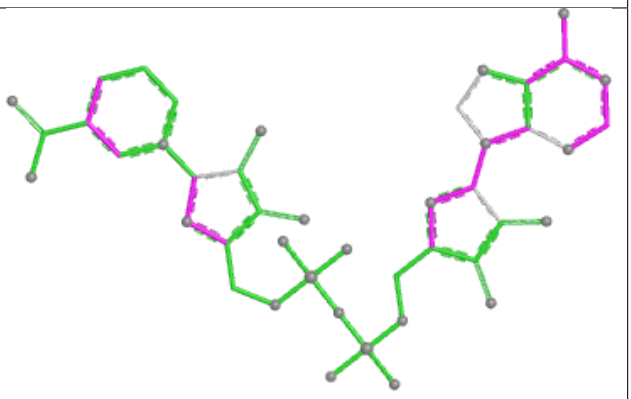
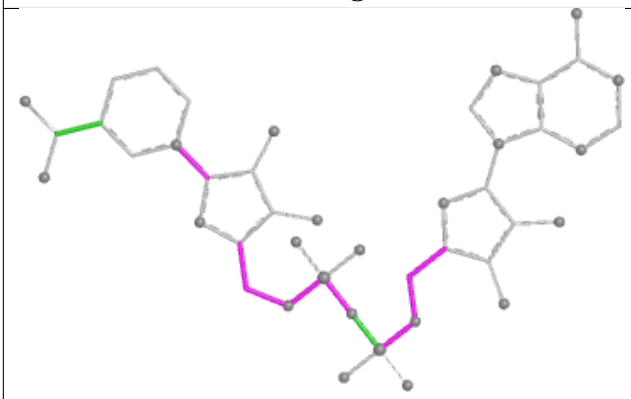
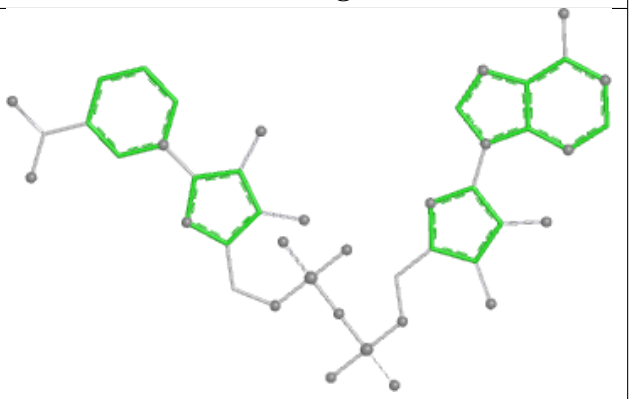


Bond angles

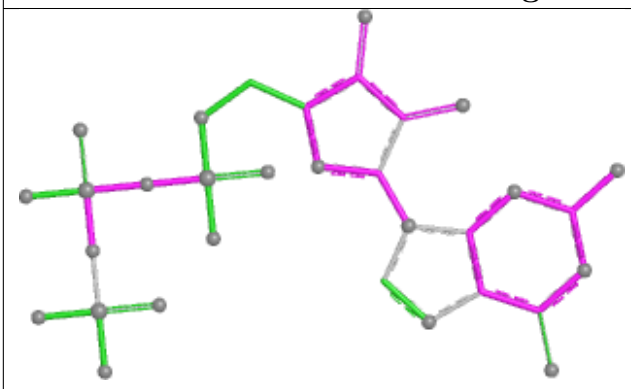


Torsions



Rings

Ligand GTP A 601



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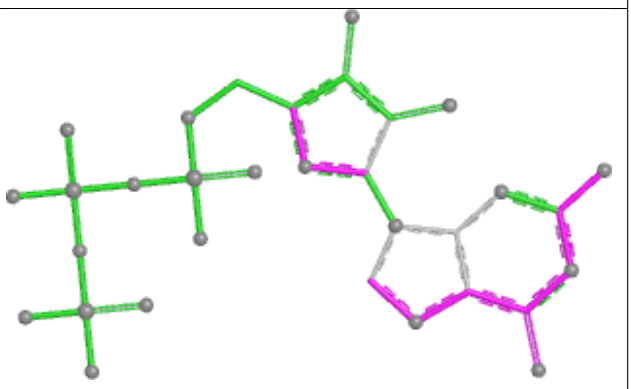
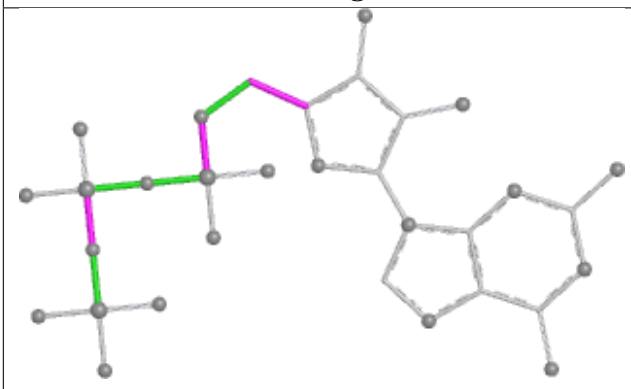
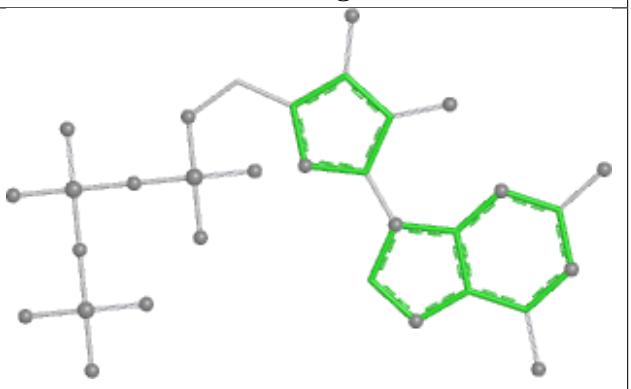


Bond angles

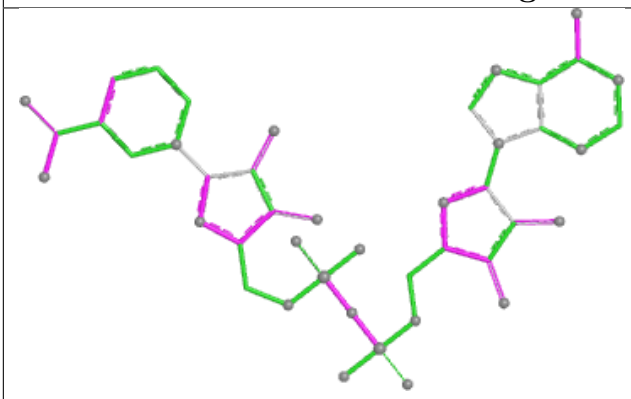


Torsions

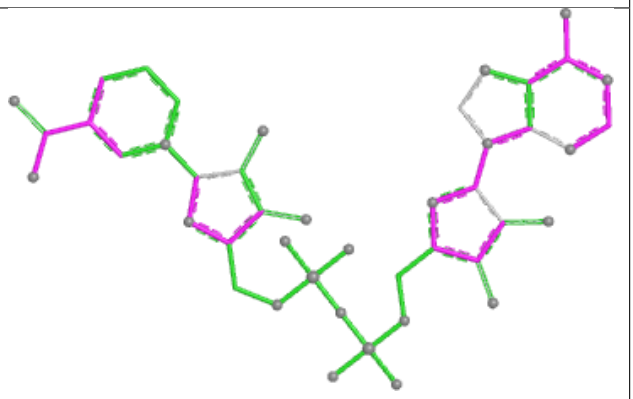


Rings

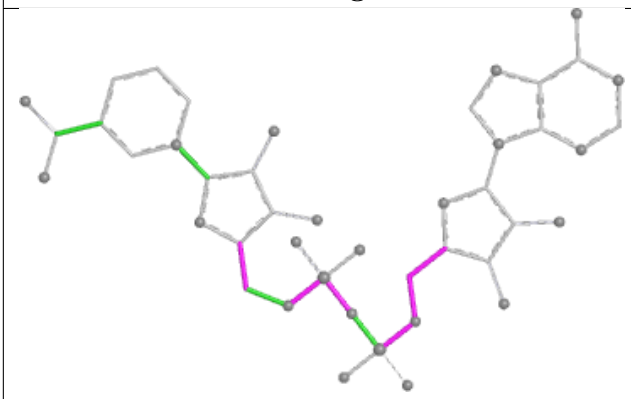
Ligand NAD G 605



Bond lengths



Bond angles



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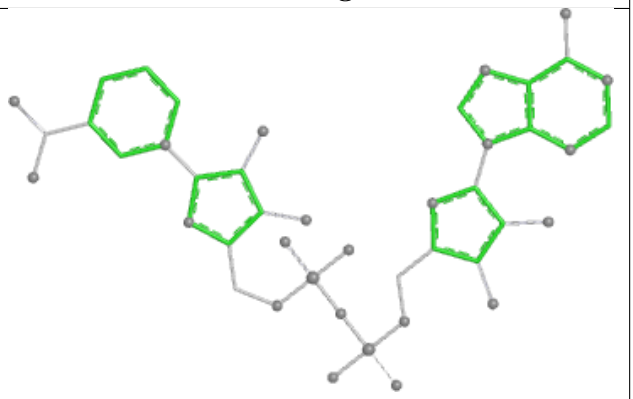
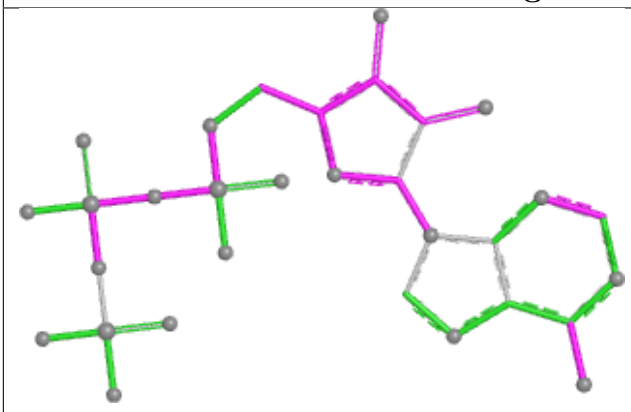


Rings

Ligand ATP A 603



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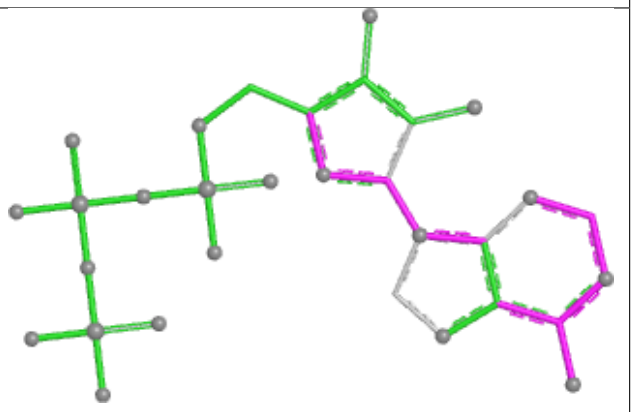
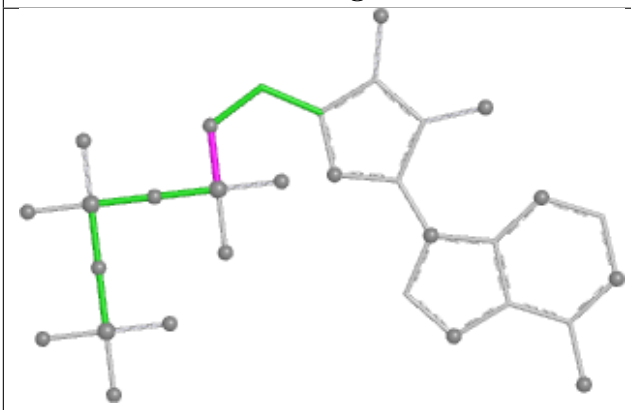


Bond angles



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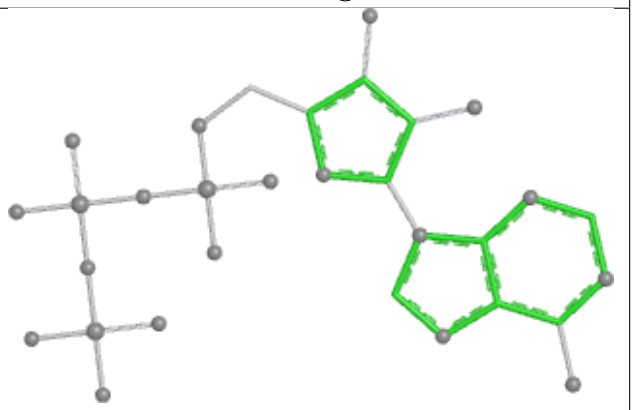
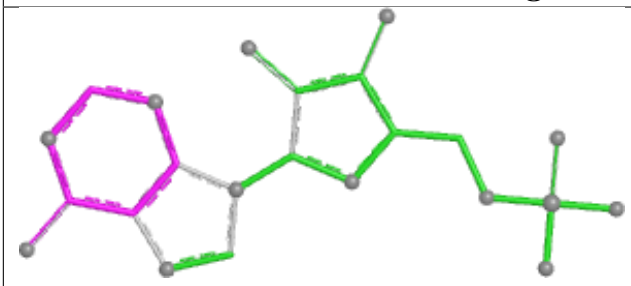


Rings

Ligand IMP A 604



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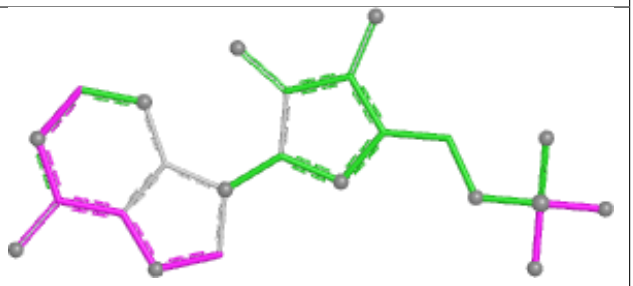
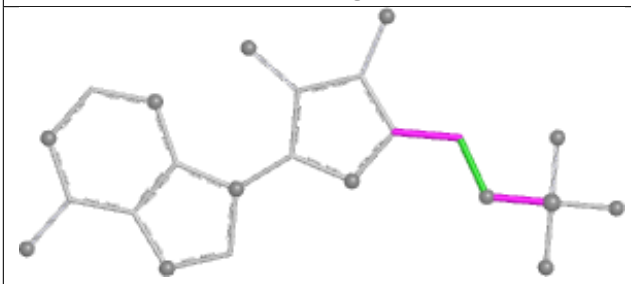


Bond angles



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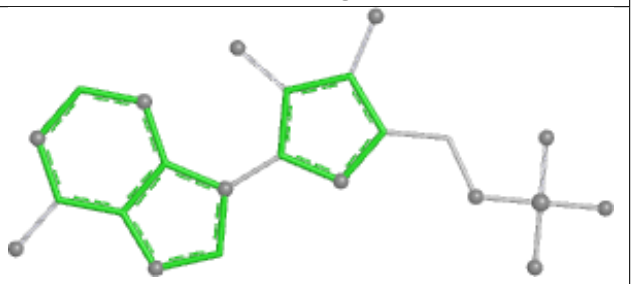
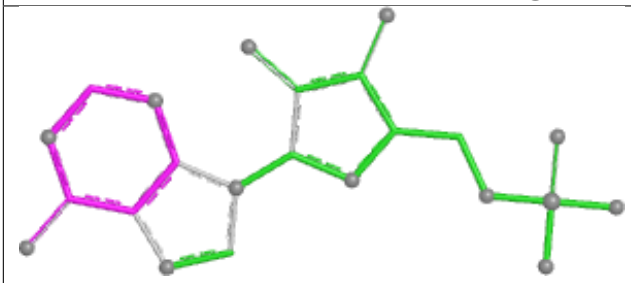


Rings

Ligand IMP E 604



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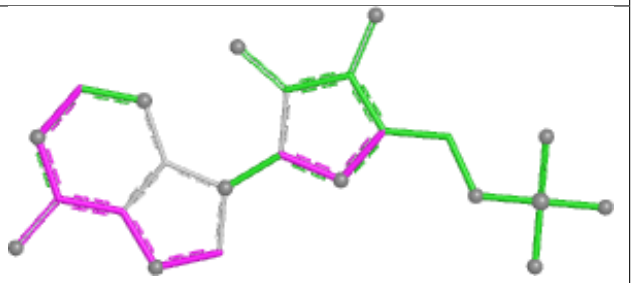
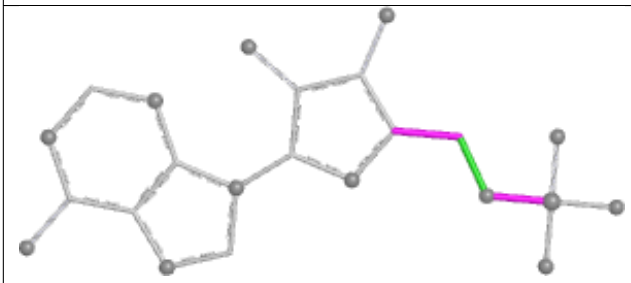


Bond angles



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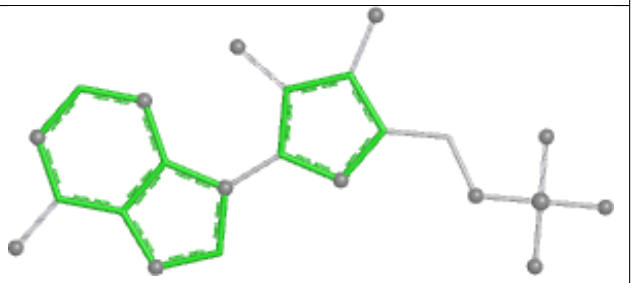
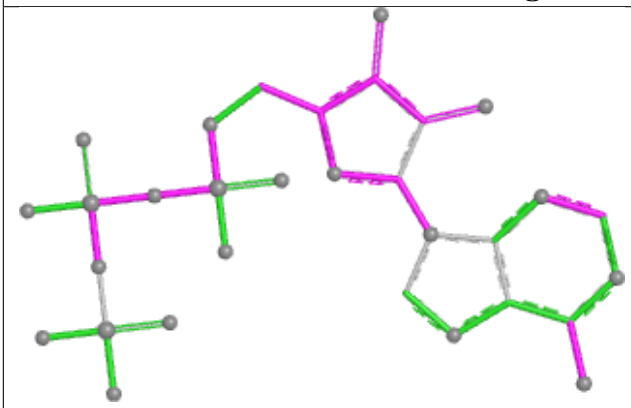


Rings

Ligand ATP G 603



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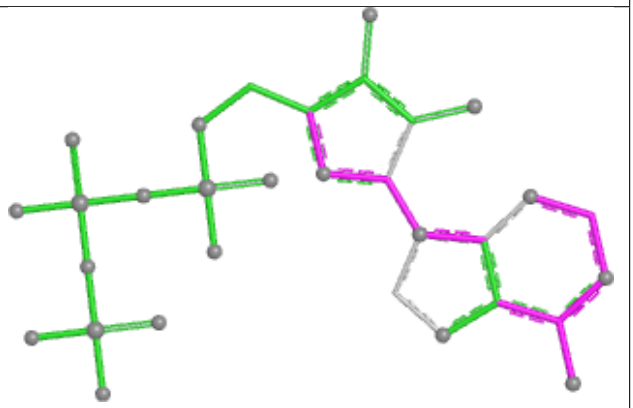
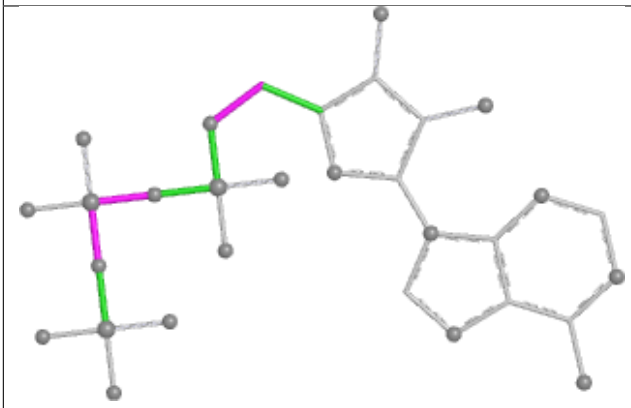


Bond angles



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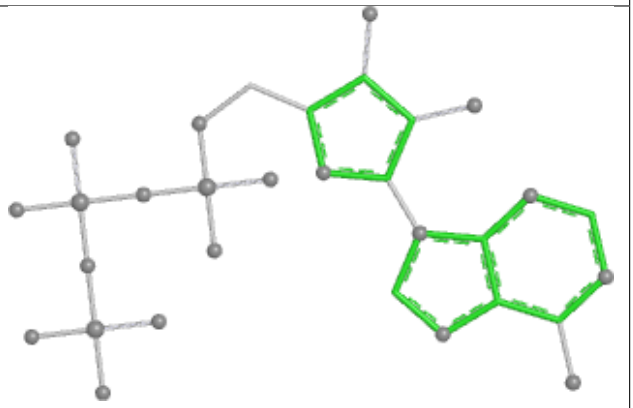
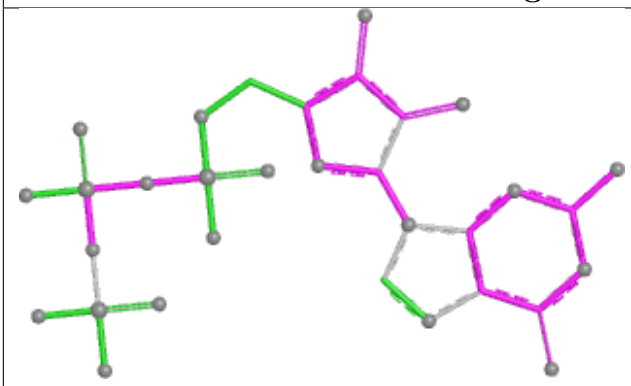
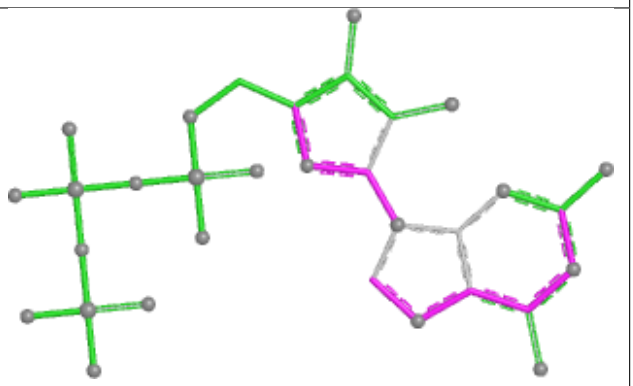


Rings

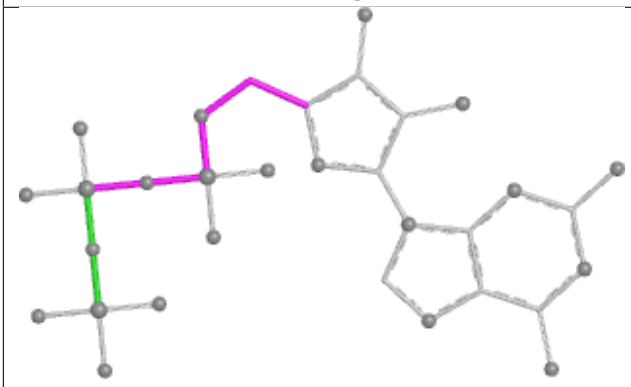
Ligand GTP E 602



Bond lengths



Bond angles



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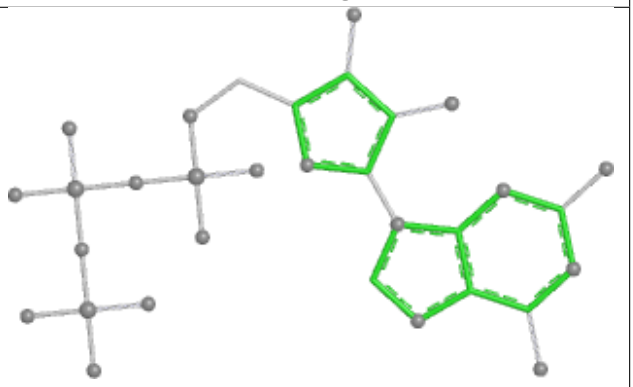
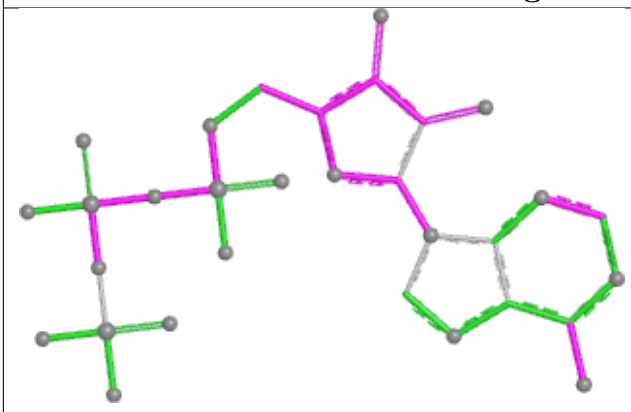


Rings

Ligand ATP H 601



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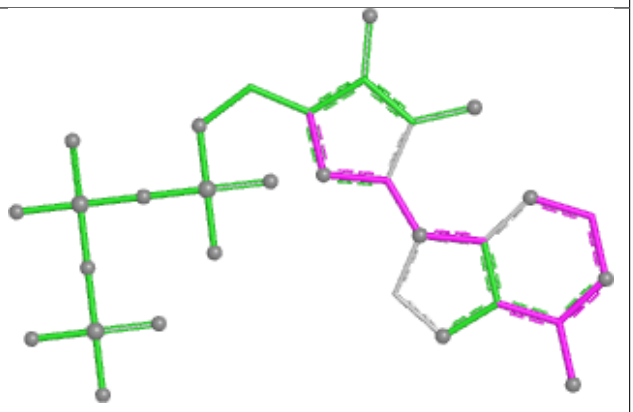
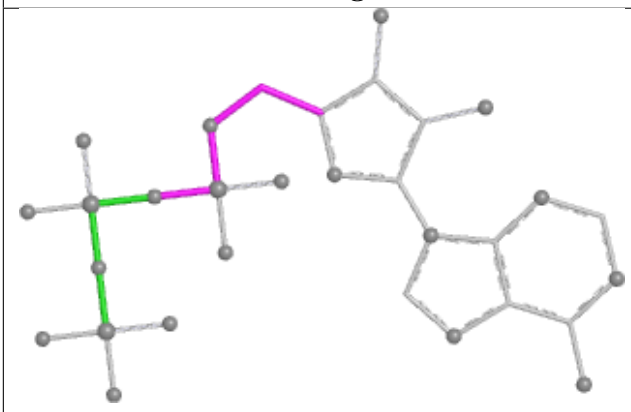
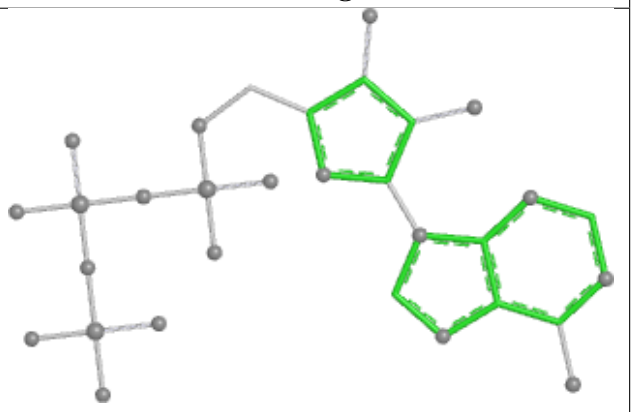


Bond angles

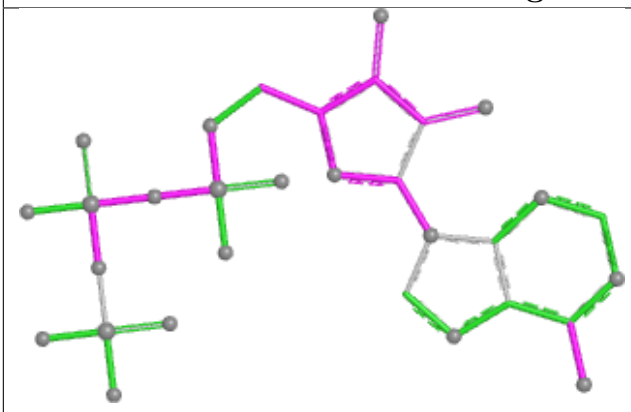


Torsions



Rings

Ligand ATP F 603



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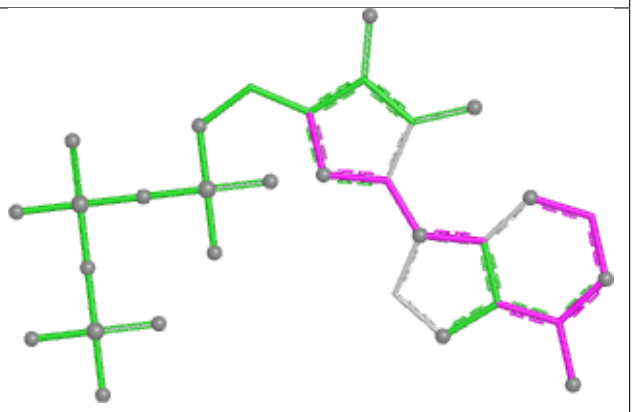
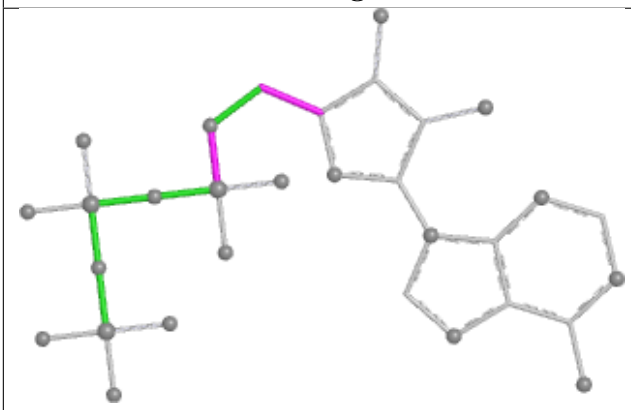


Bond angles



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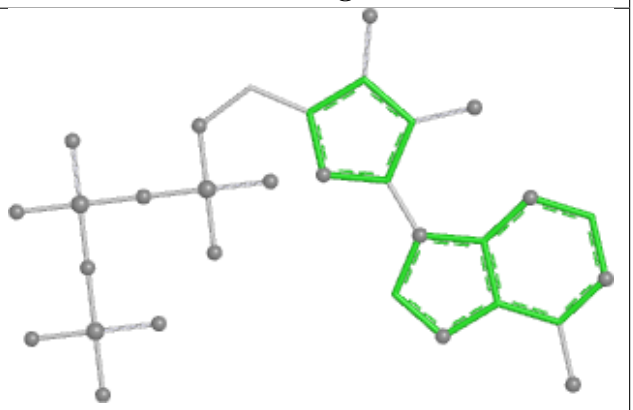
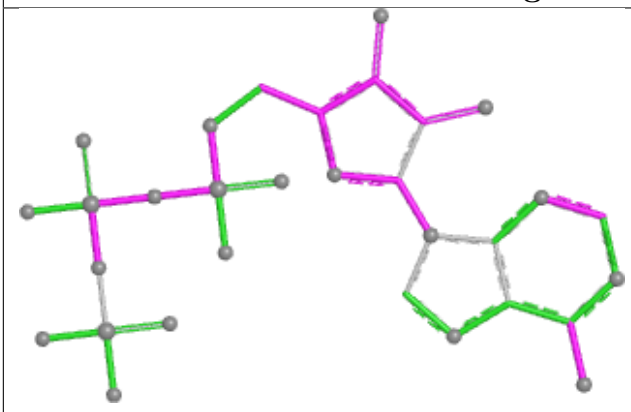


Rings

Ligand ATP G 602



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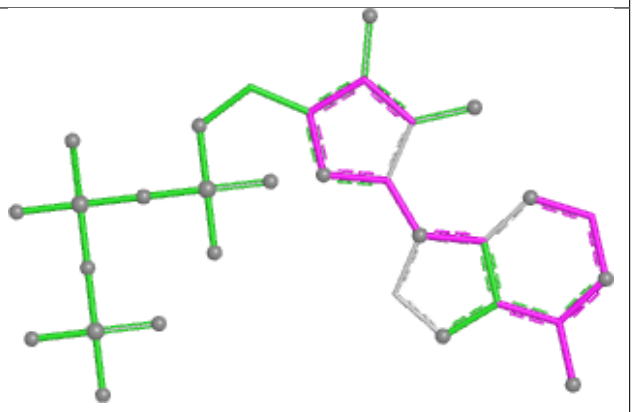
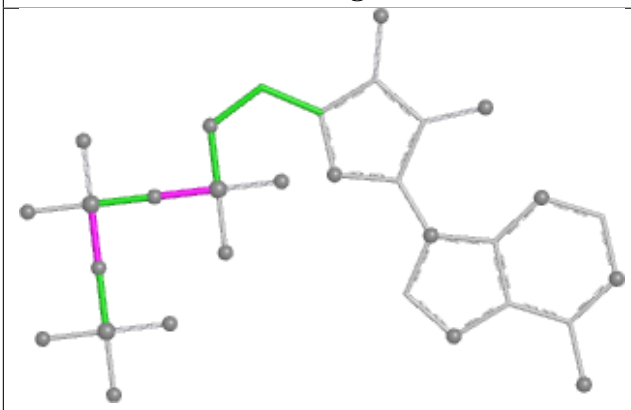


Bond angles



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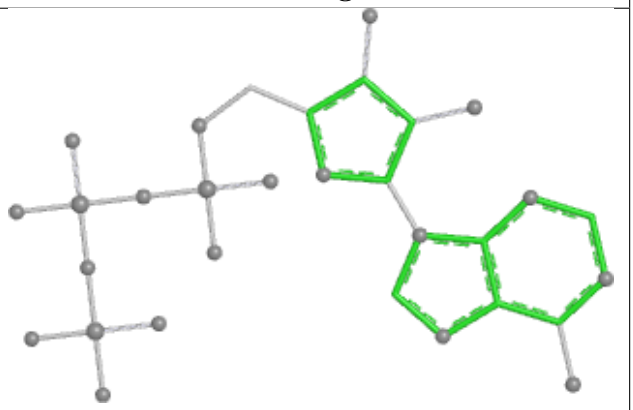
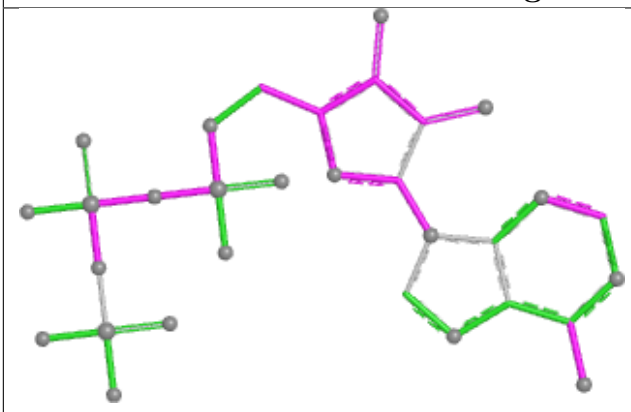
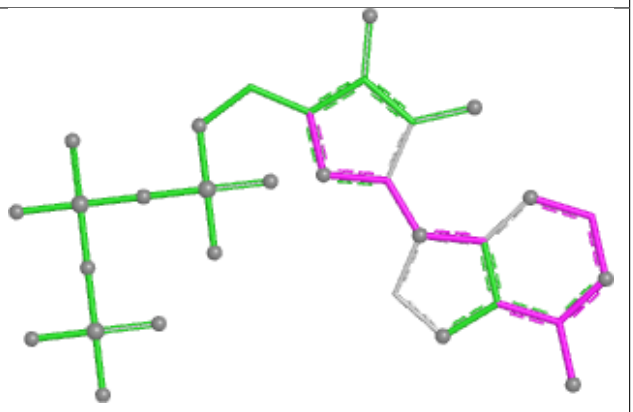


Rings

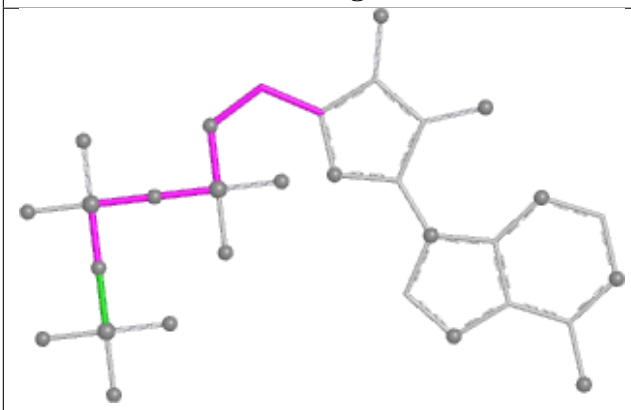
Ligand ATP D 601



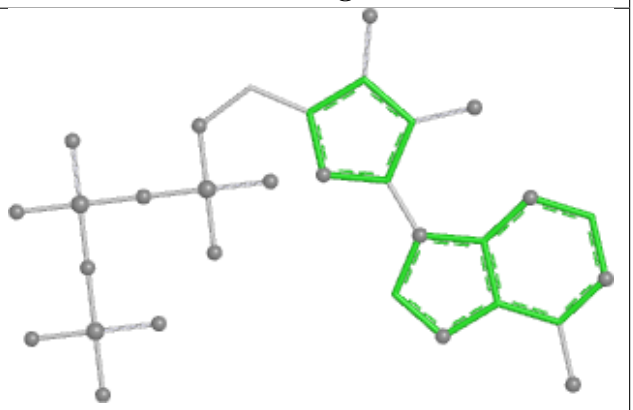
Bond lengths



Bond angles

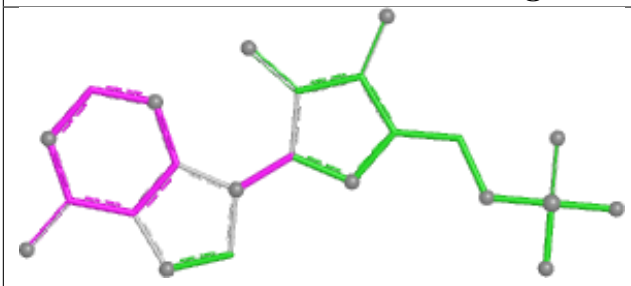


Torsions

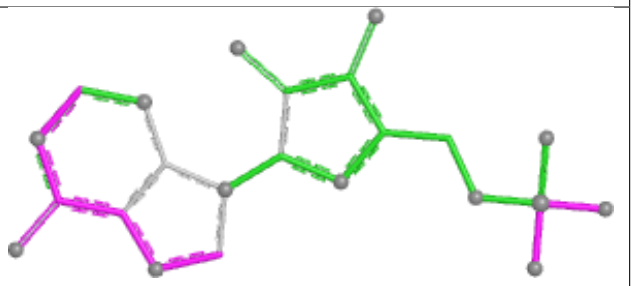


Rings

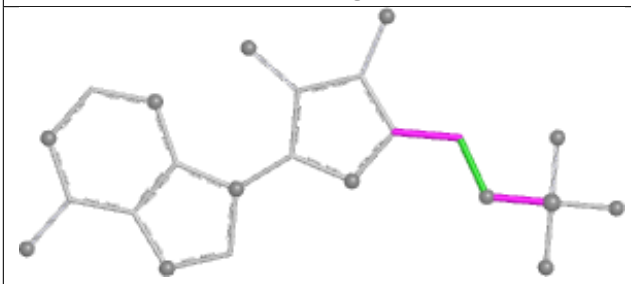
Ligand IMP G 604



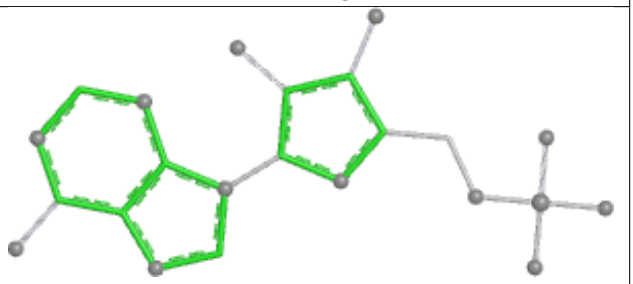
Bond lengths



Bond angles

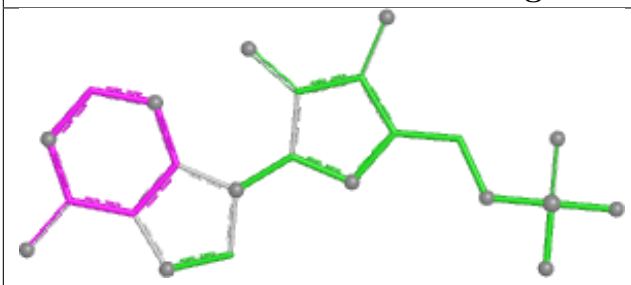


Torsions

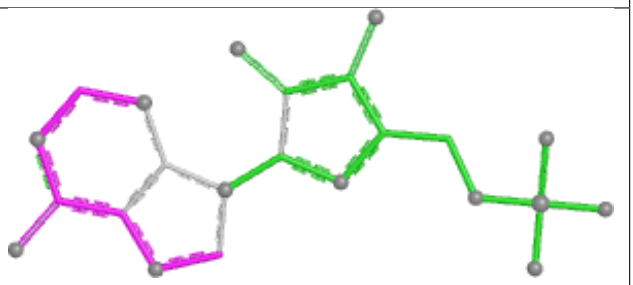


Rings

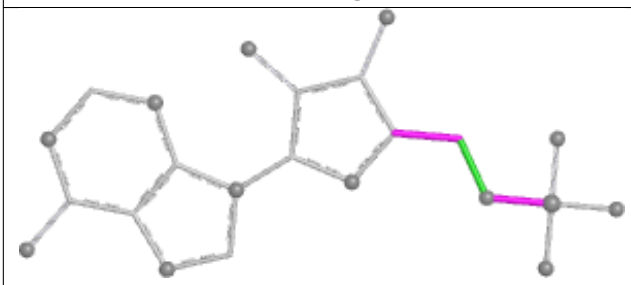
Ligand IMP D 602



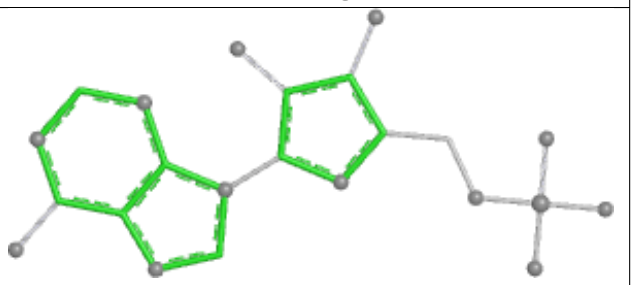
Bond lengths



Bond angles

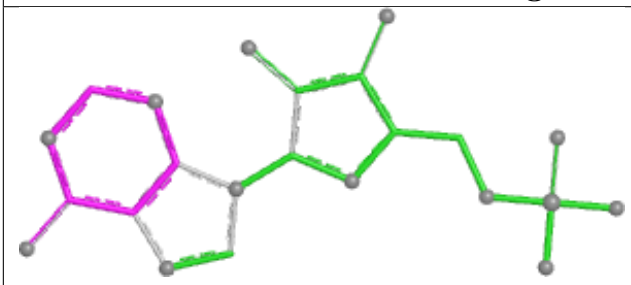


Torsions

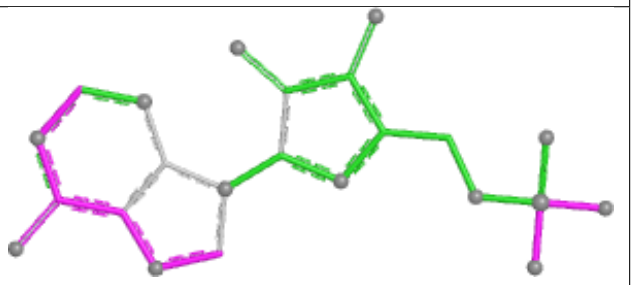


Rings

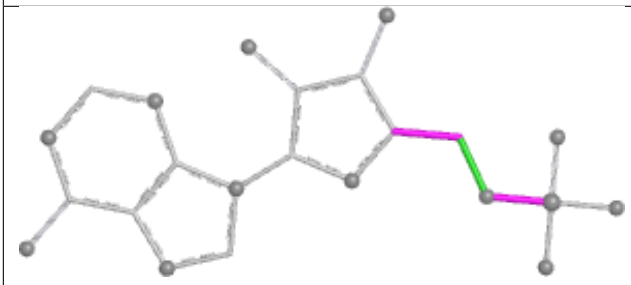
Ligand IMP C 603



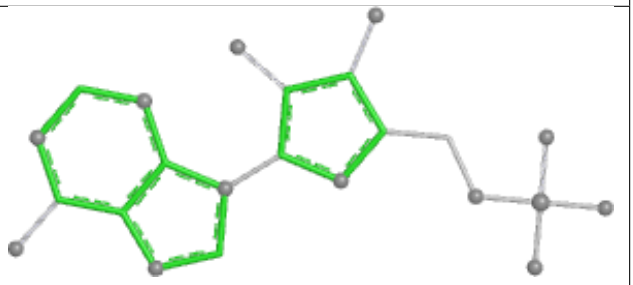
Bond lengths



Bond angles

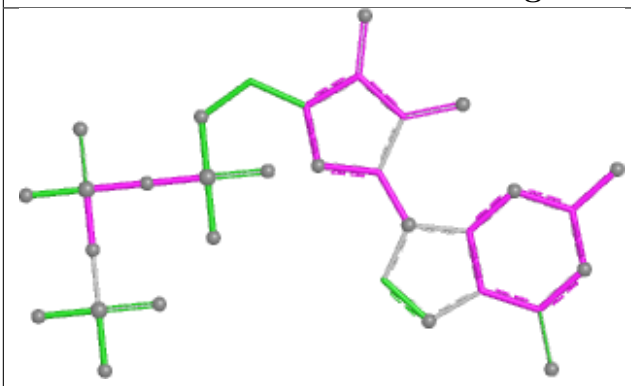


Torsions

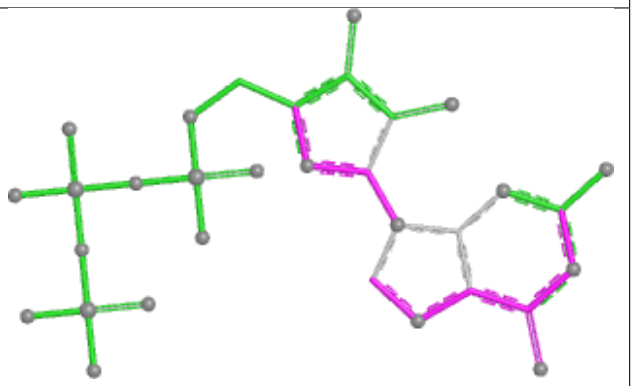


Rings

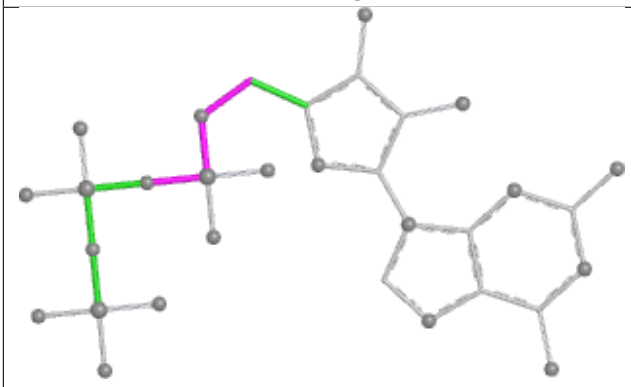
Ligand GTP F 602



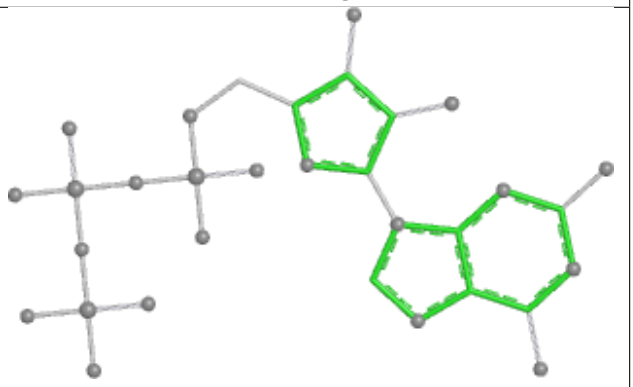
Bond lengths



Bond angles

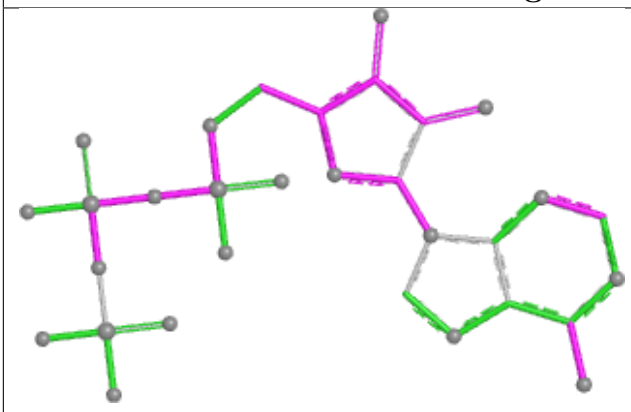


Torsions

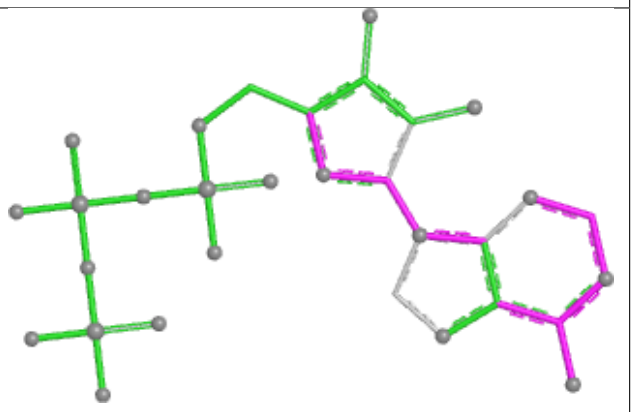


Rings

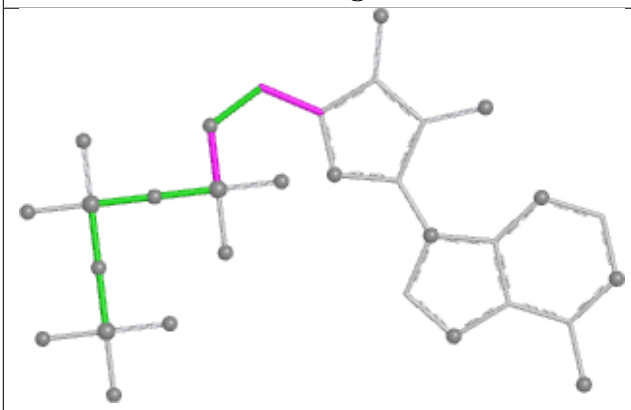
Ligand ATP C 601



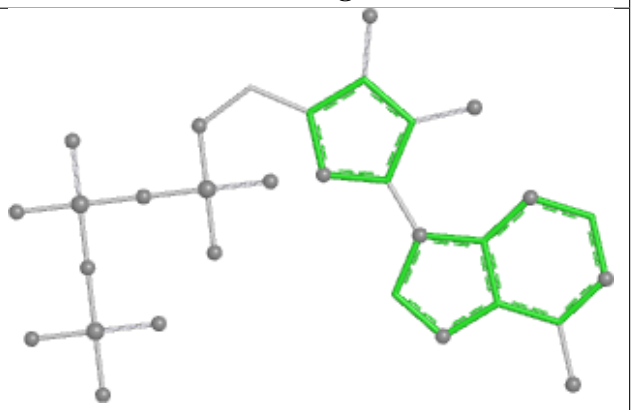
Bond lengths



Bond angles

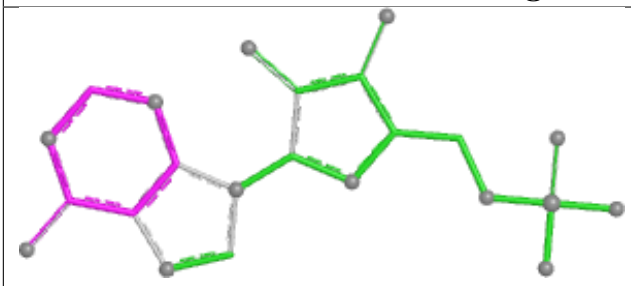


Torsions

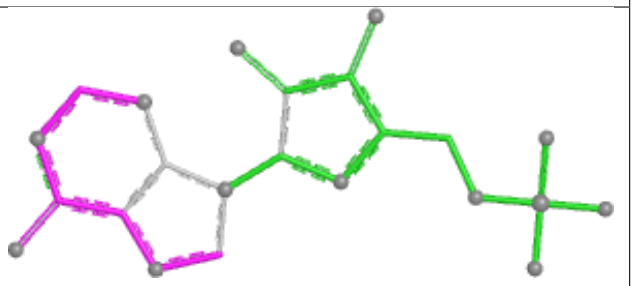


Rings

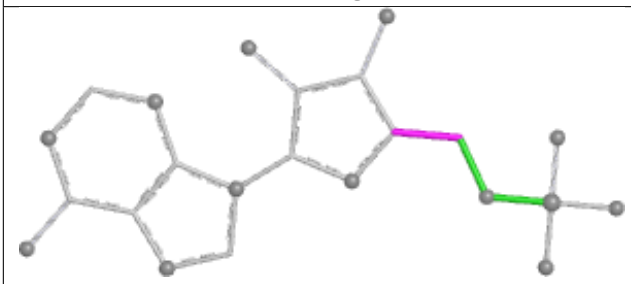
Ligand IMP H 602



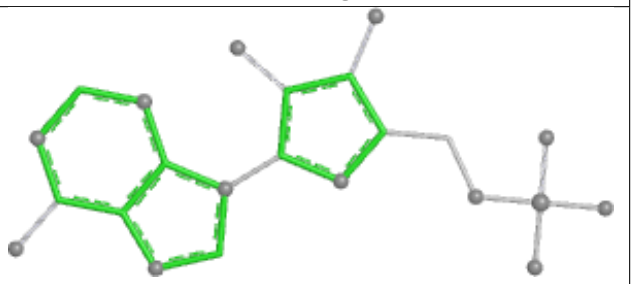
Bond lengths



Bond angles

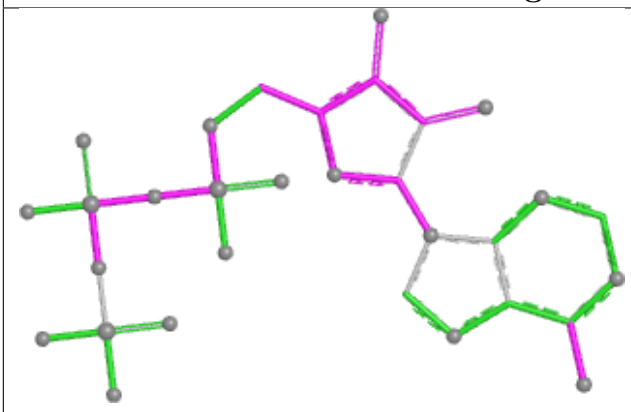


Torsions

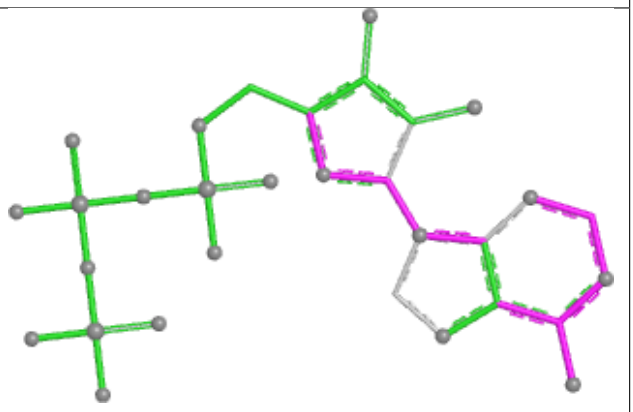


Rings

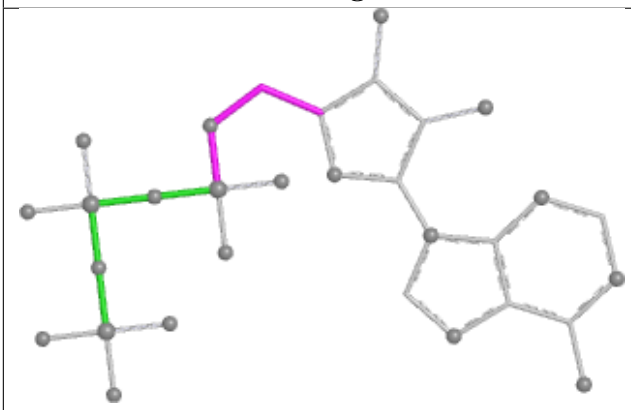
Ligand ATP C 605



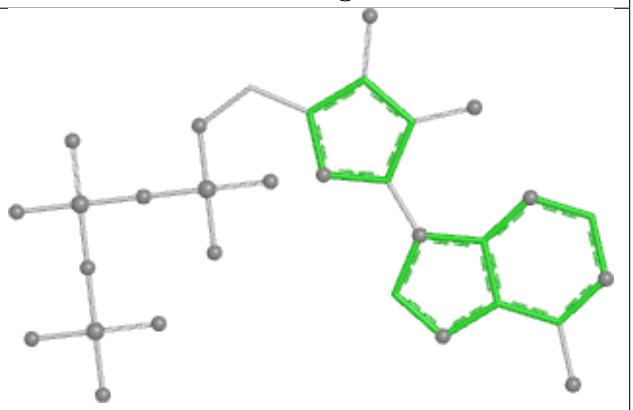
Bond lengths



Bond angles

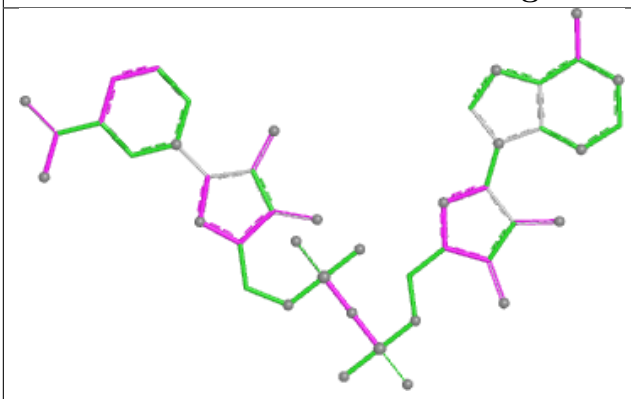


Torsions

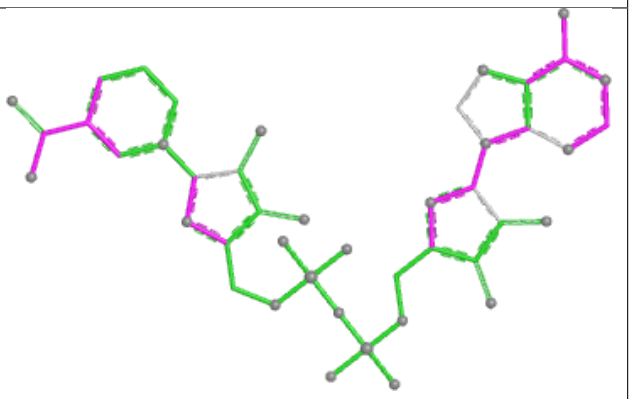


Rings

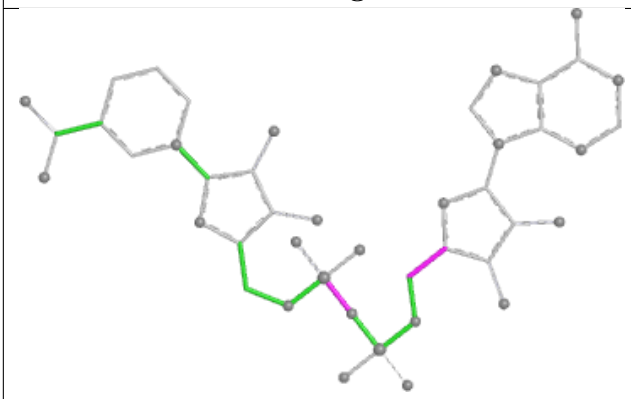
Ligand NAD E 605



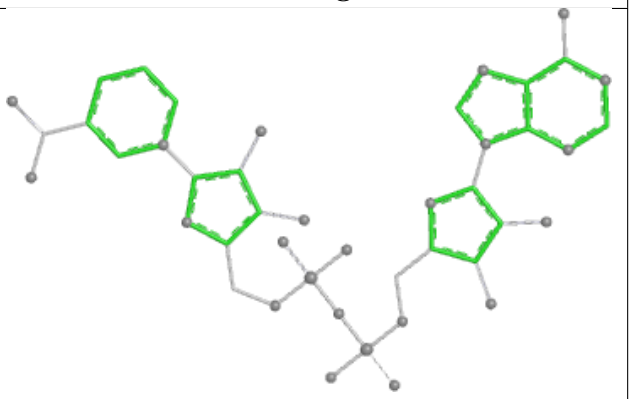
Bond lengths



Bond angles

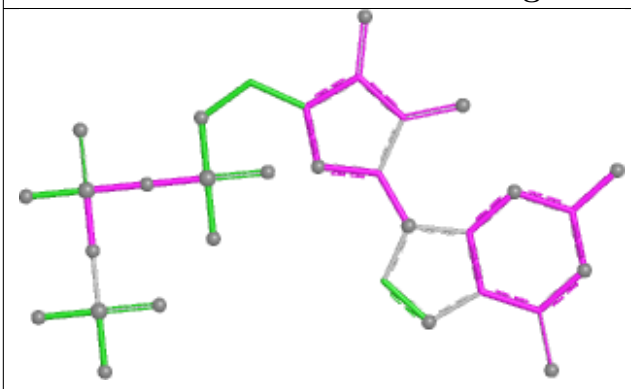


Torsions

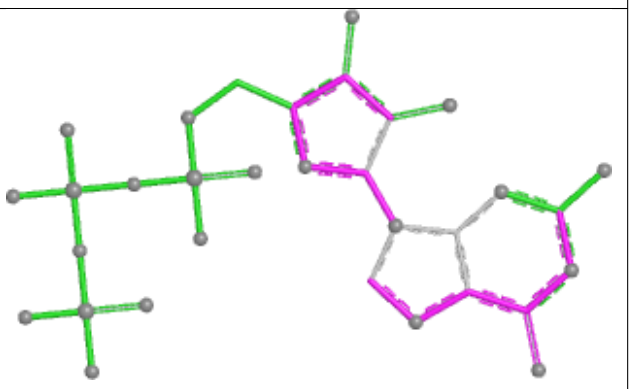


Rings

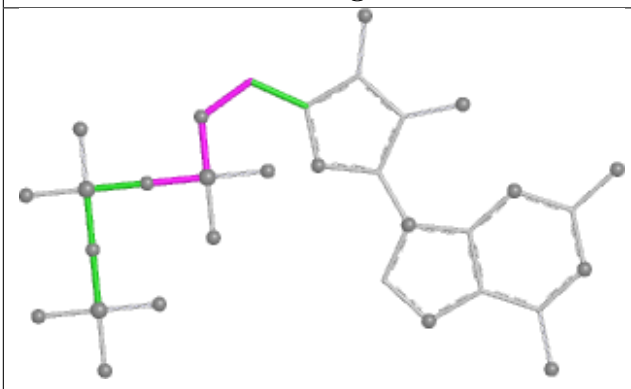
Ligand GTP B 602



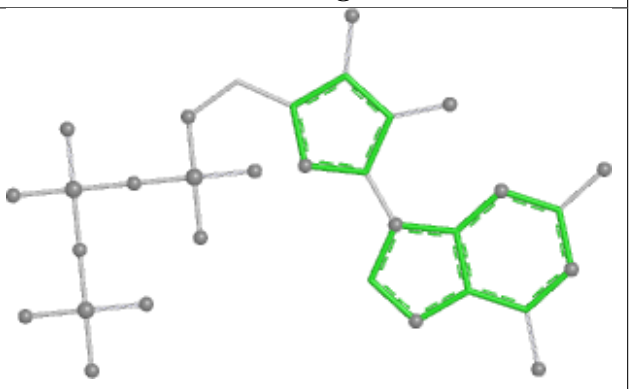
Bond lengths



Bond angles

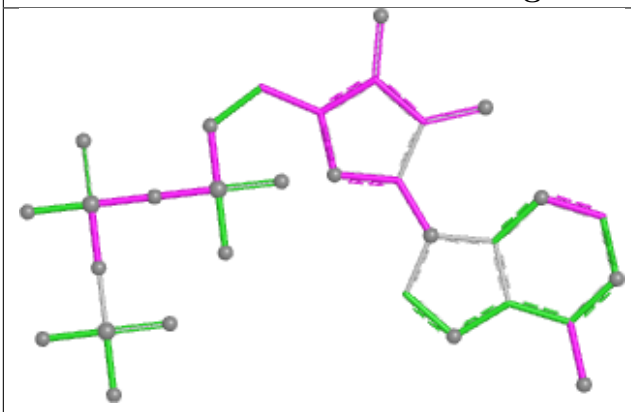


Torsions

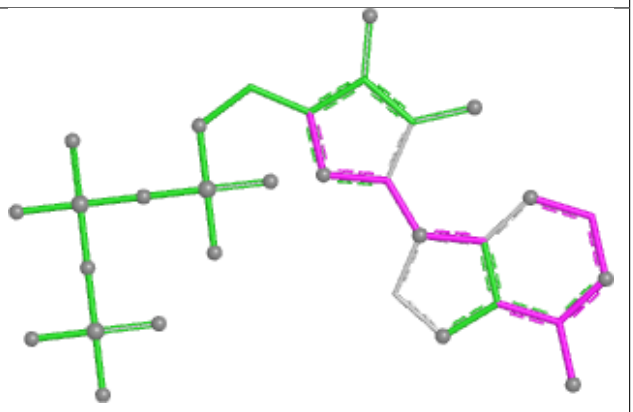


Rings

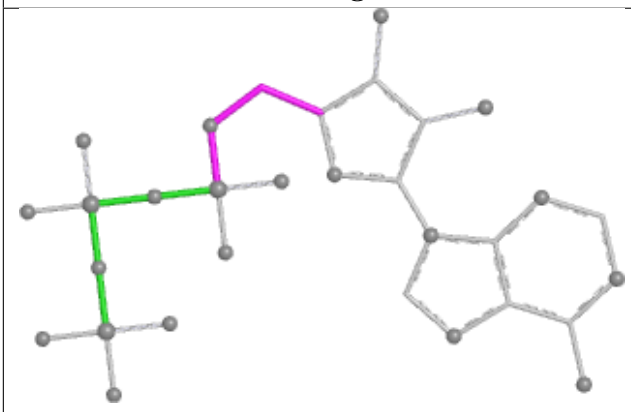
Ligand ATP G 601



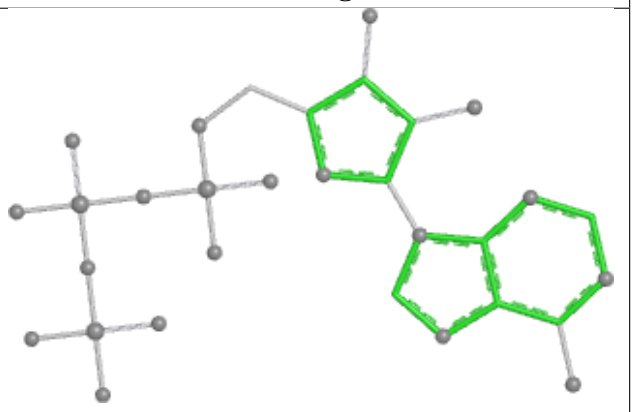
Bond lengths



Bond angles

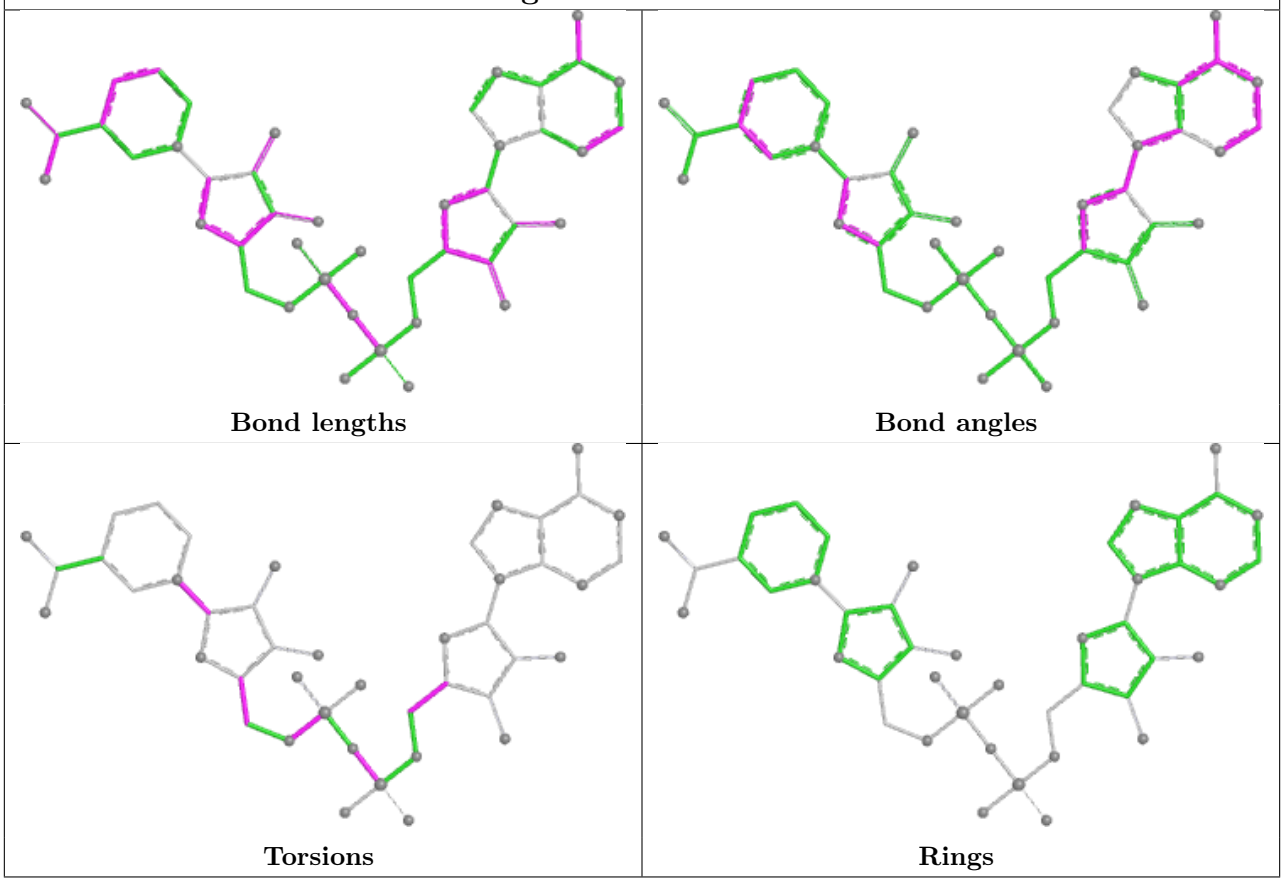


Torsions



Rings

Ligand NAD B 605



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.

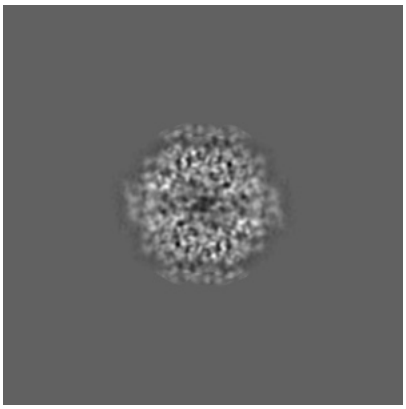
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20704. These allow visual inspection of the internal detail of the map and identification of artifacts.

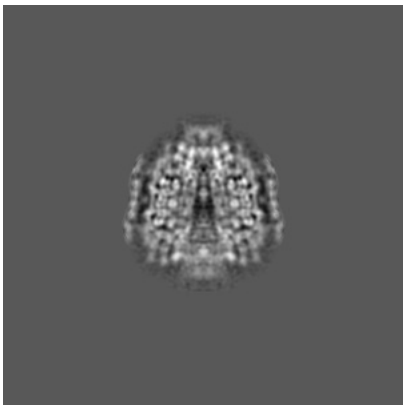
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

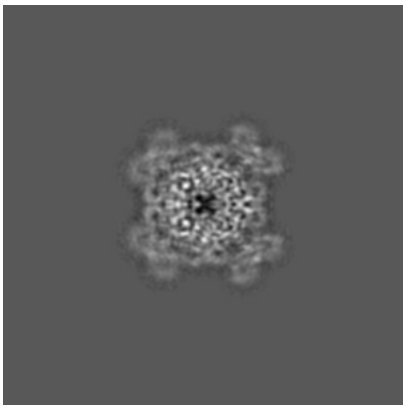
6.1.1 Primary map



X

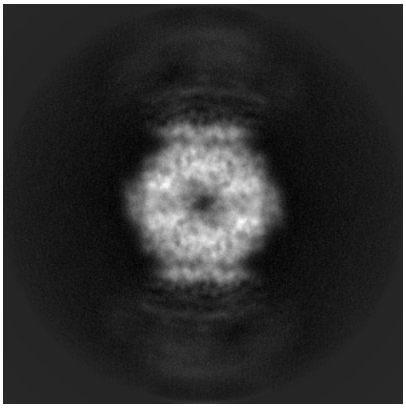


Y

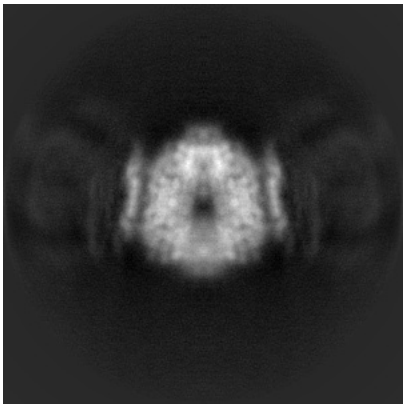


Z

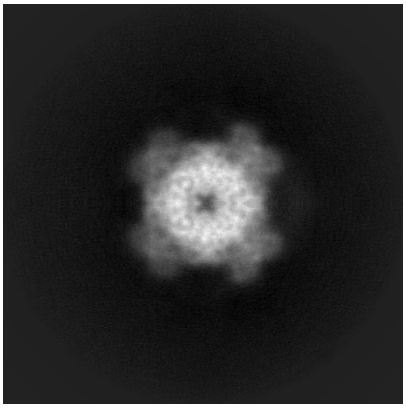
6.1.2 Raw map



X



Y

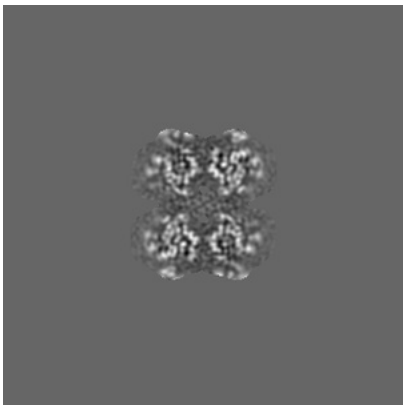


Z

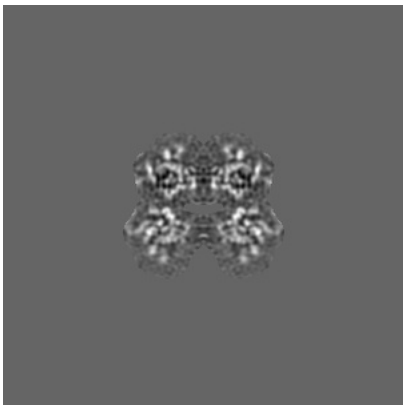
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

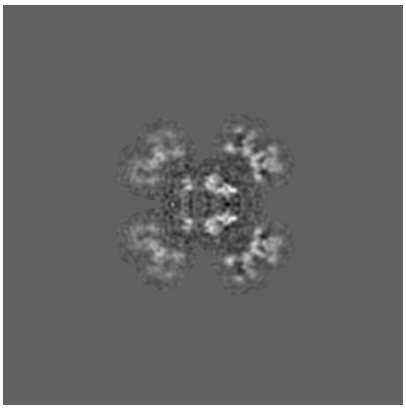
6.2.1 Primary map



X Index: 160

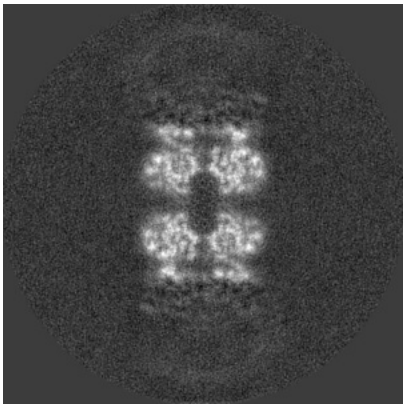


Y Index: 160

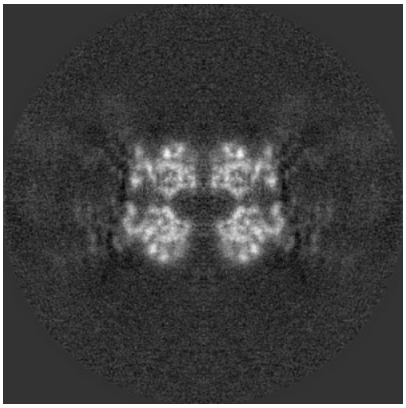


Z Index: 160

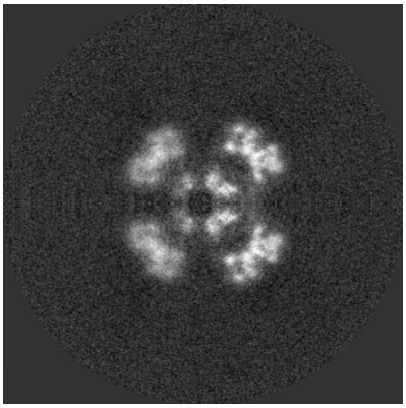
6.2.2 Raw map



X Index: 160



Y Index: 160

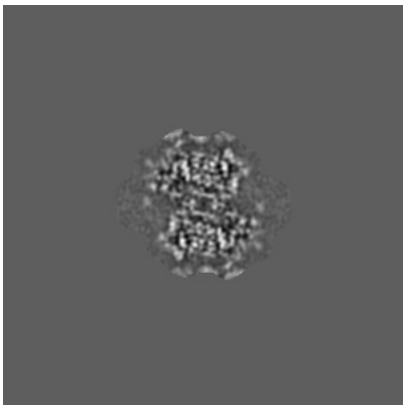


Z Index: 160

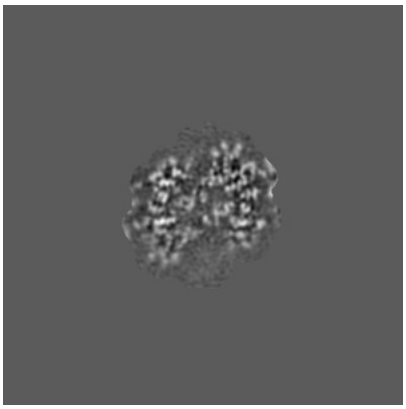
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

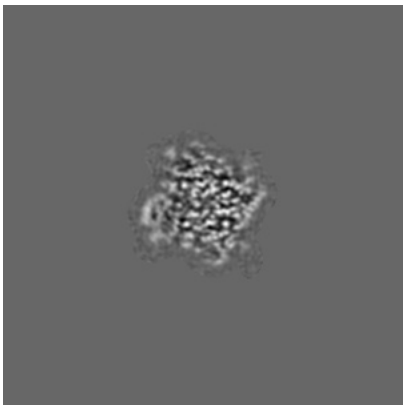
6.3.1 Primary map



X Index: 178

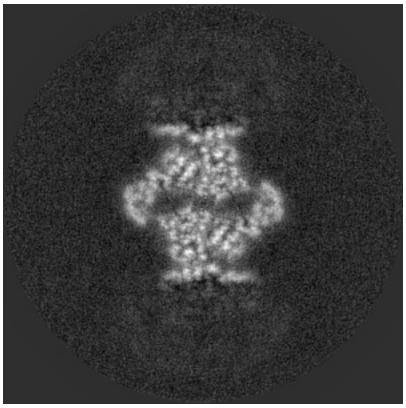


Y Index: 175

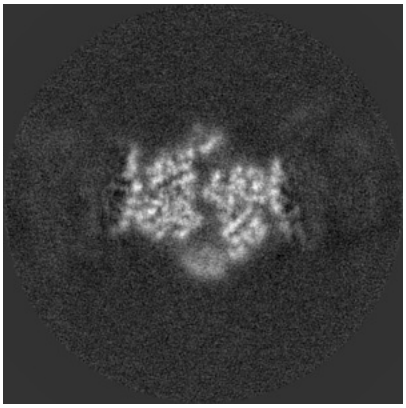


Z Index: 191

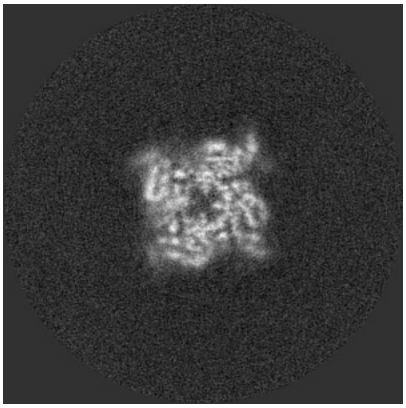
6.3.2 Raw map



X Index: 187



Y Index: 137

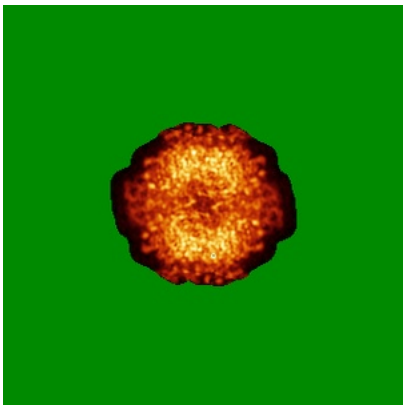


Z Index: 138

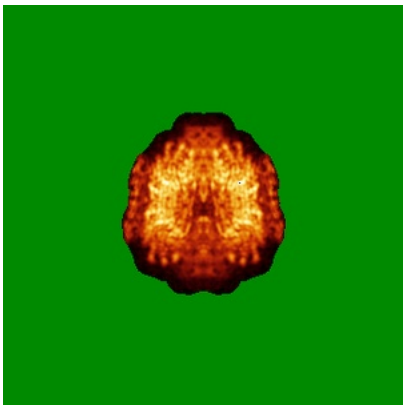
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

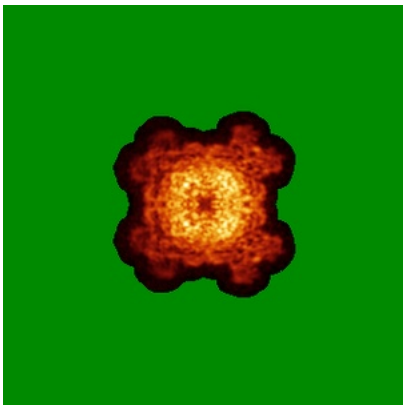
6.4.1 Primary map



X

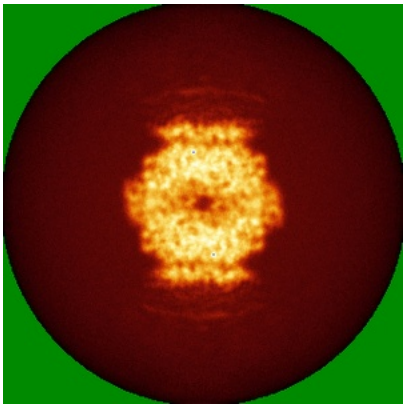


Y

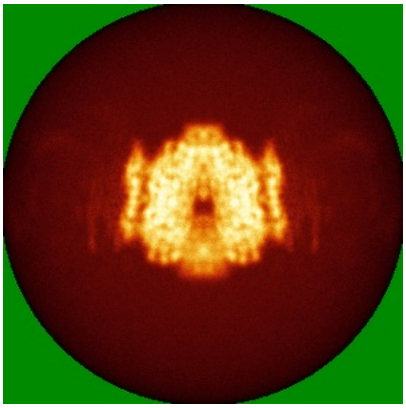


Z

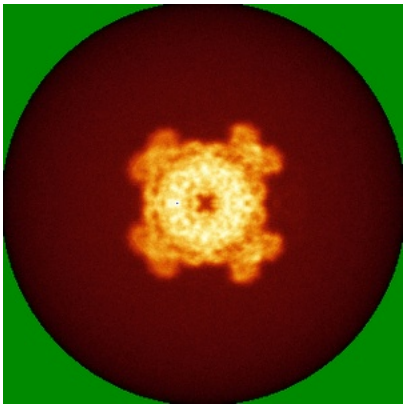
6.4.2 Raw map



X



Y

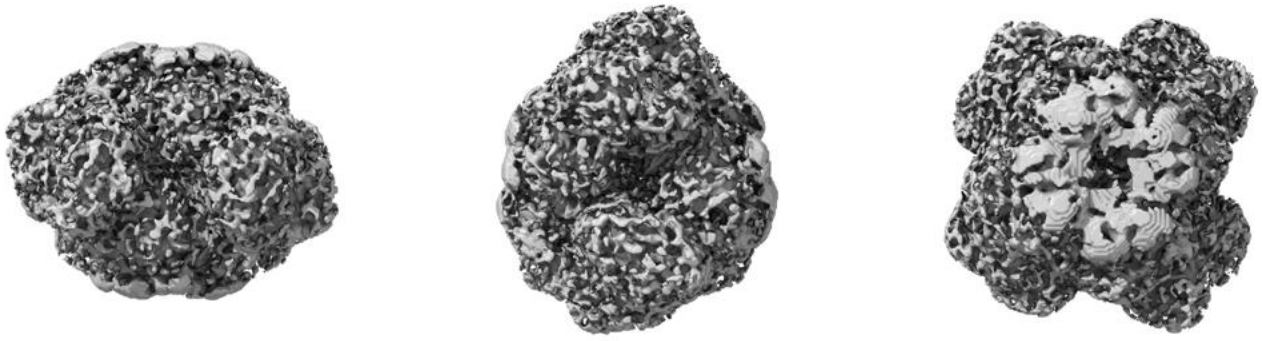


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

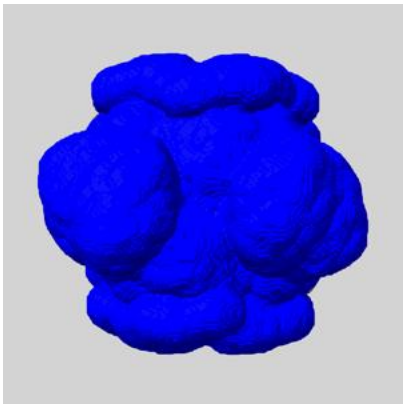
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

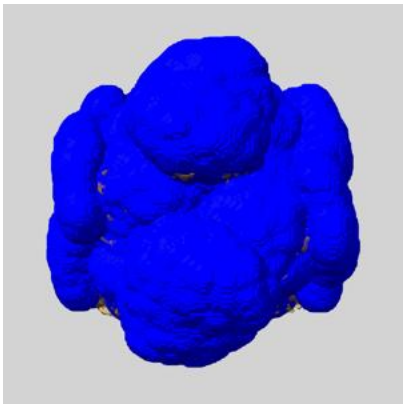
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

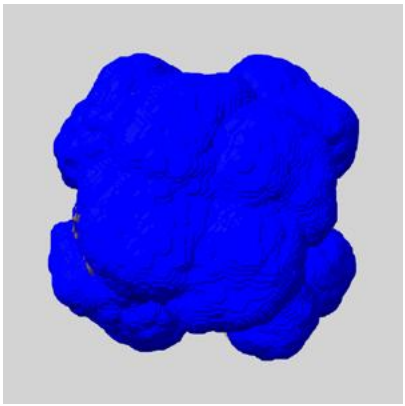
6.6.1 emd_20704_msk_1.map (i)



X



Y

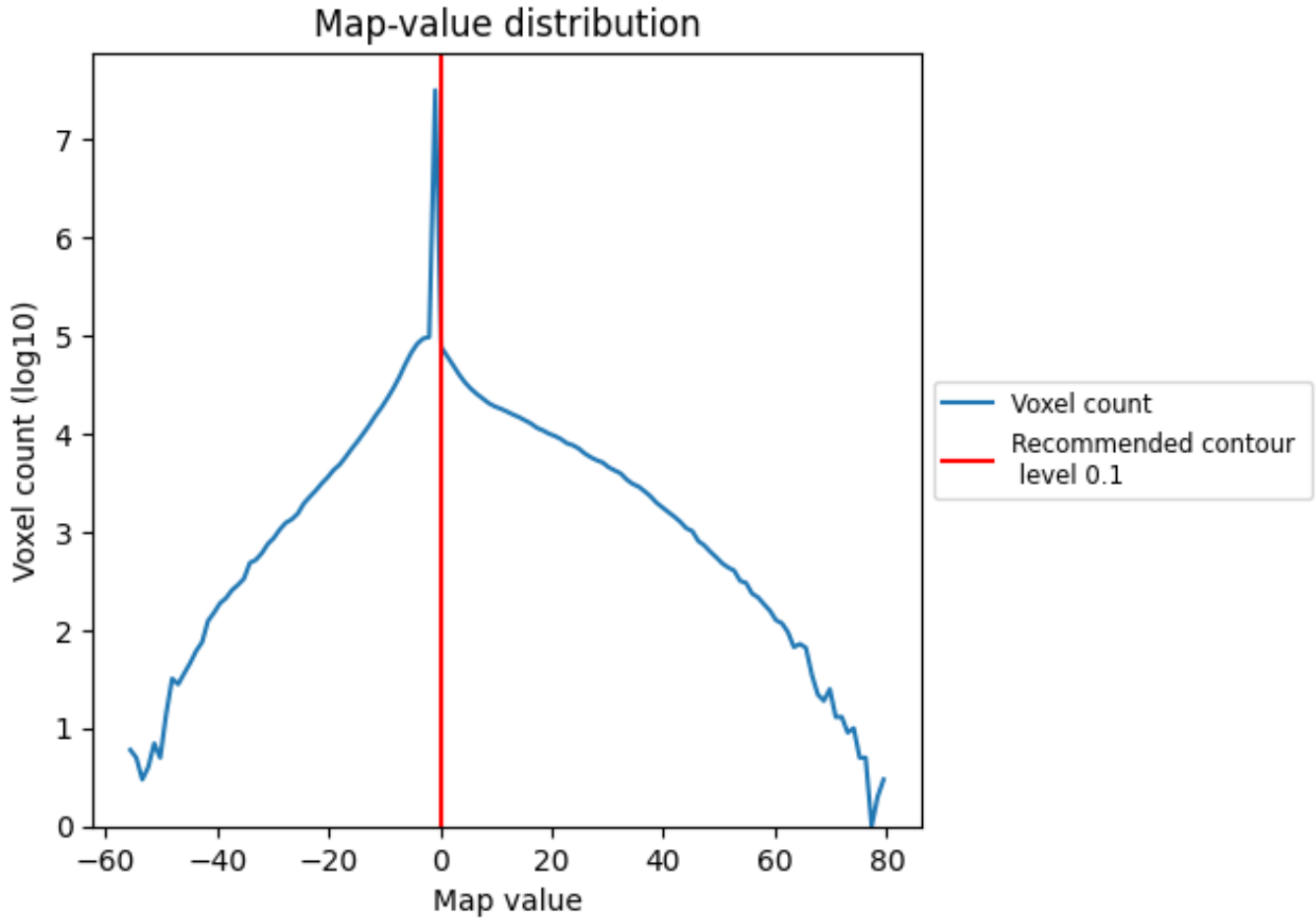


Z

7 Map analysis

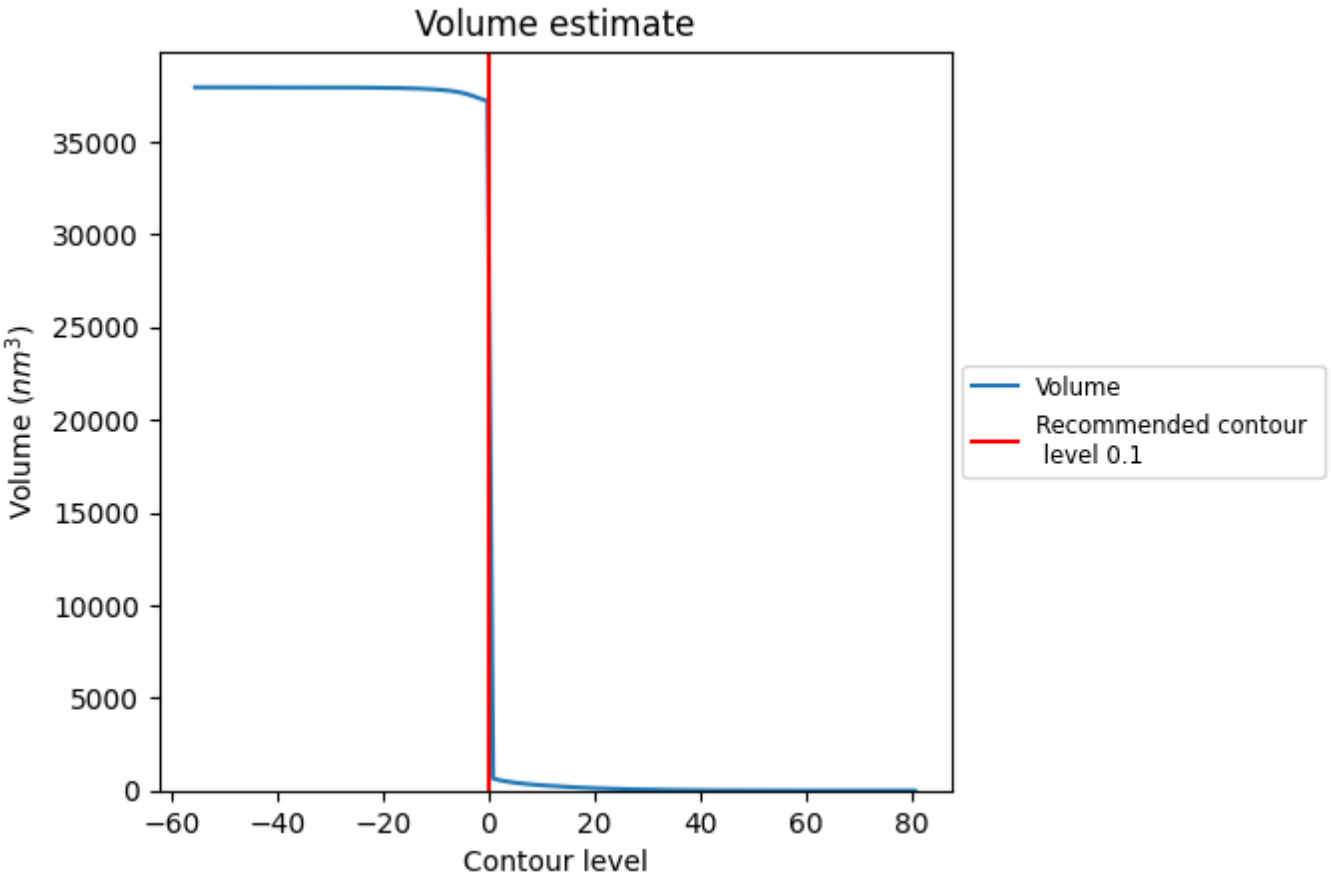
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

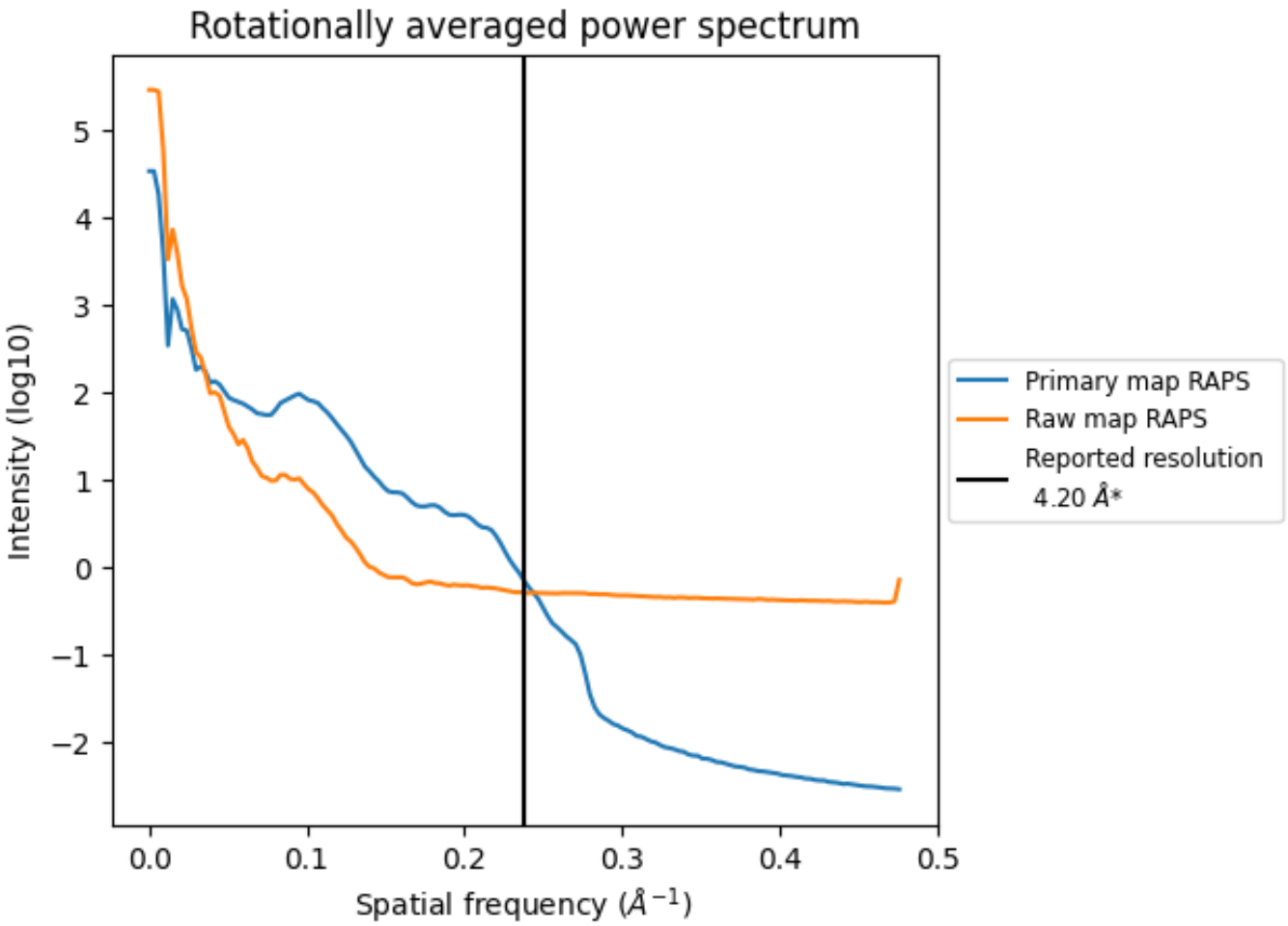
7.2 Volume estimate



The volume at the recommended contour level is 25305 nm^3; this corresponds to an approximate mass of 22859 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

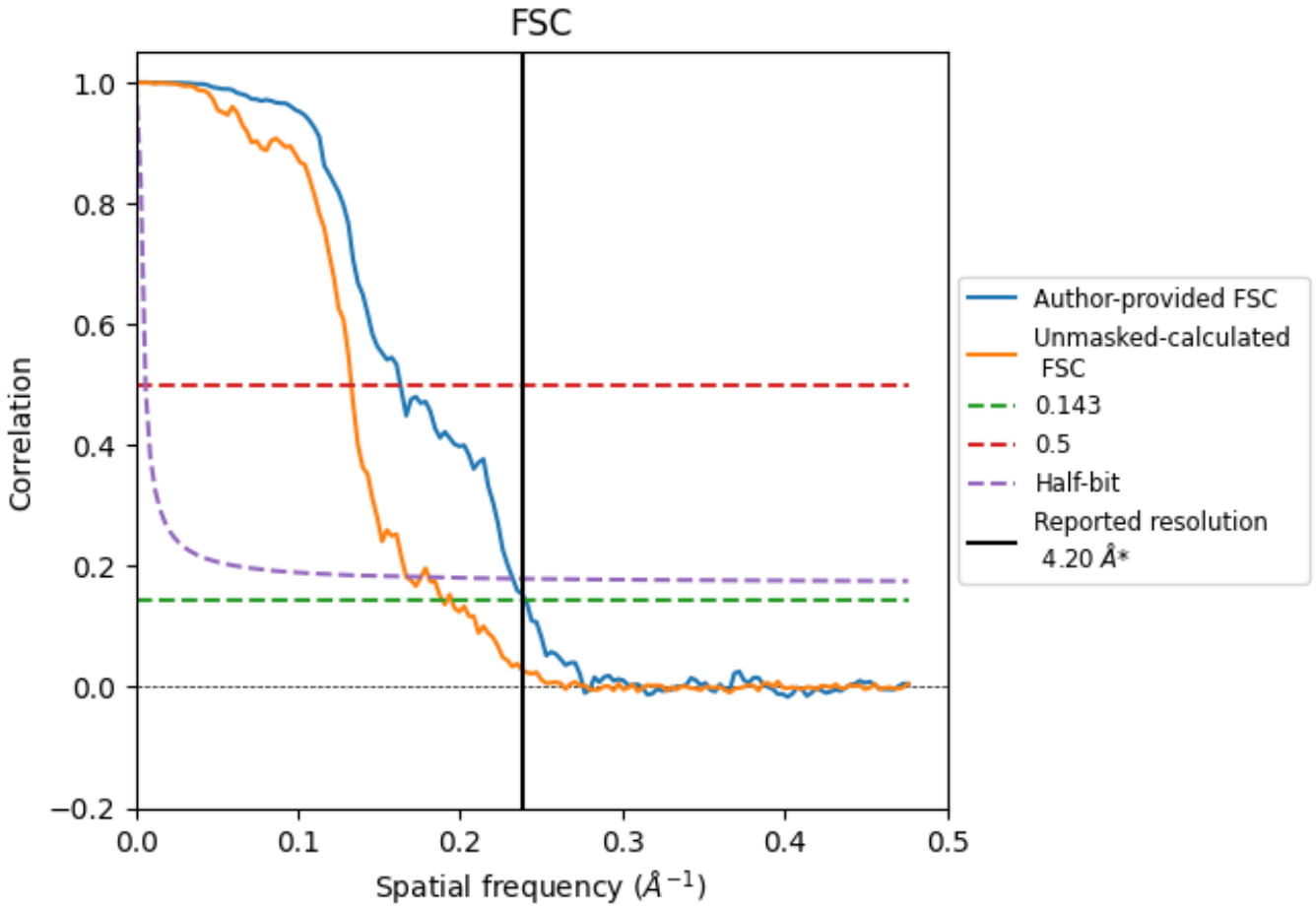


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

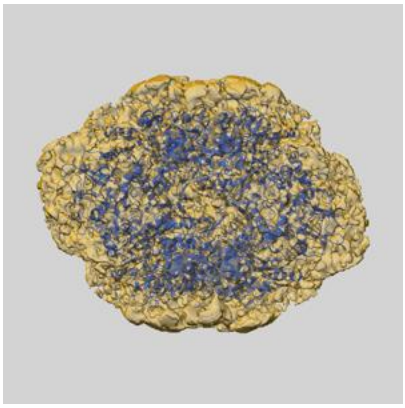
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.16	6.13	4.30
Unmasked-calculated*	5.29	7.53	6.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.29 differs from the reported value 4.2 by more than 10 %

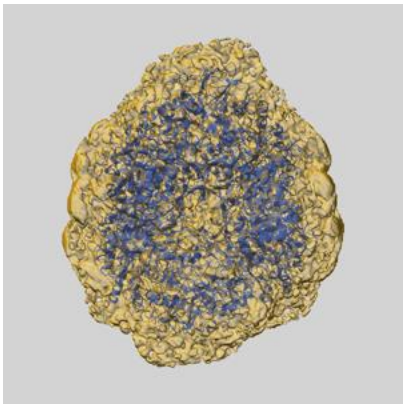
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20704 and PDB model 6UA2. Per-residue inclusion information can be found in section 3 on page 11.

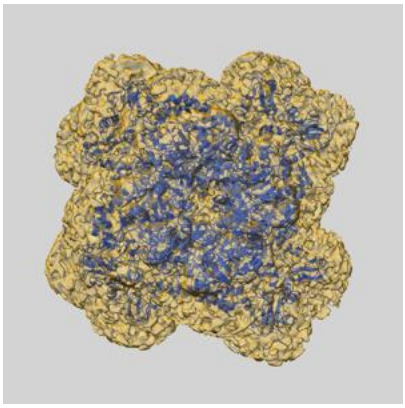
9.1 Map-model overlay



X



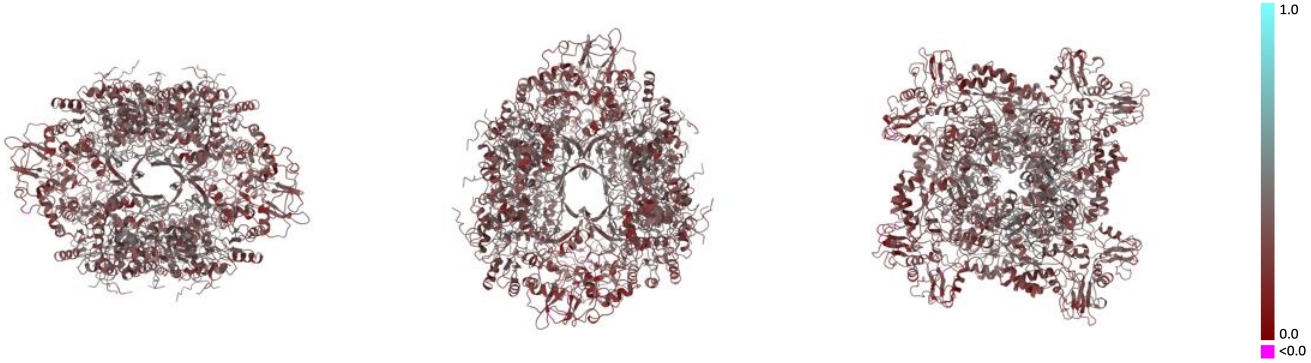
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

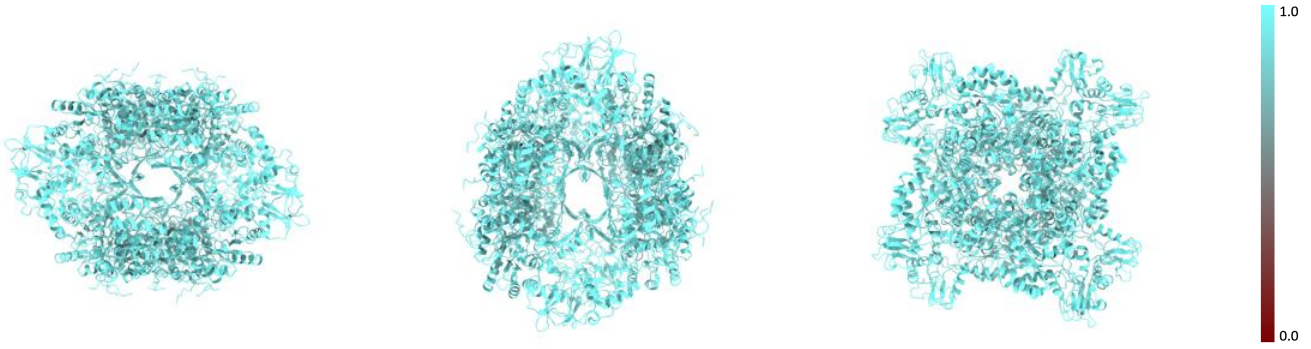
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

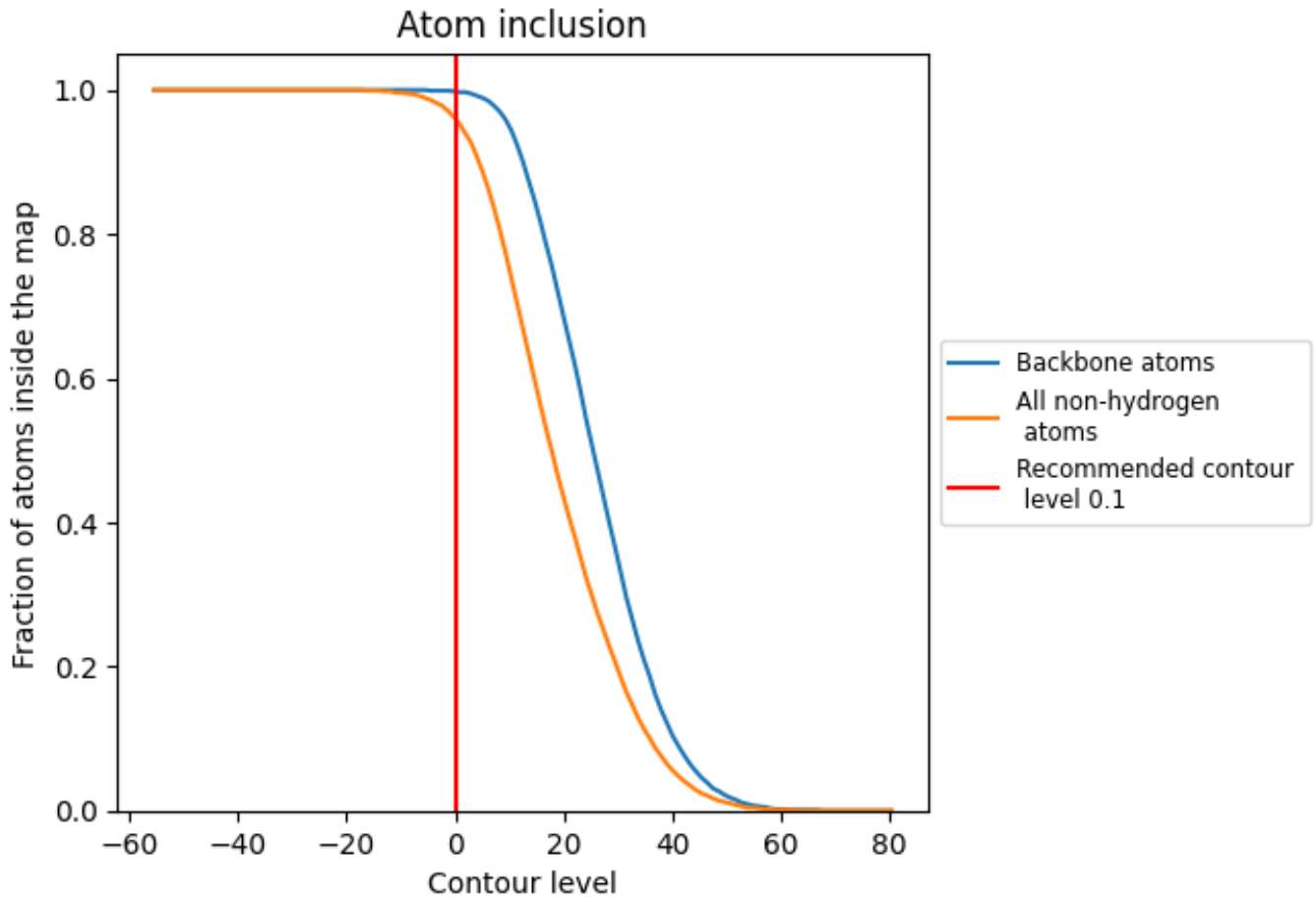
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9600	0.3310
A	0.9590	0.3440
B	0.9530	0.3510
C	0.9660	0.3200
D	0.9620	0.3090
E	0.9590	0.3440
F	0.9510	0.3510
G	0.9650	0.3190
H	0.9610	0.3100
I	0.9800	0.3530
J	0.9800	0.3190
K	1.0000	0.3260
L	1.0000	0.3170
M	0.9800	0.3610
N	0.9800	0.3120
O	1.0000	0.3200
P	0.9800	0.3190