



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2026 – 01:24 pm BST

PDB ID : 7R50 / pdb_00007r50
Title : Crystal structure of GMP reductase from mycobacterium smegmatis in complex with GMP.
Authors : Dolezal, M.; Klima, M.; Pichova, I.
Deposited on : 2022-02-09
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

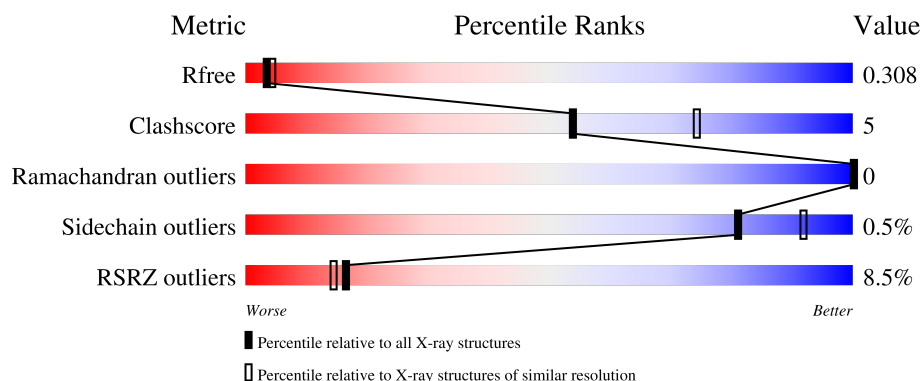
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	496	6% 86% 9% 5%
1	B	496	8% 79% 10% 10%
1	C	496	4% 80% 10% 10%
1	D	496	5% 84% 10% 6%
1	E	496	5% 83% 11% 6%

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Mol	Chain	Length	Quality of chain
1	F	496	
1	G	496	
1	H	496	
1	I	496	
1	J	496	
1	K	496	
1	L	496	
1	M	496	
1	N	496	
1	O	496	
1	P	496	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	5GP	K	501	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 53060 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GMP reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3403	2125	603	661	14			
1	B	447	Total	C	N	O	S	0	0	0
			3230	2017	572	628	13			
1	C	446	Total	C	N	O	S	0	0	0
			3235	2024	574	624	13			
1	D	468	Total	C	N	O	S	0	0	0
			3389	2118	601	656	14			
1	E	468	Total	C	N	O	S	0	0	0
			3390	2119	601	656	14			
1	F	440	Total	C	N	O	S	0	0	0
			3168	1986	561	608	13			
1	G	424	Total	C	N	O	S	0	0	0
			3017	1896	521	587	13			
1	H	468	Total	C	N	O	S	0	0	0
			3378	2107	601	656	14			
1	I	466	Total	C	N	O	S	0	0	0
			3375	2110	599	652	14			
1	J	440	Total	C	N	O	S	0	0	0
			3154	1976	551	614	13			
1	K	450	Total	C	N	O	S	0	0	0
			3216	2021	566	617	12			
1	L	465	Total	C	N	O	S	0	0	0
			3346	2089	594	649	14			
1	M	471	Total	C	N	O	S	0	0	0
			3376	2114	592	656	14			
1	N	461	Total	C	N	O	S	0	0	0
			3350	2093	597	646	14			
1	O	455	Total	C	N	O	S	0	0	0
			3280	2049	582	636	13			
1	P	465	Total	C	N	O	S	0	0	0
			3369	2108	601	646	14			

There are 304 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0QYE8
A	2	VAL	-	expression tag	UNP A0QYE8
A	480	THR	-	expression tag	UNP A0QYE8
A	481	ALA	-	expression tag	UNP A0QYE8
A	482	ALA	-	expression tag	UNP A0QYE8
A	483	ALA	-	expression tag	UNP A0QYE8
A	484	LYS	-	expression tag	UNP A0QYE8
A	485	GLU	-	expression tag	UNP A0QYE8
A	486	ASP	-	expression tag	UNP A0QYE8
A	487	LEU	-	expression tag	UNP A0QYE8
A	488	GLU	-	expression tag	UNP A0QYE8
A	489	HIS	-	expression tag	UNP A0QYE8
A	490	HIS	-	expression tag	UNP A0QYE8
A	491	HIS	-	expression tag	UNP A0QYE8
A	492	HIS	-	expression tag	UNP A0QYE8
A	493	HIS	-	expression tag	UNP A0QYE8
A	494	HIS	-	expression tag	UNP A0QYE8
A	495	HIS	-	expression tag	UNP A0QYE8
A	496	HIS	-	expression tag	UNP A0QYE8
B	1	MET	-	initiating methionine	UNP A0QYE8
B	2	VAL	-	expression tag	UNP A0QYE8
B	480	THR	-	expression tag	UNP A0QYE8
B	481	ALA	-	expression tag	UNP A0QYE8
B	482	ALA	-	expression tag	UNP A0QYE8
B	483	ALA	-	expression tag	UNP A0QYE8
B	484	LYS	-	expression tag	UNP A0QYE8
B	485	GLU	-	expression tag	UNP A0QYE8
B	486	ASP	-	expression tag	UNP A0QYE8
B	487	LEU	-	expression tag	UNP A0QYE8
B	488	GLU	-	expression tag	UNP A0QYE8
B	489	HIS	-	expression tag	UNP A0QYE8
B	490	HIS	-	expression tag	UNP A0QYE8
B	491	HIS	-	expression tag	UNP A0QYE8
B	492	HIS	-	expression tag	UNP A0QYE8
B	493	HIS	-	expression tag	UNP A0QYE8
B	494	HIS	-	expression tag	UNP A0QYE8
B	495	HIS	-	expression tag	UNP A0QYE8
B	496	HIS	-	expression tag	UNP A0QYE8
C	1	MET	-	initiating methionine	UNP A0QYE8
C	2	VAL	-	expression tag	UNP A0QYE8
C	480	THR	-	expression tag	UNP A0QYE8
C	481	ALA	-	expression tag	UNP A0QYE8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	482	ALA	-	expression tag	UNP A0QYE8
C	483	ALA	-	expression tag	UNP A0QYE8
C	484	LYS	-	expression tag	UNP A0QYE8
C	485	GLU	-	expression tag	UNP A0QYE8
C	486	ASP	-	expression tag	UNP A0QYE8
C	487	LEU	-	expression tag	UNP A0QYE8
C	488	GLU	-	expression tag	UNP A0QYE8
C	489	HIS	-	expression tag	UNP A0QYE8
C	490	HIS	-	expression tag	UNP A0QYE8
C	491	HIS	-	expression tag	UNP A0QYE8
C	492	HIS	-	expression tag	UNP A0QYE8
C	493	HIS	-	expression tag	UNP A0QYE8
C	494	HIS	-	expression tag	UNP A0QYE8
C	495	HIS	-	expression tag	UNP A0QYE8
C	496	HIS	-	expression tag	UNP A0QYE8
D	1	MET	-	initiating methionine	UNP A0QYE8
D	2	VAL	-	expression tag	UNP A0QYE8
D	480	THR	-	expression tag	UNP A0QYE8
D	481	ALA	-	expression tag	UNP A0QYE8
D	482	ALA	-	expression tag	UNP A0QYE8
D	483	ALA	-	expression tag	UNP A0QYE8
D	484	LYS	-	expression tag	UNP A0QYE8
D	485	GLU	-	expression tag	UNP A0QYE8
D	486	ASP	-	expression tag	UNP A0QYE8
D	487	LEU	-	expression tag	UNP A0QYE8
D	488	GLU	-	expression tag	UNP A0QYE8
D	489	HIS	-	expression tag	UNP A0QYE8
D	490	HIS	-	expression tag	UNP A0QYE8
D	491	HIS	-	expression tag	UNP A0QYE8
D	492	HIS	-	expression tag	UNP A0QYE8
D	493	HIS	-	expression tag	UNP A0QYE8
D	494	HIS	-	expression tag	UNP A0QYE8
D	495	HIS	-	expression tag	UNP A0QYE8
D	496	HIS	-	expression tag	UNP A0QYE8
E	1	MET	-	initiating methionine	UNP A0QYE8
E	2	VAL	-	expression tag	UNP A0QYE8
E	480	THR	-	expression tag	UNP A0QYE8
E	481	ALA	-	expression tag	UNP A0QYE8
E	482	ALA	-	expression tag	UNP A0QYE8
E	483	ALA	-	expression tag	UNP A0QYE8
E	484	LYS	-	expression tag	UNP A0QYE8
E	485	GLU	-	expression tag	UNP A0QYE8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	486	ASP	-	expression tag	UNP A0QYE8
E	487	LEU	-	expression tag	UNP A0QYE8
E	488	GLU	-	expression tag	UNP A0QYE8
E	489	HIS	-	expression tag	UNP A0QYE8
E	490	HIS	-	expression tag	UNP A0QYE8
E	491	HIS	-	expression tag	UNP A0QYE8
E	492	HIS	-	expression tag	UNP A0QYE8
E	493	HIS	-	expression tag	UNP A0QYE8
E	494	HIS	-	expression tag	UNP A0QYE8
E	495	HIS	-	expression tag	UNP A0QYE8
E	496	HIS	-	expression tag	UNP A0QYE8
F	1	MET	-	initiating methionine	UNP A0QYE8
F	2	VAL	-	expression tag	UNP A0QYE8
F	480	THR	-	expression tag	UNP A0QYE8
F	481	ALA	-	expression tag	UNP A0QYE8
F	482	ALA	-	expression tag	UNP A0QYE8
F	483	ALA	-	expression tag	UNP A0QYE8
F	484	LYS	-	expression tag	UNP A0QYE8
F	485	GLU	-	expression tag	UNP A0QYE8
F	486	ASP	-	expression tag	UNP A0QYE8
F	487	LEU	-	expression tag	UNP A0QYE8
F	488	GLU	-	expression tag	UNP A0QYE8
F	489	HIS	-	expression tag	UNP A0QYE8
F	490	HIS	-	expression tag	UNP A0QYE8
F	491	HIS	-	expression tag	UNP A0QYE8
F	492	HIS	-	expression tag	UNP A0QYE8
F	493	HIS	-	expression tag	UNP A0QYE8
F	494	HIS	-	expression tag	UNP A0QYE8
F	495	HIS	-	expression tag	UNP A0QYE8
F	496	HIS	-	expression tag	UNP A0QYE8
G	1	MET	-	initiating methionine	UNP A0QYE8
G	2	VAL	-	expression tag	UNP A0QYE8
G	480	THR	-	expression tag	UNP A0QYE8
G	481	ALA	-	expression tag	UNP A0QYE8
G	482	ALA	-	expression tag	UNP A0QYE8
G	483	ALA	-	expression tag	UNP A0QYE8
G	484	LYS	-	expression tag	UNP A0QYE8
G	485	GLU	-	expression tag	UNP A0QYE8
G	486	ASP	-	expression tag	UNP A0QYE8
G	487	LEU	-	expression tag	UNP A0QYE8
G	488	GLU	-	expression tag	UNP A0QYE8
G	489	HIS	-	expression tag	UNP A0QYE8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	490	HIS	-	expression tag	UNP A0QYE8
G	491	HIS	-	expression tag	UNP A0QYE8
G	492	HIS	-	expression tag	UNP A0QYE8
G	493	HIS	-	expression tag	UNP A0QYE8
G	494	HIS	-	expression tag	UNP A0QYE8
G	495	HIS	-	expression tag	UNP A0QYE8
G	496	HIS	-	expression tag	UNP A0QYE8
H	1	MET	-	initiating methionine	UNP A0QYE8
H	2	VAL	-	expression tag	UNP A0QYE8
H	480	THR	-	expression tag	UNP A0QYE8
H	481	ALA	-	expression tag	UNP A0QYE8
H	482	ALA	-	expression tag	UNP A0QYE8
H	483	ALA	-	expression tag	UNP A0QYE8
H	484	LYS	-	expression tag	UNP A0QYE8
H	485	GLU	-	expression tag	UNP A0QYE8
H	486	ASP	-	expression tag	UNP A0QYE8
H	487	LEU	-	expression tag	UNP A0QYE8
H	488	GLU	-	expression tag	UNP A0QYE8
H	489	HIS	-	expression tag	UNP A0QYE8
H	490	HIS	-	expression tag	UNP A0QYE8
H	491	HIS	-	expression tag	UNP A0QYE8
H	492	HIS	-	expression tag	UNP A0QYE8
H	493	HIS	-	expression tag	UNP A0QYE8
H	494	HIS	-	expression tag	UNP A0QYE8
H	495	HIS	-	expression tag	UNP A0QYE8
H	496	HIS	-	expression tag	UNP A0QYE8
I	1	MET	-	initiating methionine	UNP A0QYE8
I	2	VAL	-	expression tag	UNP A0QYE8
I	480	THR	-	expression tag	UNP A0QYE8
I	481	ALA	-	expression tag	UNP A0QYE8
I	482	ALA	-	expression tag	UNP A0QYE8
I	483	ALA	-	expression tag	UNP A0QYE8
I	484	LYS	-	expression tag	UNP A0QYE8
I	485	GLU	-	expression tag	UNP A0QYE8
I	486	ASP	-	expression tag	UNP A0QYE8
I	487	LEU	-	expression tag	UNP A0QYE8
I	488	GLU	-	expression tag	UNP A0QYE8
I	489	HIS	-	expression tag	UNP A0QYE8
I	490	HIS	-	expression tag	UNP A0QYE8
I	491	HIS	-	expression tag	UNP A0QYE8
I	492	HIS	-	expression tag	UNP A0QYE8
I	493	HIS	-	expression tag	UNP A0QYE8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	494	HIS	-	expression tag	UNP A0QYE8
I	495	HIS	-	expression tag	UNP A0QYE8
I	496	HIS	-	expression tag	UNP A0QYE8
J	1	MET	-	initiating methionine	UNP A0QYE8
J	2	VAL	-	expression tag	UNP A0QYE8
J	480	THR	-	expression tag	UNP A0QYE8
J	481	ALA	-	expression tag	UNP A0QYE8
J	482	ALA	-	expression tag	UNP A0QYE8
J	483	ALA	-	expression tag	UNP A0QYE8
J	484	LYS	-	expression tag	UNP A0QYE8
J	485	GLU	-	expression tag	UNP A0QYE8
J	486	ASP	-	expression tag	UNP A0QYE8
J	487	LEU	-	expression tag	UNP A0QYE8
J	488	GLU	-	expression tag	UNP A0QYE8
J	489	HIS	-	expression tag	UNP A0QYE8
J	490	HIS	-	expression tag	UNP A0QYE8
J	491	HIS	-	expression tag	UNP A0QYE8
J	492	HIS	-	expression tag	UNP A0QYE8
J	493	HIS	-	expression tag	UNP A0QYE8
J	494	HIS	-	expression tag	UNP A0QYE8
J	495	HIS	-	expression tag	UNP A0QYE8
J	496	HIS	-	expression tag	UNP A0QYE8
K	1	MET	-	initiating methionine	UNP A0QYE8
K	2	VAL	-	expression tag	UNP A0QYE8
K	480	THR	-	expression tag	UNP A0QYE8
K	481	ALA	-	expression tag	UNP A0QYE8
K	482	ALA	-	expression tag	UNP A0QYE8
K	483	ALA	-	expression tag	UNP A0QYE8
K	484	LYS	-	expression tag	UNP A0QYE8
K	485	GLU	-	expression tag	UNP A0QYE8
K	486	ASP	-	expression tag	UNP A0QYE8
K	487	LEU	-	expression tag	UNP A0QYE8
K	488	GLU	-	expression tag	UNP A0QYE8
K	489	HIS	-	expression tag	UNP A0QYE8
K	490	HIS	-	expression tag	UNP A0QYE8
K	491	HIS	-	expression tag	UNP A0QYE8
K	492	HIS	-	expression tag	UNP A0QYE8
K	493	HIS	-	expression tag	UNP A0QYE8
K	494	HIS	-	expression tag	UNP A0QYE8
K	495	HIS	-	expression tag	UNP A0QYE8
K	496	HIS	-	expression tag	UNP A0QYE8
L	1	MET	-	initiating methionine	UNP A0QYE8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	2	VAL	-	expression tag	UNP A0QYE8
L	480	THR	-	expression tag	UNP A0QYE8
L	481	ALA	-	expression tag	UNP A0QYE8
L	482	ALA	-	expression tag	UNP A0QYE8
L	483	ALA	-	expression tag	UNP A0QYE8
L	484	LYS	-	expression tag	UNP A0QYE8
L	485	GLU	-	expression tag	UNP A0QYE8
L	486	ASP	-	expression tag	UNP A0QYE8
L	487	LEU	-	expression tag	UNP A0QYE8
L	488	GLU	-	expression tag	UNP A0QYE8
L	489	HIS	-	expression tag	UNP A0QYE8
L	490	HIS	-	expression tag	UNP A0QYE8
L	491	HIS	-	expression tag	UNP A0QYE8
L	492	HIS	-	expression tag	UNP A0QYE8
L	493	HIS	-	expression tag	UNP A0QYE8
L	494	HIS	-	expression tag	UNP A0QYE8
L	495	HIS	-	expression tag	UNP A0QYE8
L	496	HIS	-	expression tag	UNP A0QYE8
M	1	MET	-	initiating methionine	UNP A0QYE8
M	2	VAL	-	expression tag	UNP A0QYE8
M	480	THR	-	expression tag	UNP A0QYE8
M	481	ALA	-	expression tag	UNP A0QYE8
M	482	ALA	-	expression tag	UNP A0QYE8
M	483	ALA	-	expression tag	UNP A0QYE8
M	484	LYS	-	expression tag	UNP A0QYE8
M	485	GLU	-	expression tag	UNP A0QYE8
M	486	ASP	-	expression tag	UNP A0QYE8
M	487	LEU	-	expression tag	UNP A0QYE8
M	488	GLU	-	expression tag	UNP A0QYE8
M	489	HIS	-	expression tag	UNP A0QYE8
M	490	HIS	-	expression tag	UNP A0QYE8
M	491	HIS	-	expression tag	UNP A0QYE8
M	492	HIS	-	expression tag	UNP A0QYE8
M	493	HIS	-	expression tag	UNP A0QYE8
M	494	HIS	-	expression tag	UNP A0QYE8
M	495	HIS	-	expression tag	UNP A0QYE8
M	496	HIS	-	expression tag	UNP A0QYE8
N	1	MET	-	initiating methionine	UNP A0QYE8
N	2	VAL	-	expression tag	UNP A0QYE8
N	480	THR	-	expression tag	UNP A0QYE8
N	481	ALA	-	expression tag	UNP A0QYE8
N	482	ALA	-	expression tag	UNP A0QYE8

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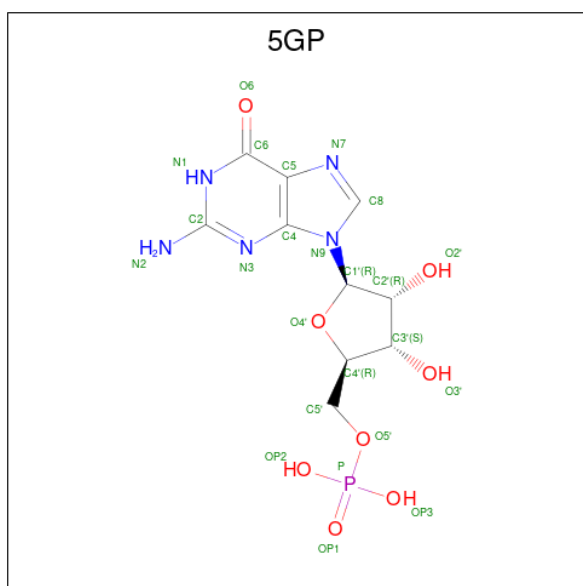
Chain	Residue	Modelled	Actual	Comment	Reference
N	483	ALA	-	expression tag	UNP A0QYE8
N	484	LYS	-	expression tag	UNP A0QYE8
N	485	GLU	-	expression tag	UNP A0QYE8
N	486	ASP	-	expression tag	UNP A0QYE8
N	487	LEU	-	expression tag	UNP A0QYE8
N	488	GLU	-	expression tag	UNP A0QYE8
N	489	HIS	-	expression tag	UNP A0QYE8
N	490	HIS	-	expression tag	UNP A0QYE8
N	491	HIS	-	expression tag	UNP A0QYE8
N	492	HIS	-	expression tag	UNP A0QYE8
N	493	HIS	-	expression tag	UNP A0QYE8
N	494	HIS	-	expression tag	UNP A0QYE8
N	495	HIS	-	expression tag	UNP A0QYE8
N	496	HIS	-	expression tag	UNP A0QYE8
O	1	MET	-	initiating methionine	UNP A0QYE8
O	2	VAL	-	expression tag	UNP A0QYE8
O	480	THR	-	expression tag	UNP A0QYE8
O	481	ALA	-	expression tag	UNP A0QYE8
O	482	ALA	-	expression tag	UNP A0QYE8
O	483	ALA	-	expression tag	UNP A0QYE8
O	484	LYS	-	expression tag	UNP A0QYE8
O	485	GLU	-	expression tag	UNP A0QYE8
O	486	ASP	-	expression tag	UNP A0QYE8
O	487	LEU	-	expression tag	UNP A0QYE8
O	488	GLU	-	expression tag	UNP A0QYE8
O	489	HIS	-	expression tag	UNP A0QYE8
O	490	HIS	-	expression tag	UNP A0QYE8
O	491	HIS	-	expression tag	UNP A0QYE8
O	492	HIS	-	expression tag	UNP A0QYE8
O	493	HIS	-	expression tag	UNP A0QYE8
O	494	HIS	-	expression tag	UNP A0QYE8
O	495	HIS	-	expression tag	UNP A0QYE8
O	496	HIS	-	expression tag	UNP A0QYE8
P	1	MET	-	initiating methionine	UNP A0QYE8
P	2	VAL	-	expression tag	UNP A0QYE8
P	480	THR	-	expression tag	UNP A0QYE8
P	481	ALA	-	expression tag	UNP A0QYE8
P	482	ALA	-	expression tag	UNP A0QYE8
P	483	ALA	-	expression tag	UNP A0QYE8
P	484	LYS	-	expression tag	UNP A0QYE8
P	485	GLU	-	expression tag	UNP A0QYE8
P	486	ASP	-	expression tag	UNP A0QYE8

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Chain	Residue	Modelled	Actual	Comment	Reference
P	487	LEU	-	expression tag	UNP A0QYE8
P	488	GLU	-	expression tag	UNP A0QYE8
P	489	HIS	-	expression tag	UNP A0QYE8
P	490	HIS	-	expression tag	UNP A0QYE8
P	491	HIS	-	expression tag	UNP A0QYE8
P	492	HIS	-	expression tag	UNP A0QYE8
P	493	HIS	-	expression tag	UNP A0QYE8
P	494	HIS	-	expression tag	UNP A0QYE8
P	495	HIS	-	expression tag	UNP A0QYE8
P	496	HIS	-	expression tag	UNP A0QYE8

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: $C_{10}H_{14}N_5O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	B	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	D	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	E	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	F	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

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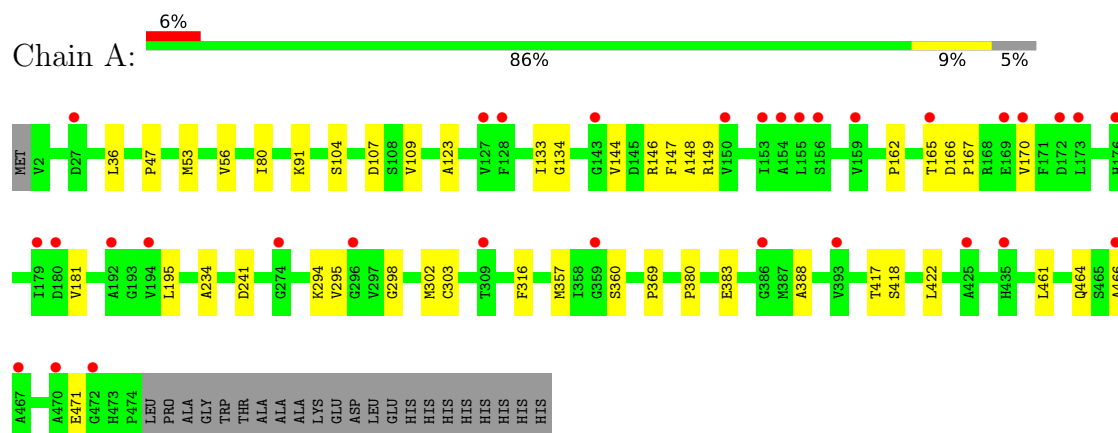
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	H	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	I	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	J	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	K	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	L	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	M	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	N	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	O	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
2	P	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

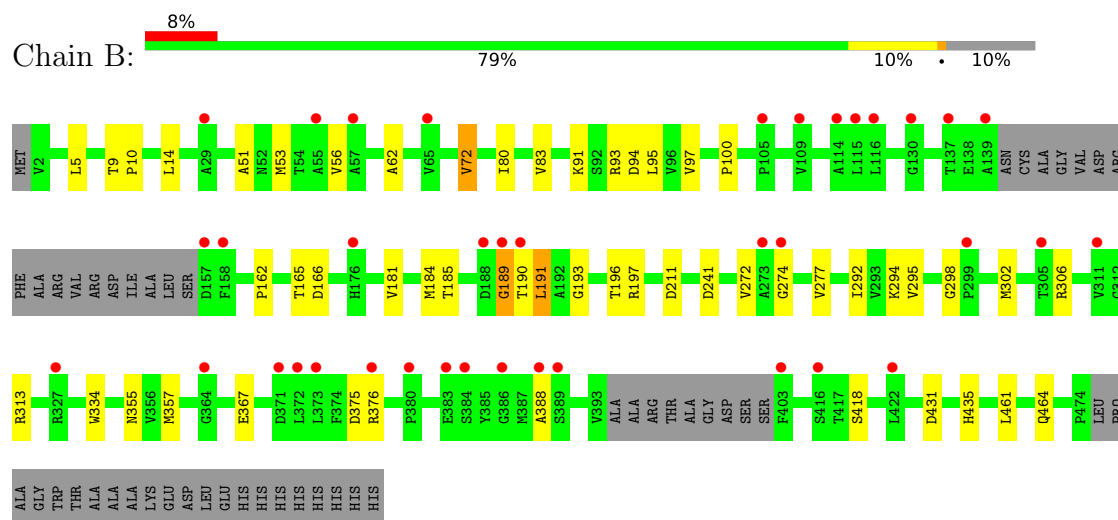
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

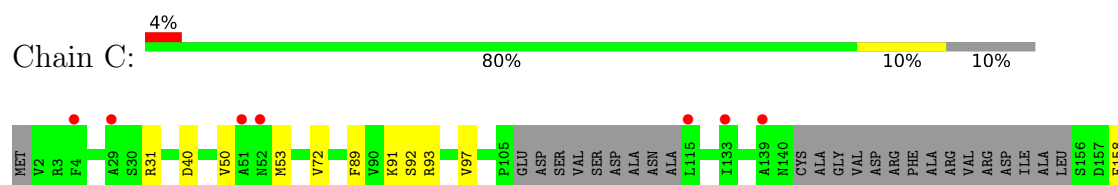
• Molecule 1: GMP reductase

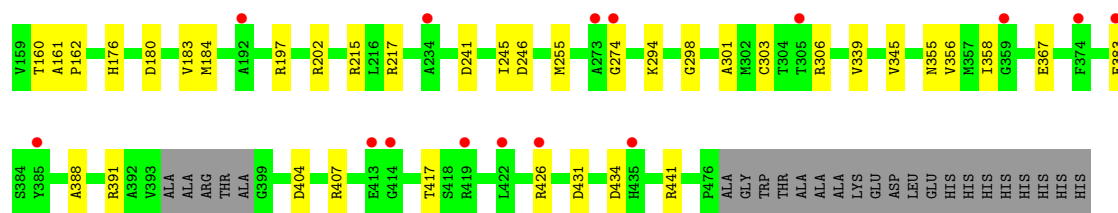


• Molecule 1: GMP reductase

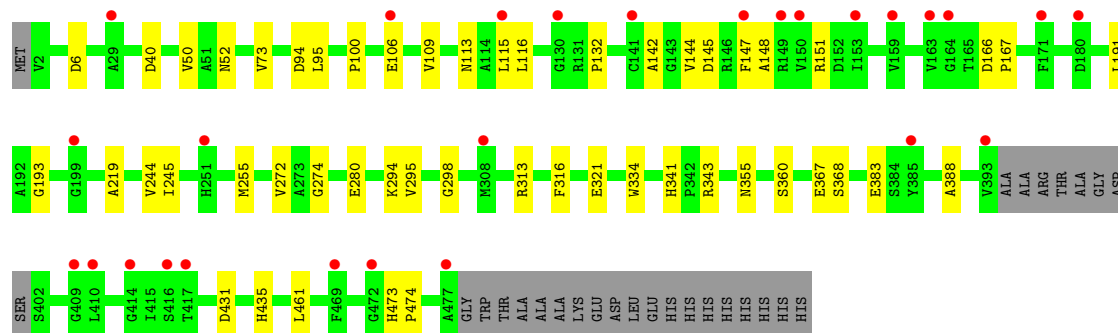
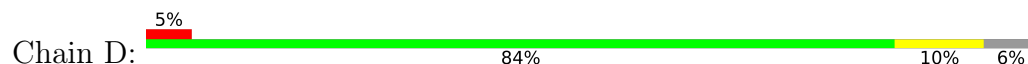


• Molecule 1: GMP reductase

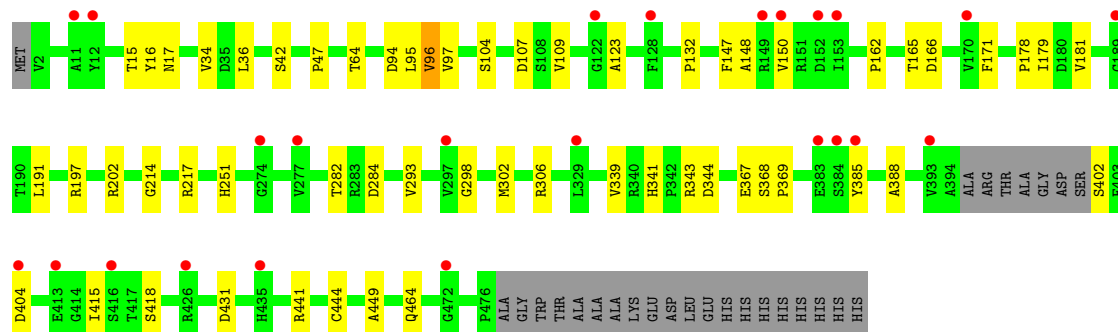
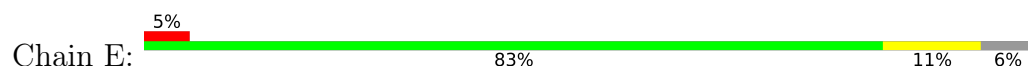




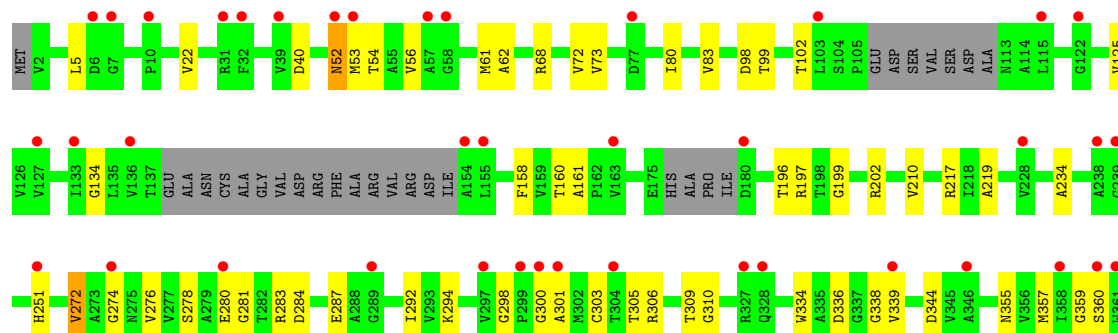
● Molecule 1: GMP reductase

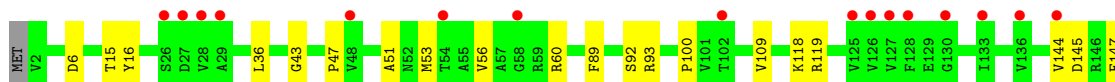
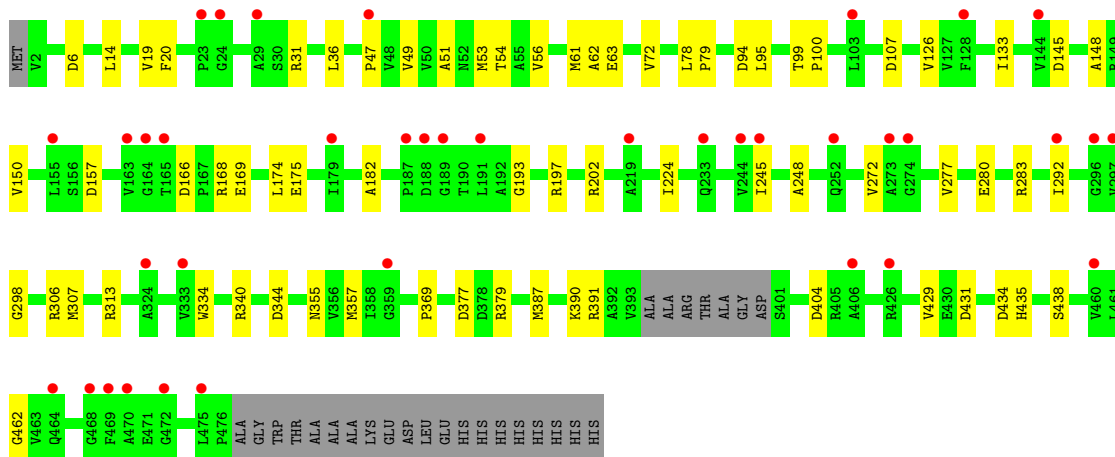
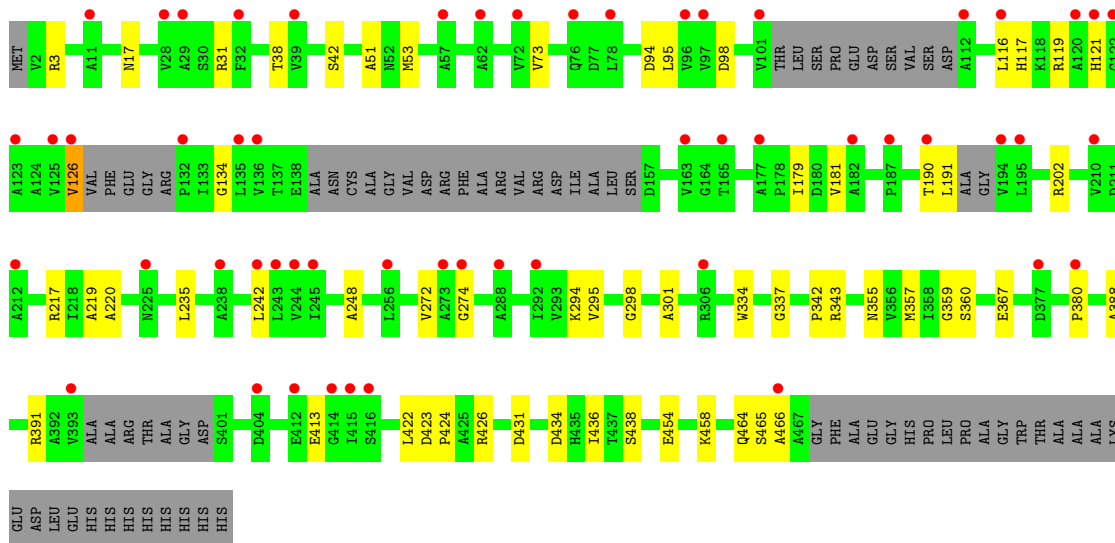


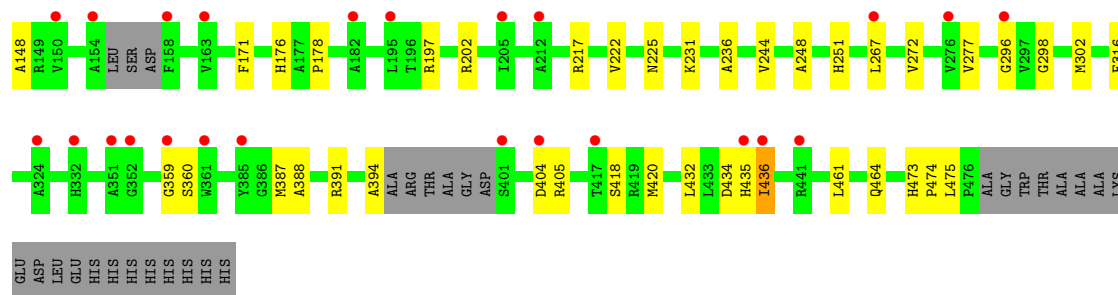
● Molecule 1: GMP reductase



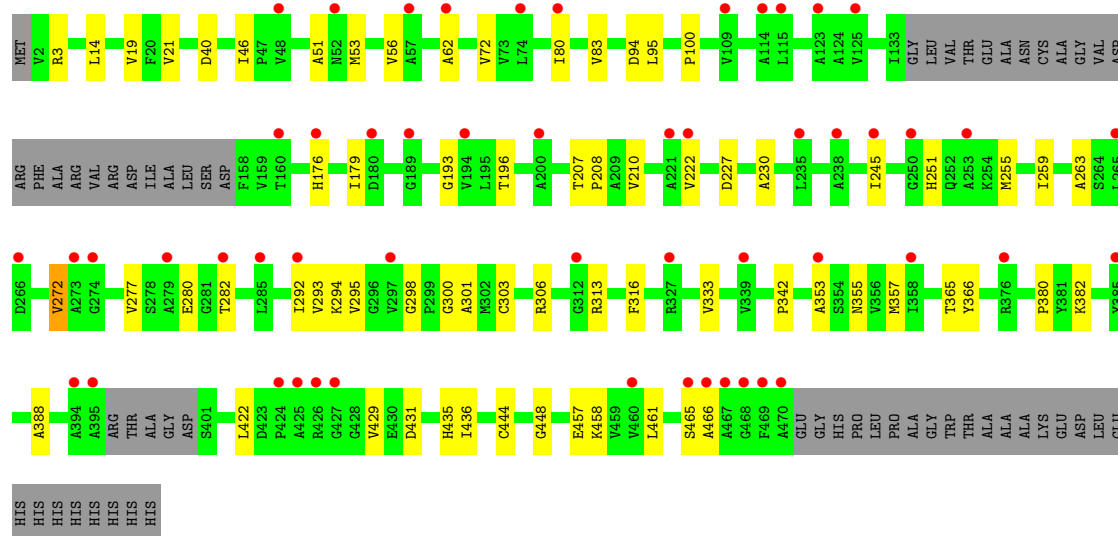
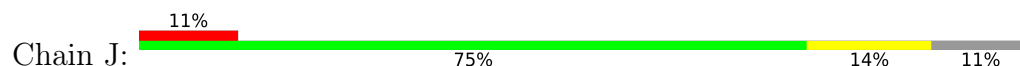
● Molecule 1: GMP reductase



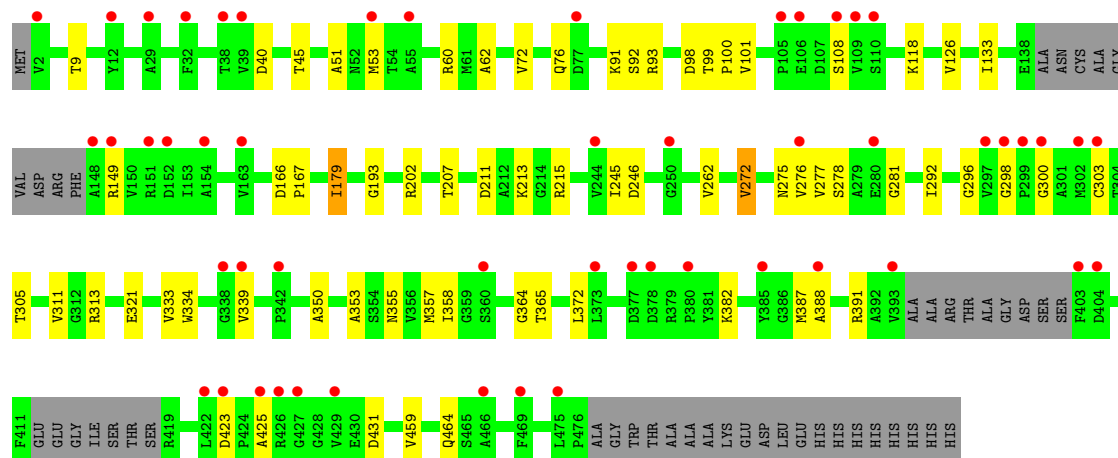
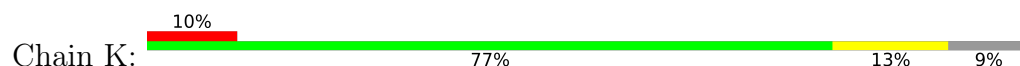




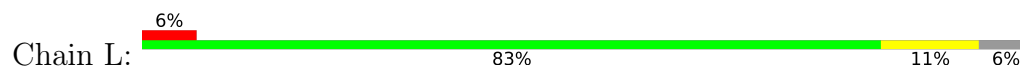
• Molecule 1: GMP reductase

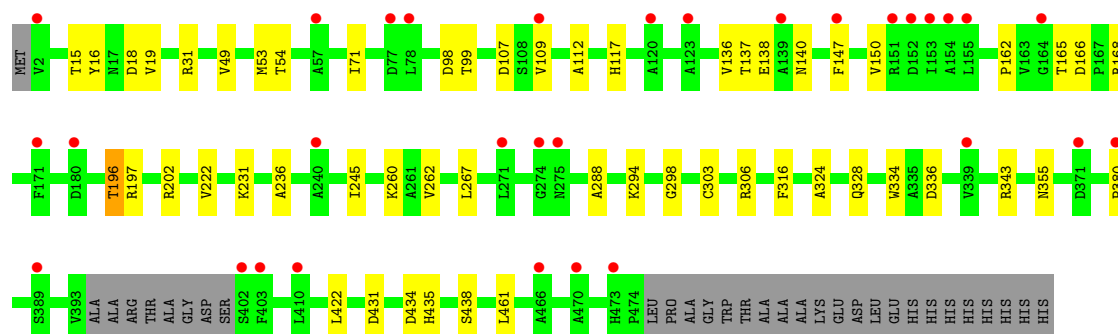


• Molecule 1: GMP reductase

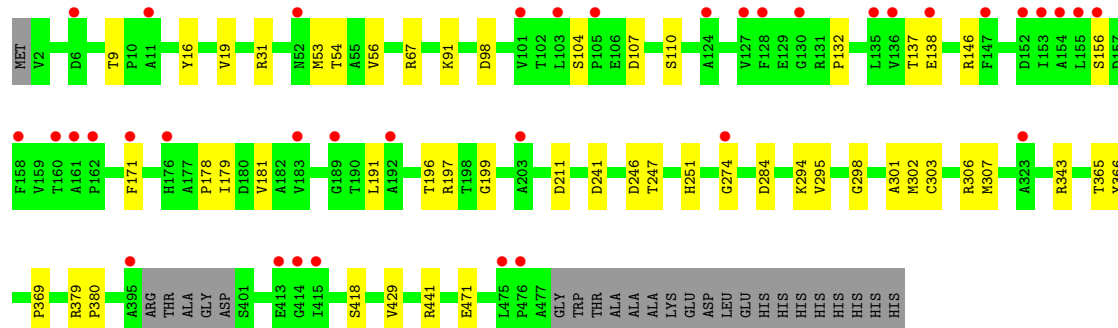
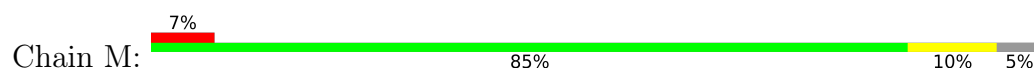


• Molecule 1: GMP reductase

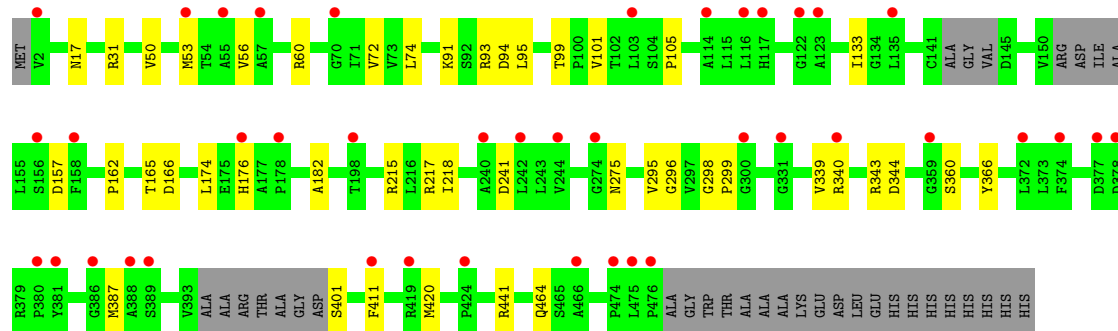
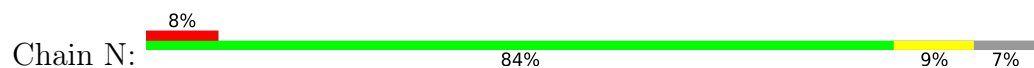




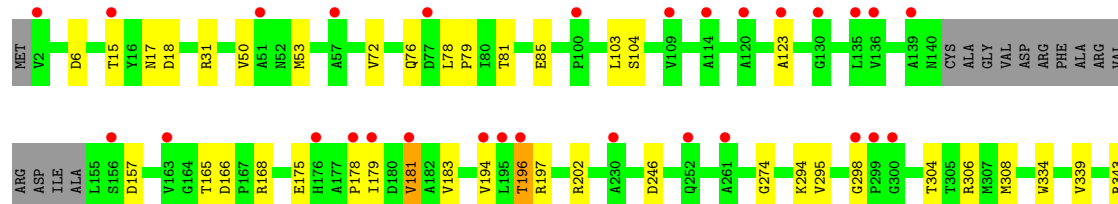
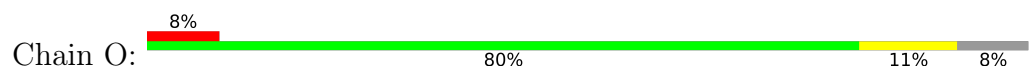
- Molecule 1: GMP reductase

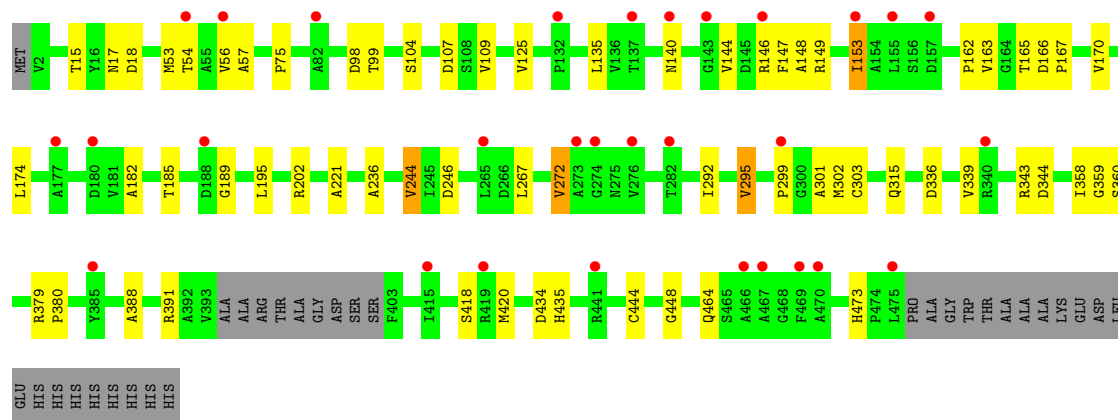


- Molecule 1: GMP reductase



- Molecule 1: GMP reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	104.79Å 105.10Å 170.47Å 76.92° 81.86° 69.01°	Depositor
Resolution (Å)	47.69 – 2.50 47.69 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.1 (47.69-2.50) 91.0 (47.69-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.263 , 0.306 0.266 , 0.308	Depositor DCC
R_{free} test set	10296 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	53060	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5GP

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	0.30	0/3460	0.76	5/4717 (0.1%)
1	B	0.32	0/3283	0.79	6/4474 (0.1%)
1	C	0.29	0/3289	0.75	3/4478 (0.1%)
1	D	0.31	0/3446	0.78	8/4696 (0.2%)
1	E	0.30	0/3447	0.74	3/4697 (0.1%)
1	F	0.30	0/3218	0.77	4/4381 (0.1%)
1	G	0.31	0/3063	0.76	6/4176 (0.1%)
1	H	0.30	0/3433	0.76	2/4678 (0.0%)
1	I	0.30	0/3431	0.75	3/4673 (0.1%)
1	J	0.35	0/3206	0.82	5/4372 (0.1%)
1	K	0.31	0/3270	0.78	3/4462 (0.1%)
1	L	0.30	0/3401	0.76	2/4637 (0.0%)
1	M	0.30	0/3433	0.76	3/4683 (0.1%)
1	N	0.30	0/3405	0.73	3/4635 (0.1%)
1	O	0.31	0/3334	0.76	4/4544 (0.1%)
1	P	0.31	0/3425	0.78	4/4665 (0.1%)
All	All	0.31	0/53544	0.77	64/72968 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	210	VAL	N-CA-C	13.26	124.76	112.17
1	P	189	GLY	N-CA-C	10.17	126.79	114.69
1	B	190	THR	N-CA-C	9.03	123.89	110.52
1	K	108	SER	CA-C-N	-6.98	114.19	122.22
1	K	108	SER	C-N-CA	-6.98	114.19	122.22
1	F	298	GLY	CA-C-N	-6.76	111.38	119.84
1	F	298	GLY	C-N-CA	-6.76	111.38	119.84
1	H	298	GLY	CA-C-N	-6.22	113.28	119.56
1	H	298	GLY	C-N-CA	-6.22	113.28	119.56
1	F	414	GLY	N-CA-C	6.22	120.67	110.97
1	A	298	GLY	CA-C-N	-6.16	113.34	119.56
1	A	298	GLY	C-N-CA	-6.16	113.34	119.56
1	B	191	LEU	N-CA-C	6.05	118.78	110.24
1	C	298	GLY	CA-C-N	-6.05	113.45	119.56
1	C	298	GLY	C-N-CA	-6.05	113.45	119.56
1	M	298	GLY	CA-C-N	-6.00	113.50	119.56
1	M	298	GLY	C-N-CA	-6.00	113.50	119.56
1	D	115	LEU	N-CA-C	-5.99	98.04	110.80
1	M	295	VAL	N-CA-C	5.97	116.60	107.77
1	J	295	VAL	N-CA-C	5.96	116.76	107.28
1	E	298	GLY	CA-C-N	-5.92	113.58	119.56
1	E	298	GLY	C-N-CA	-5.92	113.58	119.56
1	N	298	GLY	CA-C-N	-5.87	113.63	119.56
1	N	298	GLY	C-N-CA	-5.87	113.63	119.56
1	D	298	GLY	CA-C-N	-5.84	113.66	119.56
1	D	298	GLY	C-N-CA	-5.84	113.66	119.56
1	G	116	LEU	CA-C-N	-5.79	114.15	123.23
1	G	116	LEU	C-N-CA	-5.79	114.15	123.23
1	J	298	GLY	CA-C-N	-5.62	113.88	119.56
1	J	298	GLY	C-N-CA	-5.62	113.88	119.56
1	N	295	VAL	N-CA-C	5.59	116.05	107.77
1	L	298	GLY	CA-C-N	-5.59	113.92	119.56
1	L	298	GLY	C-N-CA	-5.59	113.92	119.56
1	F	298	GLY	N-CA-C	5.56	123.68	112.34
1	O	298	GLY	CA-C-N	-5.46	114.04	119.56
1	O	298	GLY	C-N-CA	-5.46	114.04	119.56
1	B	295	VAL	N-CA-C	5.45	116.40	107.24
1	E	388	ALA	CB-CA-C	-5.43	109.85	117.23
1	D	368	SER	CA-C-N	5.42	125.24	119.28
1	D	368	SER	C-N-CA	5.42	125.24	119.28
1	G	298	GLY	CA-C-N	-5.41	114.10	119.56
1	G	298	GLY	C-N-CA	-5.41	114.10	119.56
1	P	295	VAL	N-CA-C	5.38	115.83	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	ALA	CB-CA-C	-5.38	109.92	117.23
1	P	388	ALA	CB-CA-C	-5.36	109.94	117.23
1	D	388	ALA	CB-CA-C	-5.34	109.97	117.23
1	I	388	ALA	CB-CA-C	-5.34	109.97	117.23
1	P	153	ILE	N-CA-C	5.33	116.81	111.00
1	B	388	ALA	CB-CA-C	-5.29	110.04	117.23
1	G	295	VAL	N-CA-C	5.28	116.11	107.24
1	I	298	GLY	CA-C-N	-5.28	114.23	119.56
1	I	298	GLY	C-N-CA	-5.28	114.23	119.56
1	D	295	VAL	N-CA-C	5.27	116.09	107.24
1	D	116	LEU	CA-CB-CG	5.25	134.68	116.30
1	G	388	ALA	CB-CA-C	-5.25	110.09	117.23
1	B	298	GLY	CA-C-N	-5.23	114.27	119.56
1	B	298	GLY	C-N-CA	-5.23	114.27	119.56
1	C	388	ALA	CB-CA-C	-5.23	110.12	117.23
1	O	388	ALA	CB-CA-C	-5.22	110.12	117.23
1	A	295	VAL	N-CA-C	5.19	115.96	107.24
1	J	388	ALA	CB-CA-C	-5.19	110.18	117.23
1	O	295	VAL	N-CA-C	5.10	115.81	107.24
1	K	298	GLY	N-CA-C	5.09	122.72	112.34
1	A	466	ALA	CB-CA-C	-5.07	110.33	117.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	189	GLY	Peptide
1	G	117	HIS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3403	0	3371	23	0
1	B	3230	0	3204	29	1
1	C	3235	0	3222	28	0
1	D	3389	0	3370	27	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3390	0	3372	33	0
1	F	3168	0	3163	48	0
1	G	3017	0	2977	37	0
1	H	3378	0	3358	45	0
1	I	3375	0	3358	40	0
1	J	3154	0	3119	41	0
1	K	3216	0	3177	41	0
1	L	3346	0	3312	33	0
1	M	3376	0	3339	32	1
1	N	3350	0	3336	27	0
1	O	3280	0	3262	38	1
1	P	3369	0	3360	41	0
2	A	24	0	12	2	0
2	B	24	0	12	0	0
2	C	24	0	12	3	0
2	D	24	0	12	1	0
2	E	24	0	12	0	0
2	F	24	0	12	3	0
2	G	24	0	12	5	0
2	H	24	0	12	0	0
2	I	24	0	12	2	0
2	J	24	0	12	3	0
2	K	24	0	12	7	0
2	L	24	0	12	2	0
2	M	24	0	12	3	0
2	N	24	0	12	1	0
2	O	24	0	12	2	0
2	P	24	0	12	4	0
All	All	53060	0	52492	520	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (520) 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:O:175:GLU:OE2	1:O:197:ARG:NH2	2.14	0.80
1:K:372:LEU:H	1:K:382:LYS:HE3	1.47	0.79
1:B:185:THR:OG1	1:B:189:GLY:O	2.00	0.78
1:G:202:ARG:NH1	1:G:434:ASP:OD2	2.16	0.78
1:H:272:VAL:HG12	1:H:292:ILE:HB	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:ILE:HG13	1:O:178:PRO:HG3	1.67	0.76
1:E:306:ARG:NH1	1:F:471:GLU:OE2	2.21	0.74
1:H:31:ARG:NH2	1:H:438:SER:OG	2.20	0.74
1:P:53:MET:HB2	1:P:56:VAL:HG22	1.70	0.74
1:J:40:ASP:OD2	1:J:355:ASN:ND2	2.21	0.73
1:B:162:PRO:O	1:B:165:THR:OG1	2.05	0.73
1:F:202:ARG:NH2	1:F:434:ASP:OD2	2.18	0.73
1:O:360:SER:N	2:O:501:5GP:OP3	2.22	0.72
1:J:333:VAL:HG23	1:J:353:ALA:HA	1.72	0.72
1:L:31:ARG:NH2	1:L:438:SER:OG	2.22	0.71
1:F:40:ASP:OD2	1:F:355:ASN:ND2	2.22	0.71
1:D:106:GLU:OE2	1:D:151:ARG:NH1	2.24	0.71
1:E:306:ARG:NH2	1:F:464:GLN:OE1	2.24	0.71
1:K:40:ASP:OD2	1:K:355:ASN:ND2	2.24	0.71
1:P:144:VAL:O	1:P:146:ARG:NH1	2.24	0.71
1:C:383:GLU:OE2	1:C:417:THR:OG1	2.08	0.70
1:E:171:PHE:O	1:E:197:ARG:NH1	2.24	0.70
1:K:275:ASN:OD1	1:K:391:ARG:NH2	2.25	0.70
1:H:175:GLU:OE1	1:H:197:ARG:NH2	2.26	0.69
1:K:464:GLN:OE1	1:L:306:ARG:NH2	2.26	0.69
1:F:52:ASN:OD1	1:F:52:ASN:N	2.25	0.69
1:M:53:MET:HB2	1:M:56:VAL:HG22	1.75	0.69
1:N:401:SER:OG	1:O:168:ARG:NH2	2.25	0.69
1:O:383:GLU:OE2	1:O:417:THR:OG1	2.10	0.69
1:O:31:ARG:NH1	1:O:438:SER:OG	2.26	0.68
1:B:464:GLN:OE1	1:C:306:ARG:NH2	2.26	0.68
1:A:53:MET:HB2	1:A:56:VAL:HG12	1.76	0.67
1:B:53:MET:HB2	1:B:56:VAL:HG12	1.76	0.67
1:J:53:MET:HB2	1:J:56:VAL:HG22	1.77	0.67
1:J:365:THR:HG21	1:J:429:VAL:HB	1.77	0.67
1:N:53:MET:HB2	1:N:56:VAL:HG12	1.76	0.67
1:P:147:PHE:O	1:P:149:ARG:NH2	2.29	0.66
1:N:60:ARG:NH2	1:N:366:TYR:O	2.29	0.65
1:J:303:CYS:SG	2:J:501:5GP:N2	2.70	0.64
1:P:272:VAL:HG12	1:P:292:ILE:HB	1.78	0.64
1:I:92:SER:OG	1:I:93:ARG:NH1	2.31	0.64
1:F:53:MET:HB2	1:F:56:VAL:HG22	1.79	0.63
1:G:31:ARG:NH2	1:G:438:SER:OG	2.31	0.63
1:G:98:ASP:OD2	1:G:121:HIS:NE2	2.31	0.63
1:G:301:ALA:N	2:G:501:5GP:OP3	2.31	0.63
1:B:91:LYS:NZ	1:B:241:ASP:OD2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:VAL:O	1:A:146:ARG:NH1	2.31	0.62
1:A:464:GLN:OE1	1:B:306:ARG:NH2	2.32	0.62
1:D:40:ASP:OD2	1:D:355:ASN:ND2	2.29	0.62
1:D:367:GLU:OE2	1:D:367:GLU:N	2.31	0.62
1:F:54:THR:H	1:F:387:MET:HE3	1.64	0.62
1:N:299:PRO:HA	1:O:471:GLU:HG2	1.80	0.62
1:K:60:ARG:NH1	1:K:118:LYS:O	2.33	0.62
1:N:17:ASN:OD1	1:N:340:ARG:NH2	2.33	0.61
1:H:431:ASP:O	1:H:435:HIS:ND1	2.33	0.61
1:C:301:ALA:N	2:C:501:5GP:OP3	2.29	0.61
1:L:117:HIS:NE2	1:L:138:GLU:OE2	2.34	0.61
1:K:40:ASP:OD1	1:K:40:ASP:N	2.32	0.61
1:L:202:ARG:NH1	1:L:434:ASP:OD2	2.34	0.61
1:M:365:THR:HG21	1:M:429:VAL:HB	1.82	0.61
1:E:162:PRO:O	1:E:165:THR:OG1	2.19	0.61
1:K:305:THR:OG1	2:K:501:5GP:N2	2.34	0.60
1:O:339:VAL:HG13	1:O:344:ASP:HB2	1.83	0.60
1:K:53:MET:HE2	2:K:501:5GP:H8	1.82	0.60
1:A:303:CYS:SG	2:A:501:5GP:N2	2.75	0.60
1:M:471:GLU:HG3	1:P:299:PRO:HA	1.84	0.60
1:P:315:GLN:NE2	1:P:336:ASP:O	2.35	0.60
1:H:6:ASP:OD2	1:K:9:THR:OG1	2.11	0.60
1:C:367:GLU:OE2	1:C:367:GLU:N	2.33	0.60
1:F:56:VAL:HG11	1:F:359:GLY:O	2.02	0.59
1:O:202:ARG:NH2	1:O:431:ASP:OD1	2.35	0.58
1:J:176:HIS:ND1	1:O:157:ASP:OD2	2.35	0.58
1:I:360:SER:N	2:I:501:5GP:OP1	2.35	0.58
1:K:202:ARG:NH2	1:K:431:ASP:OD1	2.33	0.58
1:K:276:VAL:HG22	1:K:278:SER:H	1.69	0.58
1:E:464:GLN:OE1	1:H:306:ARG:NH2	2.37	0.57
1:I:171:PHE:O	1:I:197:ARG:NH1	2.37	0.57
1:K:387:MET:N	2:K:501:5GP:O6	2.36	0.57
1:E:178:PRO:HG2	1:E:179:ILE:HD12	1.86	0.57
1:C:202:ARG:NH1	1:C:434:ASP:OD2	2.37	0.57
1:F:300:GLY:HA3	1:F:303:CYS:HB3	1.87	0.56
1:F:301:ALA:HB1	1:F:360:SER:HB3	1.86	0.56
1:L:431:ASP:O	1:L:435:HIS:ND1	2.38	0.56
1:M:301:ALA:N	2:M:501:5GP:OP1	2.39	0.56
1:K:51:ALA:HA	1:K:357:MET:HE2	1.86	0.56
1:P:56:VAL:HG11	1:P:359:GLY:O	2.06	0.56
1:G:17:ASN:O	1:G:464:GLN:NE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:91:LYS:HB3	1:N:215:ARG:HD2	1.87	0.56
1:B:367:GLU:N	1:B:367:GLU:OE2	2.39	0.56
1:J:316:PHE:HZ	1:J:461:LEU:HD13	1.70	0.55
1:M:132:PRO:HD3	1:M:191:LEU:HB2	1.88	0.55
1:K:388:ALA:N	2:K:501:5GP:O6	2.39	0.55
1:I:248:ALA:N	1:I:391:ARG:O	2.39	0.55
1:J:342:PRO:HB3	1:J:436:ILE:HA	1.89	0.55
1:F:367:GLU:N	1:F:367:GLU:OE1	2.40	0.54
1:E:282:THR:HG23	1:E:293:VAL:HG21	1.90	0.54
1:M:306:ARG:NH2	1:N:464:GLN:OE1	2.40	0.54
1:O:306:ARG:NH2	1:P:464:GLN:OE1	2.39	0.54
1:H:277:VAL:O	1:H:313:ARG:NH1	2.40	0.54
1:P:336:ASP:OD2	2:P:501:5GP:O3'	2.25	0.54
1:I:56:VAL:HG11	1:I:359:GLY:O	2.07	0.54
1:N:53:MET:HE2	2:N:501:5GP:H8	1.88	0.54
1:G:360:SER:N	2:G:501:5GP:OP2	2.39	0.54
1:K:92:SER:OG	1:K:93:ARG:NH1	2.40	0.54
1:B:94:ASP:OD1	1:B:95:LEU:N	2.41	0.54
1:K:303:CYS:SG	2:K:501:5GP:N2	2.81	0.54
1:L:137:THR:H	1:L:140:ASN:ND2	2.06	0.54
1:H:168:ARG:HG3	1:H:169:GLU:H	1.73	0.53
1:B:431:ASP:O	1:B:435:HIS:ND1	2.38	0.53
1:B:375:ASP:OD1	1:B:376:ARG:N	2.39	0.53
1:L:98:ASP:OD1	1:L:99:THR:N	2.42	0.53
1:M:171:PHE:O	1:M:197:ARG:NH1	2.40	0.53
1:C:92:SER:OG	1:C:93:ARG:NH1	2.42	0.53
1:C:176:HIS:NE2	1:H:157:ASP:OD2	2.41	0.53
1:G:367:GLU:N	1:G:367:GLU:OE2	2.41	0.53
1:L:107:ASP:O	1:L:150:VAL:HG23	2.09	0.53
1:I:225:ASN:OD1	1:I:394:ALA:N	2.40	0.52
1:A:133:ILE:HG13	1:A:134:GLY:H	1.73	0.52
1:L:16:TYR:O	1:L:343:ARG:NH2	2.42	0.52
1:G:42:SER:O	1:G:217:ARG:NE	2.42	0.52
1:L:49:VAL:HG22	1:L:71:ILE:HG22	1.91	0.52
1:J:366:TYR:O	1:J:382:LYS:NZ	2.42	0.52
1:P:174:LEU:HD21	1:P:182:ALA:HB2	1.91	0.52
1:M:16:TYR:O	1:M:343:ARG:NH2	2.42	0.52
1:O:81:THR:O	1:O:85:GLU:N	2.42	0.52
1:K:76:GLN:NE2	1:K:246:ASP:OD2	2.42	0.52
1:J:51:ALA:HA	1:J:357:MET:HE2	1.91	0.52
1:J:80:ILE:HA	1:J:83:VAL:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:17:ASN:OD1	1:O:343:ARG:NH2	2.43	0.52
1:F:251:HIS:NE2	1:F:284:ASP:OD2	2.41	0.52
1:J:62:ALA:HA	1:J:72:VAL:HG11	1.90	0.52
1:A:360:SER:N	2:A:501:5GP:OP2	2.40	0.52
1:F:196:THR:HG23	1:F:199:GLY:H	1.74	0.51
1:M:137:THR:HG22	1:M:138:GLU:N	2.25	0.51
1:F:80:ILE:HA	1:F:83:VAL:HG12	1.91	0.51
1:P:17:ASN:OD1	1:P:343:ARG:NH2	2.42	0.51
1:A:80:ILE:HD12	1:A:234:ALA:HB1	1.92	0.51
1:B:334:TRP:CD1	1:B:355:ASN:HB2	2.46	0.51
1:F:196:THR:OG1	1:F:197:ARG:N	2.43	0.51
1:N:162:PRO:O	1:N:165:THR:OG1	2.25	0.51
1:O:365:THR:HG22	1:O:366:TYR:H	1.74	0.51
1:E:444:CYS:O	1:E:449:ALA:N	2.44	0.51
1:B:5:LEU:N	1:B:461:LEU:O	2.41	0.51
1:H:62:ALA:HA	1:H:72:VAL:HG21	1.93	0.51
1:N:174:LEU:HD11	1:N:182:ALA:HB2	1.92	0.51
1:C:404:ASP:OD1	1:C:407:ARG:NH2	2.44	0.51
1:D:94:ASP:OD1	1:D:95:LEU:N	2.43	0.51
1:M:137:THR:HG22	1:M:138:GLU:H	1.75	0.51
1:C:40:ASP:OD2	1:C:355:ASN:ND2	2.38	0.50
1:F:388:ALA:HB1	1:F:413:GLU:HB3	1.93	0.50
1:H:166:ASP:C	1:H:168:ARG:H	2.19	0.50
1:P:53:MET:HE2	2:P:501:5GP:H8	1.93	0.50
1:H:166:ASP:O	1:H:168:ARG:N	2.41	0.50
1:L:137:THR:H	1:L:140:ASN:HD21	1.58	0.50
1:H:51:ALA:HA	1:H:357:MET:HE2	1.93	0.50
1:L:19:VAL:O	1:L:343:ARG:NH2	2.45	0.50
1:G:342:PRO:HB3	1:G:436:ILE:HA	1.94	0.50
1:I:100:PRO:O	1:I:119:ARG:NH1	2.45	0.50
1:L:303:CYS:SG	2:L:501:5GP:N2	2.85	0.50
1:F:283:ARG:HG2	1:F:287:GLU:OE2	2.11	0.50
1:O:308:MET:HG3	1:O:413:GLU:OE2	2.11	0.50
1:P:162:PRO:O	1:P:165:THR:OG1	2.20	0.50
1:P:221:ALA:HA	1:P:244:VAL:HG22	1.94	0.50
1:G:190:THR:HG23	1:G:191:LEU:H	1.77	0.50
1:H:61:MET:HE1	1:H:429:VAL:HG21	1.94	0.50
1:L:294:LYS:NZ	1:L:336:ASP:OD2	2.45	0.50
1:F:160:THR:HG22	1:F:161:ALA:H	1.77	0.49
1:K:364:GLY:O	1:K:365:THR:HG23	2.12	0.49
1:K:276:VAL:HG21	1:K:281:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:ARG:NH2	1:G:464:GLN:OE1	2.45	0.49
1:L:109:VAL:HA	1:L:112:ALA:HB3	1.94	0.49
1:J:255:MET:HE3	1:J:259:ILE:HD11	1.94	0.49
1:E:341:HIS:HB2	1:E:343:ARG:HG2	1.95	0.49
1:E:302:MET:HE1	1:E:418:SER:HB3	1.95	0.49
1:F:272:VAL:HG12	1:F:292:ILE:HB	1.93	0.49
1:G:73:VAL:HG12	1:G:219:ALA:HB3	1.93	0.49
1:G:454:GLU:HB3	1:G:458:LYS:HE3	1.93	0.49
1:P:339:VAL:HG21	1:P:358:ILE:HG12	1.93	0.49
1:G:179:ILE:HG12	1:G:181:VAL:H	1.77	0.49
1:M:365:THR:HG22	1:M:366:TYR:H	1.78	0.49
1:A:302:MET:HE1	1:A:418:SER:HB2	1.92	0.49
1:E:385:TYR:HB3	1:E:415:ILE:HD11	1.94	0.49
1:A:170:VAL:HG21	1:A:195:LEU:HD23	1.95	0.49
1:G:413:GLU:OE2	1:H:435:HIS:HA	2.13	0.49
1:O:365:THR:HG21	1:O:429:VAL:HB	1.94	0.49
1:A:162:PRO:O	1:A:165:THR:OG1	2.22	0.49
1:K:149:ARG:NH2	1:O:76:GLN:O	2.46	0.49
1:I:15:THR:HG22	1:I:16:TYR:H	1.78	0.48
1:K:45:THR:HG21	1:K:207:THR:HB	1.94	0.48
1:K:62:ALA:HA	1:K:72:VAL:HG21	1.94	0.48
1:I:43:GLY:HA3	1:I:217:ARG:CZ	2.42	0.48
1:I:144:VAL:HG12	1:I:145:ASP:H	1.78	0.48
1:D:341:HIS:HB2	1:D:343:ARG:HG2	1.94	0.48
1:L:162:PRO:O	1:L:165:THR:OG1	2.30	0.48
1:N:53:MET:HA	1:N:387:MET:SD	2.54	0.48
1:A:104:SER:N	1:A:107:ASP:OD2	2.41	0.48
1:G:17:ASN:OD1	1:G:343:ARG:NH2	2.46	0.48
1:G:94:ASP:OD1	1:G:95:LEU:N	2.46	0.48
1:H:107:ASP:O	1:H:150:VAL:HG23	2.13	0.48
1:I:202:ARG:NH2	1:I:434:ASP:OD2	2.46	0.48
1:A:316:PHE:HZ	1:A:461:LEU:HD13	1.78	0.48
1:B:302:MET:HE1	1:B:418:SER:HB2	1.95	0.48
1:E:94:ASP:OD1	1:E:95:LEU:N	2.46	0.48
1:C:31:ARG:HB3	1:C:441:ARG:HB3	1.96	0.48
1:I:53:MET:HB2	1:I:56:VAL:HG22	1.96	0.48
1:P:170:VAL:HG11	1:P:195:LEU:HD23	1.96	0.48
1:C:97:VAL:HG11	1:C:184:MET:HG3	1.95	0.48
1:H:202:ARG:NH1	1:H:434:ASP:OD2	2.46	0.48
1:J:259:ILE:O	1:J:263:ALA:N	2.41	0.48
1:C:339:VAL:HG21	1:C:358:ILE:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:31:ARG:HB2	1:N:441:ARG:HB3	1.94	0.48
1:P:109:VAL:HG23	1:P:148:ALA:O	2.13	0.48
1:P:236:ALA:HB2	1:P:267:LEU:HD23	1.96	0.48
1:E:64:THR:HG21	1:E:367:GLU:HG2	1.96	0.48
1:H:53:MET:HE3	1:H:56:VAL:HG21	1.96	0.48
1:P:303:CYS:SG	2:P:501:5GP:N2	2.87	0.48
1:D:100:PRO:HD3	1:D:193:GLY:HA2	1.96	0.47
1:H:248:ALA:N	1:H:391:ARG:O	2.46	0.47
1:O:304:THR:HG22	1:P:473:HIS:HB3	1.96	0.47
1:D:109:VAL:HG23	1:D:148:ALA:O	2.14	0.47
1:K:272:VAL:HG12	1:K:292:ILE:HB	1.97	0.47
1:O:196:THR:HG22	1:O:197:ARG:H	1.79	0.47
1:P:360:SER:HB3	1:P:420:MET:HE3	1.95	0.47
1:B:100:PRO:HD3	1:B:193:GLY:HA2	1.97	0.47
1:F:102:THR:HG22	1:F:125:VAL:HB	1.96	0.47
1:H:340:ARG:N	1:H:344:ASP:OD2	2.48	0.47
1:I:15:THR:HG22	1:I:16:TYR:N	2.30	0.47
1:I:36:LEU:HB3	1:I:47:PRO:HD3	1.96	0.47
1:J:365:THR:HG22	1:J:366:TYR:N	2.29	0.47
1:P:15:THR:HG22	1:P:18:ASP:OD2	2.14	0.47
1:D:431:ASP:O	1:D:435:HIS:ND1	2.45	0.47
1:A:383:GLU:OE1	1:A:417:THR:OG1	2.32	0.47
1:F:276:VAL:HG22	1:F:278:SER:H	1.78	0.47
1:J:431:ASP:O	1:J:435:HIS:ND1	2.47	0.47
1:M:91:LYS:NZ	1:M:241:ASP:OD2	2.46	0.47
1:B:196:THR:HG22	1:B:197:ARG:H	1.80	0.47
1:F:5:LEU:HD11	1:F:22:VAL:HG21	1.96	0.47
1:G:51:ALA:HA	1:G:357:MET:HE2	1.96	0.47
1:G:337:GLY:HA2	2:G:501:5GP:H5'1	1.97	0.47
1:H:94:ASP:OD1	1:H:95:LEU:N	2.48	0.47
1:J:294:LYS:HD2	1:J:357:MET:SD	2.55	0.47
1:P:339:VAL:HG12	1:P:344:ASP:HB3	1.97	0.47
1:G:248:ALA:N	1:G:391:ARG:O	2.41	0.47
1:I:302:MET:HE1	1:I:418:SER:HB3	1.97	0.47
1:I:435:HIS:CE1	1:I:475:LEU:HD23	2.50	0.47
1:J:365:THR:HG22	1:J:366:TYR:H	1.79	0.47
1:K:98:ASP:OD1	1:K:99:THR:N	2.47	0.47
1:E:343:ARG:HD2	1:H:307:MET:HA	1.97	0.47
1:M:179:ILE:HG22	1:M:181:VAL:H	1.79	0.47
1:B:272:VAL:HG22	1:B:292:ILE:HB	1.97	0.47
1:E:95:LEU:HD11	1:E:214:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:MET:HE3	2:F:501:5GP:H5'2	1.97	0.47
1:G:294:LYS:HD2	1:G:357:MET:SD	2.54	0.47
1:G:465:SER:OG	1:G:466:ALA:N	2.47	0.47
1:H:36:LEU:HB3	1:H:47:PRO:HD3	1.96	0.47
1:J:465:SER:OG	1:J:466:ALA:N	2.48	0.47
1:M:67:ARG:NH1	1:M:98:ASP:OD1	2.47	0.47
1:P:104:SER:N	1:P:107:ASP:OD2	2.41	0.46
1:E:36:LEU:HB3	1:E:47:PRO:HD3	1.97	0.46
1:F:73:VAL:HG12	1:F:219:ALA:HB3	1.96	0.46
1:K:91:LYS:NZ	1:K:211:ASP:OD2	2.45	0.46
1:O:123:ALA:HB2	1:O:181:VAL:HG21	1.98	0.46
1:B:181:VAL:HG12	1:B:196:THR:HG23	1.97	0.46
1:B:211:ASP:HB3	1:B:241:ASP:OD2	2.15	0.46
1:C:245:ILE:HG22	1:C:255:MET:HE1	1.97	0.46
1:D:73:VAL:HG12	1:D:219:ALA:HB3	1.98	0.46
1:O:179:ILE:HG22	1:O:181:VAL:HG23	1.97	0.46
1:A:123:ALA:HB3	1:A:181:VAL:HG21	1.98	0.46
1:B:51:ALA:HA	1:B:357:MET:HE2	1.97	0.46
1:D:145:ASP:OD2	1:H:54:THR:HG21	2.16	0.46
1:G:3:ARG:NH2	1:I:6:ASP:O	2.47	0.46
1:I:147:PHE:CZ	1:M:369:PRO:HB2	2.51	0.46
1:M:196:THR:HG23	1:M:199:GLY:H	1.81	0.46
1:O:365:THR:HG22	1:O:366:TYR:N	2.30	0.46
1:C:53:MET:SD	2:C:501:5GP:H8	2.56	0.46
1:D:109:VAL:O	1:D:113:ASN:N	2.42	0.46
1:F:364:GLY:O	1:F:422:LEU:HD23	2.15	0.46
1:K:100:PRO:HD3	1:K:193:GLY:HA2	1.97	0.46
1:M:251:HIS:NE2	1:M:284:ASP:OD2	2.46	0.46
1:C:246:ASP:OD2	1:C:391:ARG:NH1	2.49	0.46
1:H:53:MET:HG2	1:H:387:MET:HG2	1.98	0.46
1:L:324:ALA:O	1:L:328:GLN:HG2	2.16	0.46
1:O:274:GLY:O	1:O:294:LYS:HB3	2.15	0.46
1:C:91:LYS:HB3	1:C:215:ARG:HD2	1.97	0.46
1:G:219:ALA:HB2	1:G:242:LEU:HB3	1.98	0.46
1:F:210:VAL:O	1:F:217:ARG:NH1	2.48	0.45
1:H:100:PRO:HD3	1:H:193:GLY:HA2	1.98	0.45
1:L:54:THR:HB	1:P:147:PHE:HB2	1.97	0.45
1:L:380:PRO:HB2	1:L:422:LEU:HD12	1.98	0.45
1:P:246:ASP:OD1	1:P:391:ARG:NH1	2.49	0.45
1:L:222:VAL:HG23	1:L:231:LYS:HE2	1.98	0.45
1:H:283:ARG:HD3	1:L:328:GLN:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:350:ALA:HB1	1:K:459:VAL:HG21	1.99	0.45
1:L:334:TRP:CD1	1:L:355:ASN:HB3	2.52	0.45
1:M:110:SER:N	1:M:146:ARG:O	2.49	0.45
1:P:125:VAL:HA	1:P:135:LEU:HD23	1.99	0.45
1:E:15:THR:HG22	1:E:16:TYR:H	1.80	0.45
1:E:123:ALA:HB3	1:E:181:VAL:HG21	1.99	0.45
1:M:53:MET:SD	2:M:501:5GP:H8	2.55	0.45
1:E:202:ARG:NH2	1:E:431:ASP:OD1	2.50	0.45
1:I:51:ALA:HB3	1:I:359:GLY:HA2	1.99	0.45
1:K:53:MET:HE2	2:K:501:5GP:C8	2.46	0.45
1:L:166:ASP:OD2	1:L:168:ARG:HG2	2.17	0.45
1:M:104:SER:HB2	1:M:107:ASP:OD2	2.16	0.45
1:E:251:HIS:NE2	1:E:284:ASP:OD2	2.44	0.45
1:F:387:MET:HE2	1:F:387:MET:HA	1.99	0.45
1:J:3:ARG:NH2	1:J:458:LYS:O	2.50	0.45
1:O:304:THR:OG1	1:O:413:GLU:OE2	2.33	0.45
1:I:53:MET:SD	2:I:501:5GP:H8	2.56	0.45
1:M:303:CYS:SG	2:M:501:5GP:N2	2.90	0.45
1:C:345:VAL:HG13	1:C:356:VAL:HG21	1.98	0.45
1:B:97:VAL:HG11	1:B:184:MET:HG3	1.99	0.44
1:I:277:VAL:HG12	1:I:296:GLY:HA2	1.98	0.44
1:P:444:CYS:O	1:P:448:GLY:N	2.48	0.44
1:B:165:THR:HG22	1:B:166:ASP:H	1.83	0.44
1:F:294:LYS:NZ	1:F:357:MET:SD	2.90	0.44
1:N:165:THR:HG22	1:N:166:ASP:H	1.82	0.44
1:E:339:VAL:HG13	1:E:344:ASP:HB2	1.99	0.44
1:F:62:ALA:HA	1:F:72:VAL:HG21	1.99	0.44
1:C:274:GLY:O	1:C:294:LYS:HB3	2.18	0.44
1:O:165:THR:HG22	1:O:166:ASP:N	2.32	0.44
1:P:379:ARG:HA	1:P:380:PRO:HD3	1.87	0.44
1:D:145:ASP:OD2	1:H:390:LYS:NZ	2.47	0.44
1:C:180:ASP:HB2	1:C:197:ARG:HB2	2.00	0.44
1:F:276:VAL:HG21	1:F:281:GLY:HA3	1.98	0.44
1:L:196:THR:HG22	1:L:197:ARG:H	1.82	0.44
1:A:380:PRO:HB2	1:A:422:LEU:HB2	1.99	0.44
1:F:339:VAL:HG13	1:F:344:ASP:HB2	1.99	0.44
1:J:277:VAL:O	1:J:313:ARG:NH1	2.50	0.44
1:P:56:VAL:HG23	1:P:57:ALA:N	2.32	0.44
1:E:165:THR:HG22	1:E:166:ASP:H	1.82	0.44
1:F:309:THR:OG1	1:F:310:GLY:N	2.51	0.44
1:F:336:ASP:OD1	2:F:501:5GP:O3'	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:334:TRP:CD1	1:G:355:ASN:HB2	2.53	0.44
1:L:236:ALA:HB2	1:L:267:LEU:HD23	2.00	0.44
1:O:465:SER:OG	1:O:466:ALA:N	2.49	0.44
1:C:303:CYS:SG	2:C:501:5GP:N2	2.91	0.44
1:D:280:GLU:OE1	1:D:280:GLU:N	2.49	0.44
1:F:280:GLU:OE2	1:J:280:GLU:OE2	2.35	0.44
1:J:301:ALA:N	2:J:501:5GP:OP3	2.48	0.44
1:M:365:THR:HG22	1:M:366:TYR:N	2.32	0.44
1:D:147:PHE:CZ	1:H:369:PRO:HB2	2.53	0.43
1:K:277:VAL:HG12	1:K:296:GLY:HA2	2.00	0.43
1:E:132:PRO:HD3	1:E:191:LEU:HB2	1.99	0.43
1:K:339:VAL:HG21	1:K:358:ILE:HA	1.99	0.43
1:O:78:LEU:HG	1:O:79:PRO:HD2	2.00	0.43
1:D:244:VAL:HG22	1:D:272:VAL:HB	1.99	0.43
1:F:80:ILE:HD12	1:F:234:ALA:HB1	1.99	0.43
1:J:94:ASP:OD1	1:J:95:LEU:N	2.51	0.43
1:K:423:ASP:C	1:K:425:ALA:H	2.25	0.43
1:M:19:VAL:O	1:M:343:ARG:NH2	2.45	0.43
1:C:426:ARG:NH2	1:C:431:ASP:OD1	2.51	0.43
1:E:16:TYR:O	1:E:343:ARG:NH2	2.45	0.43
1:E:42:SER:O	1:E:217:ARG:NH2	2.51	0.43
1:N:217:ARG:HA	1:N:241:ASP:OD2	2.18	0.43
1:B:62:ALA:HA	1:B:72:VAL:HG21	2.01	0.43
1:E:368:SER:HA	1:E:369:PRO:HD3	1.89	0.43
1:H:49:VAL:O	1:H:357:MET:HA	2.18	0.43
1:M:302:MET:HE1	1:M:418:SER:HB2	2.01	0.43
1:N:93:ARG:NE	1:N:99:THR:OG1	2.52	0.43
1:I:178:PRO:HG3	1:N:176:HIS:HA	2.00	0.43
1:J:272:VAL:HG12	1:J:292:ILE:HB	2.01	0.43
1:J:282:THR:OG1	1:J:293:VAL:HG21	2.19	0.43
1:L:165:THR:HG22	1:L:166:ASP:H	1.83	0.43
1:B:184:MET:O	1:B:191:LEU:HA	2.17	0.43
1:E:96:VAL:HG13	1:E:97:VAL:H	1.83	0.43
1:F:53:MET:HE1	1:F:301:ALA:HB3	2.00	0.43
1:I:360:SER:HB3	1:I:420:MET:HE3	2.00	0.43
1:I:404:ASP:OD1	1:I:405:ARG:N	2.52	0.43
1:J:444:CYS:O	1:J:448:GLY:N	2.46	0.43
1:B:277:VAL:HB	1:B:313:ARG:HD3	2.01	0.42
1:E:34:VAL:O	1:E:441:ARG:NH1	2.52	0.42
1:J:100:PRO:HD3	1:J:193:GLY:HA2	2.00	0.42
1:L:245:ILE:HD11	1:L:262:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:380:PRO:HB2	1:G:422:LEU:HD22	2.00	0.42
1:L:136:VAL:HA	1:L:140:ASN:HD21	1.82	0.42
1:C:161:ALA:HA	1:C:162:PRO:HD3	1.90	0.42
1:E:402:SER:OG	1:E:404:ASP:OD1	2.31	0.42
1:H:126:VAL:HG23	1:H:133:ILE:HG13	2.00	0.42
1:L:53:MET:SD	2:L:501:5GP:H8	2.59	0.42
1:A:91:LYS:NZ	1:A:241:ASP:OD2	2.48	0.42
1:C:89:PHE:O	1:C:93:ARG:HG2	2.19	0.42
1:I:178:PRO:HD3	1:N:176:HIS:O	2.19	0.42
1:J:222:VAL:HB	1:J:245:ILE:HD13	2.01	0.42
1:N:94:ASP:OD1	1:N:95:LEU:N	2.52	0.42
1:P:98:ASP:OD1	1:P:99:THR:N	2.52	0.42
1:A:36:LEU:HB3	1:A:47:PRO:HD3	2.00	0.42
1:C:158:PHE:CE1	1:C:183:VAL:HG21	2.54	0.42
1:F:379:ARG:HA	1:F:380:PRO:HD3	1.83	0.42
1:G:53:MET:HE2	2:G:501:5GP:H8	2.01	0.42
1:H:166:ASP:OD1	1:H:168:ARG:HG2	2.20	0.42
1:I:176:HIS:NE2	1:N:157:ASP:OD1	2.52	0.42
1:I:464:GLN:OE1	1:J:306:ARG:NH1	2.52	0.42
1:F:98:ASP:OD1	1:F:99:THR:N	2.53	0.42
1:P:163:VAL:N	1:P:185:THR:O	2.51	0.42
1:A:294:LYS:HD2	1:A:357:MET:SD	2.60	0.42
1:H:145:ASP:HB3	1:H:148:ALA:HB2	2.00	0.42
1:I:53:MET:HG2	1:I:387:MET:HG2	2.02	0.42
1:K:313:ARG:NH2	1:K:321:GLU:OE1	2.45	0.42
1:O:53:MET:SD	2:O:501:5GP:H8	2.59	0.42
1:B:294:LYS:HD2	1:B:357:MET:SD	2.59	0.42
1:D:147:PHE:HB2	1:H:54:THR:HB	2.02	0.42
1:H:280:GLU:HA	1:H:283:ARG:HE	1.83	0.42
1:I:147:PHE:HB2	1:M:54:THR:HB	2.01	0.42
1:N:50:VAL:HB	1:N:72:VAL:HG12	2.01	0.42
1:C:176:HIS:CD2	1:H:157:ASP:OD2	2.73	0.42
1:F:303:CYS:SG	1:F:305:THR:OG1	2.57	0.42
1:G:220:ALA:HB3	1:G:235:LEU:HD21	2.01	0.42
1:H:63:GLU:OE2	1:H:99:THR:OG1	2.33	0.42
1:M:31:ARG:O	1:M:441:ARG:NH1	2.49	0.42
1:N:275:ASN:ND2	1:N:296:GLY:O	2.53	0.42
1:P:166:ASP:HA	1:P:167:PRO:HD3	1.93	0.42
1:B:80:ILE:HA	1:B:83:VAL:HG12	2.01	0.42
1:F:274:GLY:O	1:F:294:LYS:HB2	2.20	0.42
1:F:338:GLY:N	2:F:501:5GP:OP1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:334:TRP:CD1	1:O:355:ASN:HB2	2.55	0.42
1:C:160:THR:HG23	1:C:183:VAL:HG23	2.02	0.41
1:D:142:ALA:O	1:D:144:VAL:HG23	2.19	0.41
1:D:313:ARG:NH1	1:D:321:GLU:OE1	2.45	0.41
1:F:134:GLY:HA2	1:F:158:PHE:CE2	2.55	0.41
1:I:109:VAL:HG23	1:I:148:ALA:O	2.20	0.41
1:I:244:VAL:HG12	1:I:272:VAL:HB	2.02	0.41
1:I:316:PHE:HZ	1:I:461:LEU:HD13	1.85	0.41
1:J:380:PRO:HB2	1:J:422:LEU:HB2	2.02	0.41
1:A:166:ASP:HA	1:A:167:PRO:HD3	1.89	0.41
1:B:274:GLY:O	1:B:294:LYS:HB3	2.20	0.41
1:L:260:LYS:HE2	1:L:288:ALA:HA	2.03	0.41
1:P:202:ARG:NH2	1:P:434:ASP:OD2	2.50	0.41
1:E:17:ASN:OD1	1:E:343:ARG:NH1	2.54	0.41
1:E:104:SER:HB3	1:E:107:ASP:OD2	2.21	0.41
1:F:61:MET:HE1	1:F:429:VAL:HG21	2.01	0.41
1:G:202:ARG:NH2	1:G:431:ASP:OD1	2.53	0.41
1:H:404:ASP:OD1	1:H:404:ASP:N	2.53	0.41
1:I:222:VAL:HG12	1:I:231:LYS:HE2	2.02	0.41
1:J:21:VAL:HB	1:K:311:VAL:HA	2.01	0.41
1:M:246:ASP:OD1	1:M:247:THR:N	2.53	0.41
1:N:339:VAL:HG13	1:N:344:ASP:HB2	2.02	0.41
1:O:50:VAL:HB	1:O:72:VAL:HG22	2.02	0.41
1:O:246:ASP:OD1	1:O:391:ARG:NH1	2.52	0.41
1:P:302:MET:HE1	1:P:418:SER:HB2	2.02	0.41
1:D:334:TRP:CD1	1:D:355:ASN:HB2	2.55	0.41
1:F:426:ARG:HB3	1:F:431:ASP:OD2	2.20	0.41
1:K:179:ILE:H	1:K:179:ILE:HG13	1.68	0.41
1:M:274:GLY:O	1:M:294:LYS:HB3	2.21	0.41
1:N:360:SER:HB3	1:N:420:MET:HE3	2.01	0.41
1:A:369:PRO:HB2	1:E:147:PHE:CZ	2.55	0.41
1:B:10:PRO:CG	1:B:14:LEU:HD11	2.50	0.41
1:F:465:SER:OG	1:F:466:ALA:N	2.53	0.41
1:G:242:LEU:HD21	1:G:334:TRP:HH2	1.86	0.41
1:H:78:LEU:HD12	1:H:79:PRO:HD2	2.02	0.41
1:H:174:LEU:HD11	1:H:182:ALA:HB2	2.02	0.41
1:I:473:HIS:ND1	1:I:474:PRO:O	2.53	0.41
1:K:245:ILE:HD11	1:K:262:VAL:HG21	2.01	0.41
1:K:333:VAL:HG23	1:K:353:ALA:HA	2.02	0.41
1:O:103:LEU:HG	1:O:104:SER:H	1.86	0.41
1:O:183:VAL:HA	1:O:194:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:57:ALA:HB3	1:P:75:PRO:HD3	2.03	0.41
1:P:140:ASN:HB3	1:P:153:ILE:HG23	2.02	0.41
1:G:98:ASP:OD1	1:G:119:ARG:NH2	2.54	0.41
1:J:14:LEU:HD23	1:J:19:VAL:CG1	2.50	0.41
1:J:14:LEU:O	1:J:316:PHE:HB3	2.21	0.41
1:J:207:THR:HA	1:J:208:PRO:HD3	1.93	0.41
1:K:126:VAL:HG23	1:K:133:ILE:HG13	2.03	0.41
1:O:308:MET:HE1	1:P:435:HIS:NE2	2.36	0.41
1:A:471:GLU:OE2	1:B:306:ARG:NH1	2.53	0.41
1:D:473:HIS:ND1	1:D:474:PRO:O	2.53	0.41
1:F:334:TRP:CD1	1:F:355:ASN:HB2	2.56	0.41
1:G:38:THR:HG21	1:G:355:ASN:ND2	2.36	0.41
1:G:359:GLY:HA3	2:G:501:5GP:OP2	2.21	0.41
1:J:251:HIS:HE1	1:J:280:GLU:HG2	1.86	0.41
1:P:301:ALA:N	2:P:501:5GP:OP3	2.46	0.41
1:C:50:VAL:HB	1:C:72:VAL:HG22	2.02	0.41
1:C:217:ARG:HA	1:C:241:ASP:OD2	2.21	0.41
1:D:50:VAL:O	1:D:73:VAL:HG22	2.21	0.41
1:D:360:SER:N	2:D:501:5GP:OP1	2.54	0.41
1:E:109:VAL:HG23	1:E:148:ALA:O	2.20	0.41
1:G:274:GLY:O	1:G:294:LYS:HB3	2.21	0.41
1:G:423:ASP:HA	1:G:424:PRO:HD3	1.95	0.41
1:H:20:PHE:CZ	1:H:462:GLY:HA3	2.56	0.41
1:H:377:ASP:HB3	1:H:379:ARG:HG3	2.02	0.41
1:I:89:PHE:O	1:I:93:ARG:HG2	2.21	0.41
1:I:93:ARG:HD3	1:I:93:ARG:HA	1.79	0.41
1:J:62:ALA:HA	1:J:72:VAL:HG21	2.03	0.41
1:L:316:PHE:HZ	1:L:461:LEU:HD13	1.86	0.41
1:N:105:PRO:HG3	1:N:133:ILE:HD11	2.03	0.41
1:O:15:THR:HG22	1:O:18:ASP:OD2	2.20	0.41
1:O:362:PHE:O	1:O:368:SER:OG	2.39	0.41
1:A:109:VAL:HG23	1:A:148:ALA:O	2.21	0.41
1:D:166:ASP:HA	1:D:167:PRO:HD3	1.90	0.41
1:D:316:PHE:HZ	1:D:461:LEU:HD13	1.85	0.41
1:I:60:ARG:NH1	1:I:118:LYS:O	2.52	0.41
1:I:145:ASP:HB3	1:I:148:ALA:HB2	2.02	0.41
1:K:213:LYS:HD2	1:K:215:ARG:HH11	1.85	0.41
1:K:300:GLY:HA2	2:K:501:5GP:OP3	2.21	0.41
1:M:379:ARG:HA	1:M:380:PRO:HD3	1.95	0.41
1:N:74:LEU:HD11	1:N:218:ILE:HD11	2.03	0.41
1:H:334:TRP:CD1	1:H:355:ASN:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:227:ASP:OD1	1:J:230:ALA:N	2.46	0.40
1:J:300:GLY:HA2	2:J:501:5GP:OP3	2.21	0.40
1:M:178:PRO:HG2	1:M:179:ILE:HD12	2.02	0.40
1:A:147:PHE:O	1:A:149:ARG:NH1	2.54	0.40
1:G:126:VAL:HG22	1:G:134:GLY:H	1.86	0.40
1:J:3:ARG:NH1	1:J:457:GLU:O	2.53	0.40
1:L:147:PHE:HB2	1:P:54:THR:HB	2.02	0.40
1:M:91:LYS:NZ	1:M:211:ASP:OD2	2.35	0.40
1:D:132:PRO:HD3	1:D:191:LEU:HB2	2.03	0.40
1:K:166:ASP:HA	1:K:167:PRO:HD3	1.92	0.40
1:K:334:TRP:CD1	1:K:355:ASN:HB2	2.57	0.40
1:O:417:THR:O	1:P:473:HIS:NE2	2.52	0.40
1:D:245:ILE:HB	1:D:255:MET:HE1	2.04	0.40
1:D:274:GLY:O	1:D:294:LYS:HB3	2.22	0.40
1:F:68:ARG:NH1	1:F:430:GLU:OE2	2.54	0.40
1:G:423:ASP:OD2	1:G:426:ARG:N	2.49	0.40
1:H:224:ILE:HG22	1:H:245:ILE:HD11	2.03	0.40
1:I:236:ALA:HB2	1:I:267:LEU:HD23	2.03	0.40
1:I:432:LEU:O	1:I:436:ILE:HG22	2.22	0.40
1:N:411:PHE:O	1:O:31:ARG:NH1	2.54	0.40
1:H:14:LEU:HD23	1:H:19:VAL:CG1	2.52	0.40
1:L:15:THR:HG22	1:L:18:ASP:OD2	2.22	0.40
1:M:307:MET:HA	1:N:343:ARG:HD2	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ASP:OD2	1:M:9:THR:OG1[1_646]	1.95	0.25
1:B:9:THR:OG1	1:O:6:ASP:OD2[1_646]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	471/496 (95%)	459 (98%)	12 (2%)	0	100	100
1	B	441/496 (89%)	430 (98%)	11 (2%)	0	100	100
1	C	438/496 (88%)	425 (97%)	13 (3%)	0	100	100
1	D	464/496 (94%)	456 (98%)	8 (2%)	0	100	100
1	E	464/496 (94%)	449 (97%)	15 (3%)	0	100	100
1	F	430/496 (87%)	415 (96%)	15 (4%)	0	100	100
1	G	412/496 (83%)	395 (96%)	17 (4%)	0	100	100
1	H	464/496 (94%)	445 (96%)	19 (4%)	0	100	100
1	I	460/496 (93%)	448 (97%)	12 (3%)	0	100	100
1	J	434/496 (88%)	419 (96%)	15 (4%)	0	100	100
1	K	442/496 (89%)	423 (96%)	19 (4%)	0	100	100
1	L	461/496 (93%)	452 (98%)	9 (2%)	0	100	100
1	M	467/496 (94%)	456 (98%)	11 (2%)	0	100	100
1	N	453/496 (91%)	442 (98%)	11 (2%)	0	100	100
1	O	449/496 (90%)	434 (97%)	15 (3%)	0	100	100
1	P	461/496 (93%)	449 (97%)	12 (3%)	0	100	100
All	All	7211/7936 (91%)	6997 (97%)	214 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/372 (93%)	346 (100%)	0	100	100
1	B	331/372 (89%)	329 (99%)	2 (1%)	78	91
1	C	333/372 (90%)	333 (100%)	0	100	100
1	D	348/372 (94%)	346 (99%)	2 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	348/372 (94%)	346 (99%)	2 (1%)	78	91
1	F	324/372 (87%)	321 (99%)	3 (1%)	70	87
1	G	305/372 (82%)	303 (99%)	2 (1%)	76	89
1	H	347/372 (93%)	347 (100%)	0	100	100
1	I	346/372 (93%)	344 (99%)	2 (1%)	78	91
1	J	321/372 (86%)	318 (99%)	3 (1%)	70	87
1	K	323/372 (87%)	320 (99%)	3 (1%)	70	87
1	L	341/372 (92%)	340 (100%)	1 (0%)	86	94
1	M	343/372 (92%)	342 (100%)	1 (0%)	86	94
1	N	346/372 (93%)	345 (100%)	1 (0%)	86	94
1	O	337/372 (91%)	335 (99%)	2 (1%)	78	91
1	P	344/372 (92%)	341 (99%)	3 (1%)	70	87
All	All	5383/5952 (90%)	5356 (100%)	27 (0%)	81	92

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	72	VAL
1	B	93	ARG
1	D	52	ASN
1	D	383	GLU
1	E	96	VAL
1	E	150	VAL
1	F	52	ASN
1	F	272	VAL
1	F	413	GLU
1	G	126	VAL
1	G	272	VAL
1	I	251	HIS
1	I	436	ILE
1	J	46	ILE
1	J	196	THR
1	J	272	VAL
1	K	101	VAL
1	K	179	ILE
1	K	272	VAL
1	L	196	THR
1	M	156	SER

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Mol	Chain	Res	Type
1	N	101	VAL
1	O	181	VAL
1	O	196	THR
1	P	244	VAL
1	P	272	VAL
1	P	295	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	355	ASN
1	H	8	HIS
1	J	113	ASN
1	L	140	ASN
1	N	249	HIS
1	N	252	GLN
1	N	355	ASN
1	O	341	HIS
1	P	113	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5GP	K	501	-	26,26,26	1.13	2 (7%)	40,40,40	1.78	8 (20%)
2	5GP	F	501	-	26,26,26	1.13	2 (7%)	40,40,40	1.71	7 (17%)
2	5GP	O	501	-	26,26,26	1.13	2 (7%)	40,40,40	1.79	9 (22%)
2	5GP	A	501	-	26,26,26	1.11	2 (7%)	40,40,40	1.80	8 (20%)
2	5GP	G	501	-	26,26,26	0.98	1 (3%)	40,40,40	1.81	8 (20%)
2	5GP	C	501	-	26,26,26	1.10	2 (7%)	40,40,40	1.79	9 (22%)
2	5GP	D	501	-	26,26,26	1.12	2 (7%)	40,40,40	1.77	8 (20%)
2	5GP	J	501	-	26,26,26	1.13	2 (7%)	40,40,40	1.79	9 (22%)
2	5GP	M	501	-	26,26,26	0.97	1 (3%)	40,40,40	1.77	8 (20%)
2	5GP	E	501	-	26,26,26	1.10	2 (7%)	40,40,40	1.79	8 (20%)
2	5GP	P	501	-	26,26,26	0.99	1 (3%)	40,40,40	1.75	7 (17%)
2	5GP	N	501	-	26,26,26	0.98	1 (3%)	40,40,40	1.77	8 (20%)
2	5GP	L	501	-	26,26,26	1.13	2 (7%)	40,40,40	1.78	9 (22%)
2	5GP	I	501	-	26,26,26	1.09	2 (7%)	40,40,40	1.82	8 (20%)
2	5GP	B	501	-	26,26,26	1.10	2 (7%)	40,40,40	1.79	8 (20%)
2	5GP	H	501	-	26,26,26	0.96	1 (3%)	40,40,40	1.78	8 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5GP	K	501	-	-	5/10/26/26	0/3/3/3
2	5GP	F	501	-	-	0/10/26/26	0/3/3/3
2	5GP	O	501	-	-	1/10/26/26	0/3/3/3
2	5GP	A	501	-	-	0/10/26/26	0/3/3/3
2	5GP	G	501	-	-	5/10/26/26	0/3/3/3
2	5GP	C	501	-	-	5/10/26/26	0/3/3/3
2	5GP	D	501	-	-	5/10/26/26	0/3/3/3
2	5GP	J	501	-	-	5/10/26/26	0/3/3/3
2	5GP	M	501	-	-	5/10/26/26	0/3/3/3
2	5GP	E	501	-	-	3/10/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5GP	P	501	-	-	5/10/26/26	0/3/3/3
2	5GP	N	501	-	-	3/10/26/26	0/3/3/3
2	5GP	L	501	-	-	1/10/26/26	0/3/3/3
2	5GP	I	501	-	-	1/10/26/26	0/3/3/3
2	5GP	B	501	-	-	5/10/26/26	0/3/3/3
2	5GP	H	501	-	-	0/10/26/26	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	501	5GP	C6-N1	-3.87	1.31	1.38
2	F	501	5GP	C6-N1	-3.86	1.31	1.38
2	G	501	5GP	C6-N1	-3.83	1.31	1.38
2	L	501	5GP	C6-N1	-3.82	1.31	1.38
2	O	501	5GP	C6-N1	-3.81	1.31	1.38
2	K	501	5GP	C6-N1	-3.81	1.31	1.38
2	D	501	5GP	C6-N1	-3.81	1.31	1.38
2	P	501	5GP	C6-N1	-3.79	1.31	1.38
2	N	501	5GP	C6-N1	-3.78	1.31	1.38
2	M	501	5GP	C6-N1	-3.73	1.31	1.38
2	E	501	5GP	C6-N1	-3.73	1.31	1.38
2	H	501	5GP	C6-N1	-3.72	1.31	1.38
2	A	501	5GP	C6-N1	-3.72	1.31	1.38
2	B	501	5GP	C6-N1	-3.71	1.31	1.38
2	C	501	5GP	C6-N1	-3.63	1.32	1.38
2	I	501	5GP	C6-N1	-3.50	1.32	1.38
2	K	501	5GP	P-OP1	2.90	1.59	1.50
2	C	501	5GP	P-OP1	2.84	1.59	1.50
2	L	501	5GP	P-OP1	2.83	1.59	1.50
2	O	501	5GP	P-OP1	2.83	1.59	1.50
2	J	501	5GP	P-OP1	2.83	1.59	1.50
2	I	501	5GP	P-OP1	2.71	1.59	1.50
2	F	501	5GP	P-OP1	2.70	1.59	1.50
2	B	501	5GP	P-OP1	2.66	1.59	1.50
2	E	501	5GP	P-OP1	2.65	1.59	1.50
2	A	501	5GP	P-OP1	2.64	1.59	1.50
2	D	501	5GP	P-OP1	2.63	1.59	1.50

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	501	5GP	C2-N1-C6	-5.71	114.69	125.10
2	I	501	5GP	C2-N1-C6	-5.70	114.70	125.10
2	I	501	5GP	C5-C4-N3	-5.68	119.24	128.46
2	G	501	5GP	C2-N1-C6	-5.68	114.75	125.10
2	B	501	5GP	C2-N1-C6	-5.68	114.75	125.10
2	N	501	5GP	C2-N1-C6	-5.68	114.75	125.10
2	E	501	5GP	C2-N1-C6	-5.67	114.77	125.10
2	A	501	5GP	C2-N1-C6	-5.67	114.77	125.10
2	L	501	5GP	C2-N1-C6	-5.64	114.82	125.10
2	H	501	5GP	C2-N1-C6	-5.63	114.83	125.10
2	C	501	5GP	C2-N1-C6	-5.63	114.84	125.10
2	M	501	5GP	C2-N1-C6	-5.61	114.86	125.10
2	K	501	5GP	C2-N1-C6	-5.60	114.89	125.10
2	D	501	5GP	C2-N1-C6	-5.60	114.89	125.10
2	J	501	5GP	C2-N1-C6	-5.59	114.90	125.10
2	P	501	5GP	C2-N1-C6	-5.58	114.93	125.10
2	F	501	5GP	C2-N1-C6	-5.56	114.97	125.10
2	H	501	5GP	C5-C4-N3	-5.53	119.50	128.46
2	K	501	5GP	C5-C4-N3	-5.50	119.54	128.46
2	A	501	5GP	C5-C4-N3	-5.49	119.55	128.46
2	C	501	5GP	C5-C4-N3	-5.49	119.55	128.46
2	E	501	5GP	C5-C4-N3	-5.48	119.56	128.46
2	B	501	5GP	C5-C4-N3	-5.47	119.58	128.46
2	G	501	5GP	C5-C4-N3	-5.45	119.63	128.46
2	M	501	5GP	C5-C4-N3	-5.39	119.72	128.46
2	J	501	5GP	C5-C4-N3	-5.36	119.76	128.46
2	L	501	5GP	C5-C4-N3	-5.33	119.81	128.46
2	D	501	5GP	C5-C4-N3	-5.32	119.83	128.46
2	O	501	5GP	C5-C4-N3	-5.31	119.85	128.46
2	N	501	5GP	C5-C4-N3	-5.31	119.85	128.46
2	P	501	5GP	C5-C4-N3	-5.11	120.17	128.46
2	F	501	5GP	C5-C4-N3	-4.95	120.43	128.46
2	O	501	5GP	C5-C6-N1	3.48	122.02	113.19
2	F	501	5GP	C5-C6-N1	3.48	122.02	113.19
2	N	501	5GP	C5-C6-N1	3.46	121.98	113.19
2	J	501	5GP	C5-C6-N1	3.45	121.94	113.19
2	L	501	5GP	C5-C6-N1	3.44	121.93	113.19
2	P	501	5GP	C5-C6-N1	3.44	121.92	113.19
2	D	501	5GP	C5-C6-N1	3.43	121.90	113.19
2	G	501	5GP	C5-C6-N1	3.43	121.90	113.19
2	B	501	5GP	C5-C6-N1	3.41	121.84	113.19
2	E	501	5GP	C5-C6-N1	3.40	121.83	113.19
2	M	501	5GP	C5-C6-N1	3.39	121.81	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	501	5GP	N9-C4-N3	3.39	132.75	125.94
2	A	501	5GP	C5-C6-N1	3.37	121.76	113.19
2	H	501	5GP	C5-C6-N1	3.36	121.73	113.19
2	D	501	5GP	N9-C4-N3	3.36	132.68	125.94
2	K	501	5GP	C5-C6-N1	3.36	121.71	113.19
2	O	501	5GP	N9-C4-N3	3.34	132.65	125.94
2	C	501	5GP	C5-C6-N1	3.33	121.65	113.19
2	N	501	5GP	N9-C4-N3	3.33	132.62	125.94
2	M	501	5GP	N9-C4-N3	3.32	132.60	125.94
2	B	501	5GP	N9-C4-N3	3.30	132.56	125.94
2	I	501	5GP	C5-C6-N1	3.30	121.56	113.19
2	G	501	5GP	N9-C4-N3	3.30	132.56	125.94
2	L	501	5GP	N9-C4-N3	3.29	132.55	125.94
2	E	501	5GP	N9-C4-N3	3.29	132.54	125.94
2	H	501	5GP	N9-C4-N3	3.29	132.54	125.94
2	C	501	5GP	N9-C4-N3	3.26	132.48	125.94
2	A	501	5GP	N9-C4-N3	3.24	132.44	125.94
2	K	501	5GP	N9-C4-N3	3.19	132.35	125.94
2	P	501	5GP	N9-C4-N3	3.16	132.29	125.94
2	F	501	5GP	N9-C4-N3	3.16	132.28	125.94
2	F	501	5GP	O6-C6-C5	-2.98	118.69	126.60
2	P	501	5GP	O6-C6-C5	-2.95	118.78	126.60
2	I	501	5GP	N9-C4-N3	2.93	131.83	125.94
2	O	501	5GP	O6-C6-C5	-2.93	118.82	126.60
2	D	501	5GP	O6-C6-C5	-2.93	118.83	126.60
2	G	501	5GP	O6-C6-C5	-2.91	118.88	126.60
2	N	501	5GP	O6-C6-C5	-2.91	118.88	126.60
2	L	501	5GP	O6-C6-C5	-2.91	118.89	126.60
2	J	501	5GP	O6-C6-C5	-2.90	118.91	126.60
2	B	501	5GP	O6-C6-C5	-2.85	119.04	126.60
2	M	501	5GP	O6-C6-C5	-2.84	119.05	126.60
2	E	501	5GP	O6-C6-C5	-2.84	119.06	126.60
2	H	501	5GP	O6-C6-C5	-2.83	119.09	126.60
2	A	501	5GP	O6-C6-C5	-2.82	119.13	126.60
2	C	501	5GP	O6-C6-C5	-2.79	119.21	126.60
2	K	501	5GP	O6-C6-C5	-2.76	119.27	126.60
2	I	501	5GP	O6-C6-C5	-2.67	119.51	126.60
2	G	501	5GP	N9-C8-N7	-2.48	108.72	113.39
2	A	501	5GP	N9-C8-N7	-2.48	108.72	113.39
2	E	501	5GP	N9-C8-N7	-2.46	108.75	113.39
2	L	501	5GP	N9-C8-N7	-2.46	108.76	113.39
2	J	501	5GP	N9-C8-N7	-2.44	108.80	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	5GP	N9-C8-N7	-2.42	108.83	113.39
2	O	501	5GP	N9-C8-N7	-2.42	108.84	113.39
2	D	501	5GP	N9-C8-N7	-2.41	108.85	113.39
2	M	501	5GP	N9-C8-N7	-2.41	108.86	113.39
2	B	501	5GP	N9-C8-N7	-2.41	108.86	113.39
2	N	501	5GP	N9-C8-N7	-2.40	108.88	113.39
2	P	501	5GP	N9-C8-N7	-2.40	108.88	113.39
2	H	501	5GP	N9-C8-N7	-2.39	108.88	113.39
2	I	501	5GP	OP2-P-OP3	2.39	116.76	107.64
2	K	501	5GP	N9-C8-N7	-2.35	108.96	113.39
2	I	501	5GP	N9-C8-N7	-2.34	108.99	113.39
2	O	501	5GP	OP2-P-OP3	2.28	116.35	107.64
2	F	501	5GP	N9-C8-N7	-2.27	109.12	113.39
2	I	501	5GP	N1-C2-N3	2.25	127.52	123.32
2	C	501	5GP	OP2-P-OP3	2.24	116.19	107.64
2	A	501	5GP	C2-N3-C4	2.19	116.19	112.30
2	J	501	5GP	OP2-P-OP3	2.18	115.95	107.64
2	G	501	5GP	C2-N3-C4	2.16	116.15	112.30
2	H	501	5GP	C2-N3-C4	2.15	116.13	112.30
2	O	501	5GP	N1-C2-N3	2.15	127.34	123.32
2	L	501	5GP	C2-N3-C4	2.15	116.12	112.30
2	M	501	5GP	C2-N3-C4	2.14	116.12	112.30
2	J	501	5GP	C2-N3-C4	2.14	116.11	112.30
2	E	501	5GP	C2-N3-C4	2.14	116.11	112.30
2	N	501	5GP	N1-C2-N3	2.13	127.30	123.32
2	B	501	5GP	C2-N3-C4	2.13	116.09	112.30
2	C	501	5GP	C2-N3-C4	2.12	116.08	112.30
2	D	501	5GP	C2-N3-C4	2.12	116.08	112.30
2	B	501	5GP	N1-C2-N3	2.12	127.28	123.32
2	E	501	5GP	N1-C2-N3	2.12	127.27	123.32
2	G	501	5GP	N1-C2-N3	2.11	127.26	123.32
2	O	501	5GP	C2-N3-C4	2.11	116.05	112.30
2	K	501	5GP	N1-C2-N3	2.11	127.25	123.32
2	A	501	5GP	N1-C2-N3	2.10	127.25	123.32
2	C	501	5GP	N1-C2-N3	2.10	127.25	123.32
2	P	501	5GP	N1-C2-N3	2.10	127.24	123.32
2	H	501	5GP	N1-C2-N3	2.09	127.23	123.32
2	N	501	5GP	C2-N3-C4	2.09	116.02	112.30
2	L	501	5GP	N1-C2-N3	2.08	127.20	123.32
2	M	501	5GP	N1-C2-N3	2.08	127.20	123.32
2	J	501	5GP	N1-C2-N3	2.07	127.18	123.32
2	D	501	5GP	N1-C2-N3	2.06	127.17	123.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	501	5GP	C2-N3-C4	2.06	115.97	112.30
2	F	501	5GP	N1-C2-N3	2.06	127.17	123.32
2	L	501	5GP	OP2-P-OP3	2.01	115.31	107.64

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	5GP	C5'-O5'-P-OP1
2	B	501	5GP	C5'-O5'-P-OP3
2	B	501	5GP	C5'-O5'-P-OP2
2	B	501	5GP	C3'-C4'-C5'-O5'
2	C	501	5GP	C5'-O5'-P-OP1
2	C	501	5GP	C5'-O5'-P-OP3
2	C	501	5GP	C3'-C4'-C5'-O5'
2	D	501	5GP	C5'-O5'-P-OP1
2	D	501	5GP	C5'-O5'-P-OP3
2	D	501	5GP	C5'-O5'-P-OP2
2	D	501	5GP	C3'-C4'-C5'-O5'
2	G	501	5GP	C5'-O5'-P-OP1
2	G	501	5GP	C5'-O5'-P-OP3
2	G	501	5GP	C5'-O5'-P-OP2
2	J	501	5GP	C5'-O5'-P-OP3
2	J	501	5GP	C5'-O5'-P-OP2
2	J	501	5GP	C3'-C4'-C5'-O5'
2	K	501	5GP	C5'-O5'-P-OP1
2	K	501	5GP	C5'-O5'-P-OP3
2	M	501	5GP	C5'-O5'-P-OP1
2	M	501	5GP	C5'-O5'-P-OP3
2	M	501	5GP	C5'-O5'-P-OP2
2	M	501	5GP	C3'-C4'-C5'-O5'
2	N	501	5GP	C5'-O5'-P-OP3
2	N	501	5GP	C5'-O5'-P-OP2
2	P	501	5GP	C5'-O5'-P-OP1
2	P	501	5GP	C5'-O5'-P-OP3
2	P	501	5GP	C5'-O5'-P-OP2
2	P	501	5GP	O4'-C4'-C5'-O5'
2	P	501	5GP	C3'-C4'-C5'-O5'
2	C	501	5GP	O4'-C4'-C5'-O5'
2	E	501	5GP	C3'-C4'-C5'-O5'
2	G	501	5GP	O4'-C4'-C5'-O5'
2	G	501	5GP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	J	501	5GP	O4'-C4'-C5'-O5'
2	K	501	5GP	C3'-C4'-C5'-O5'
2	E	501	5GP	O4'-C4'-C5'-O5'
2	K	501	5GP	O4'-C4'-C5'-O5'
2	B	501	5GP	O4'-C4'-C5'-O5'
2	D	501	5GP	O4'-C4'-C5'-O5'
2	M	501	5GP	O4'-C4'-C5'-O5'
2	J	501	5GP	C5'-O5'-P-OP1
2	N	501	5GP	C5'-O5'-P-OP1
2	O	501	5GP	C5'-O5'-P-OP1
2	C	501	5GP	C5'-O5'-P-OP2
2	E	501	5GP	C5'-O5'-P-OP3
2	K	501	5GP	C5'-O5'-P-OP2
2	I	501	5GP	C3'-C4'-C5'-O5'
2	L	501	5GP	C3'-C4'-C5'-O5'

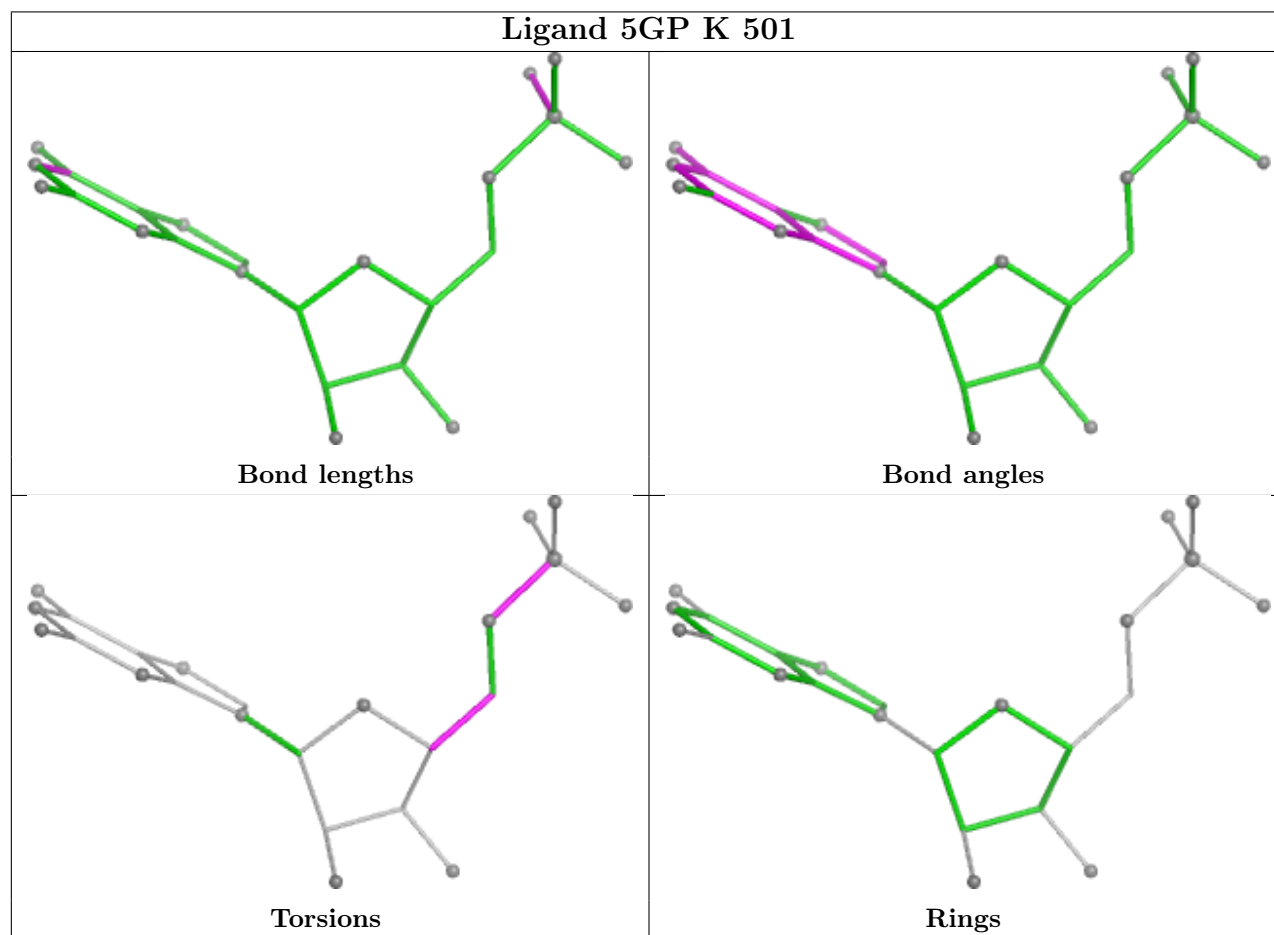
There are no ring outliers.

13 monomers are involved in 38 short contacts:

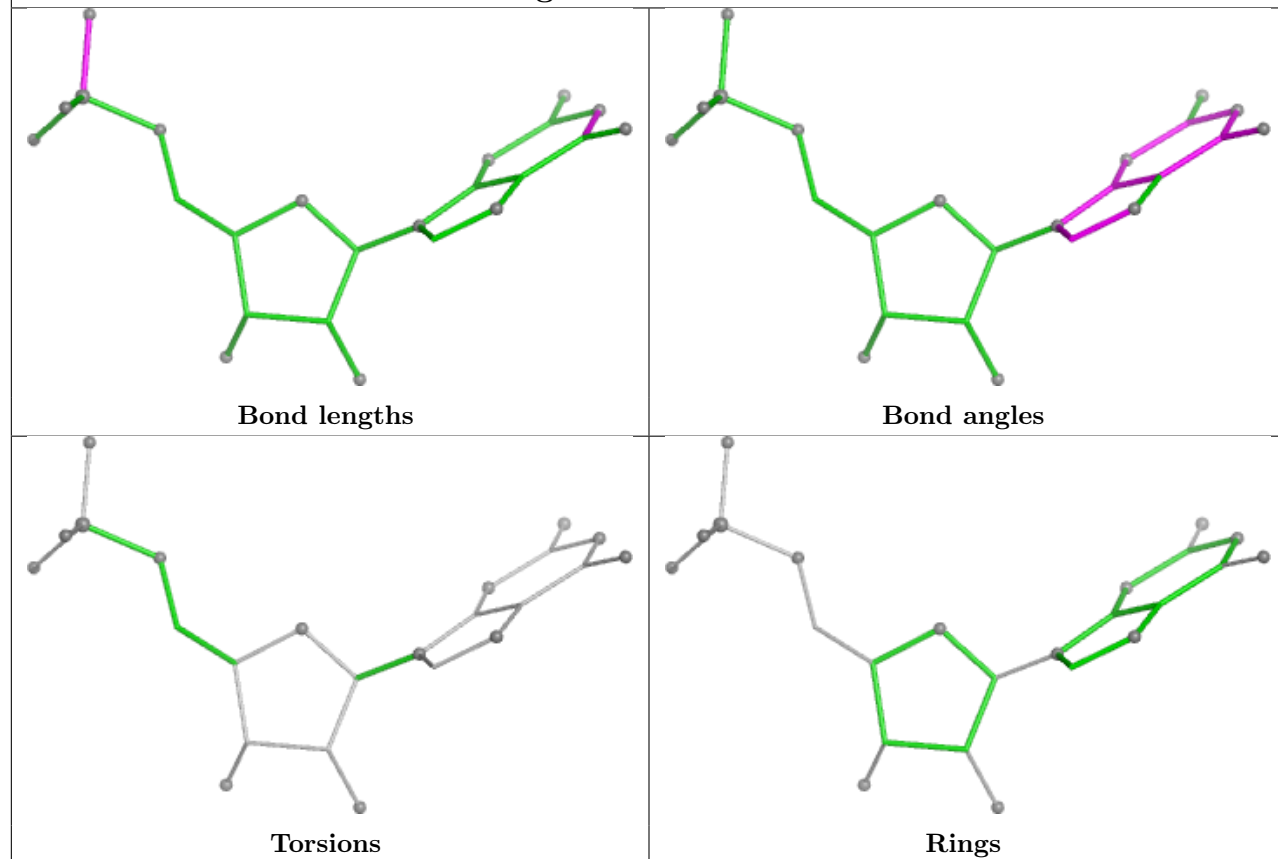
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	501	5GP	7	0
2	F	501	5GP	3	0
2	O	501	5GP	2	0
2	A	501	5GP	2	0
2	G	501	5GP	5	0
2	C	501	5GP	3	0
2	D	501	5GP	1	0
2	J	501	5GP	3	0
2	M	501	5GP	3	0
2	P	501	5GP	4	0
2	N	501	5GP	1	0
2	L	501	5GP	2	0
2	I	501	5GP	2	0

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 than 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

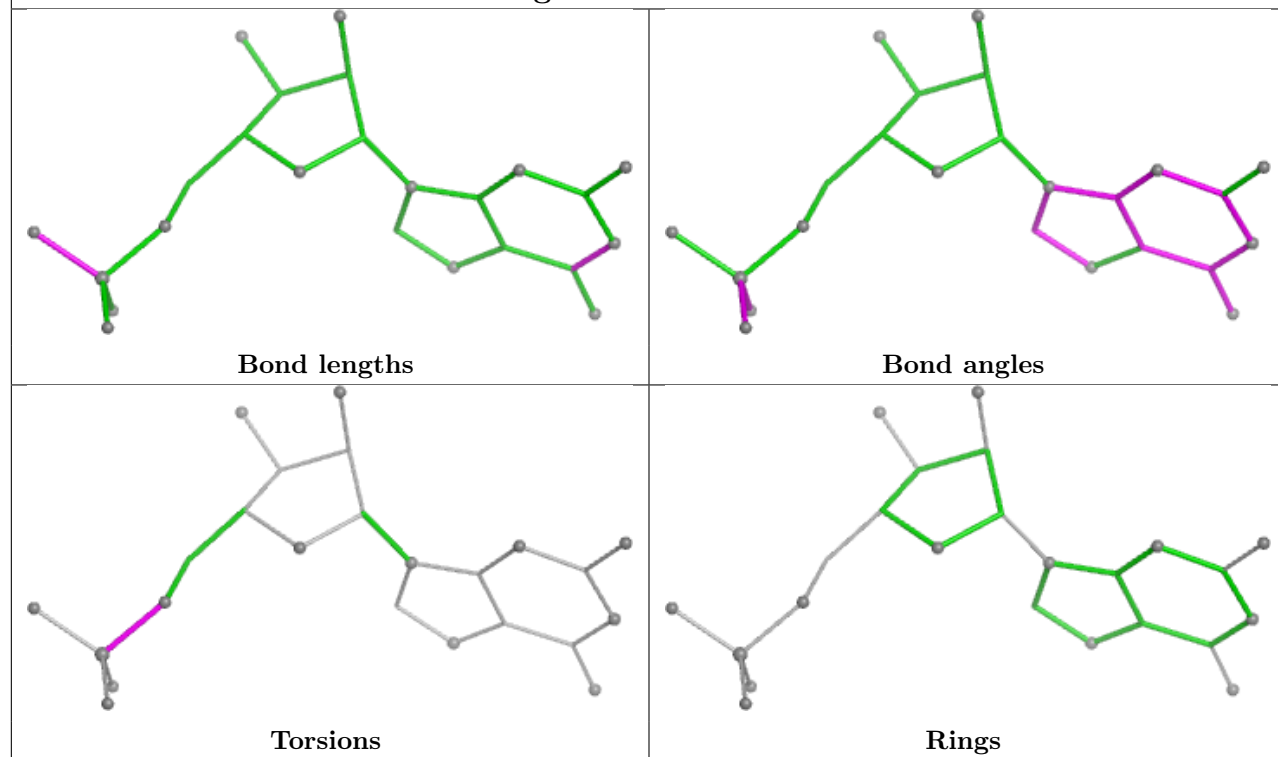
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



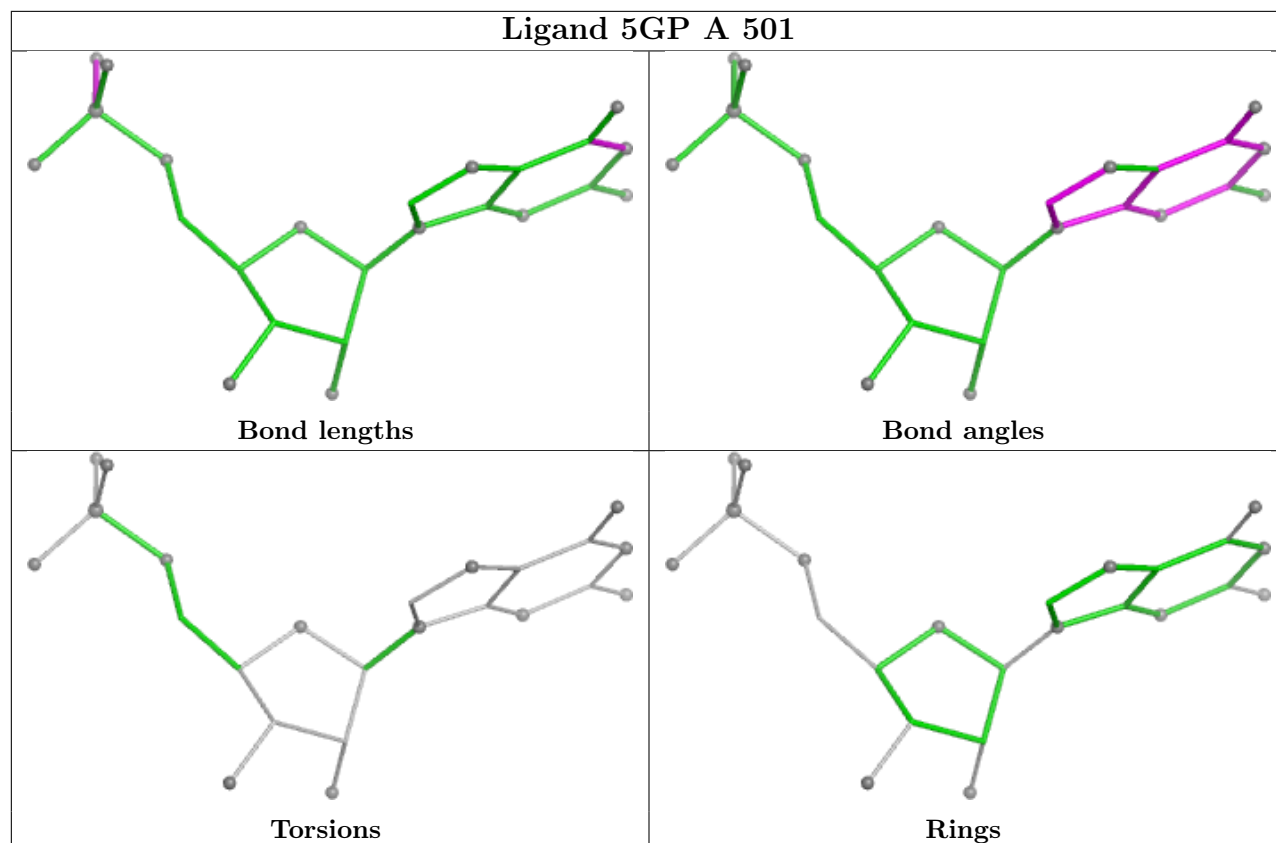
Ligand 5GP F 501



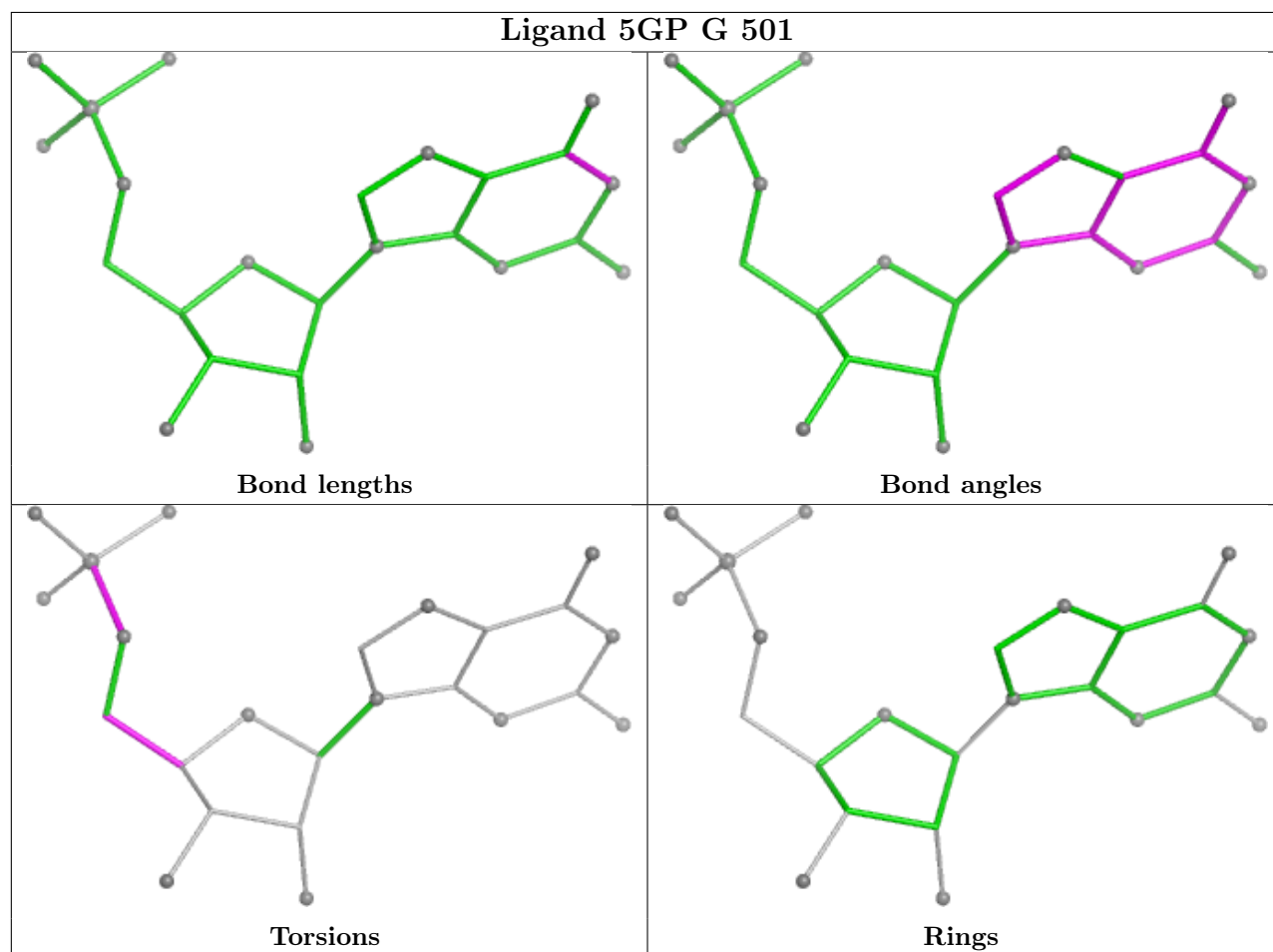
Ligand 5GP O 501



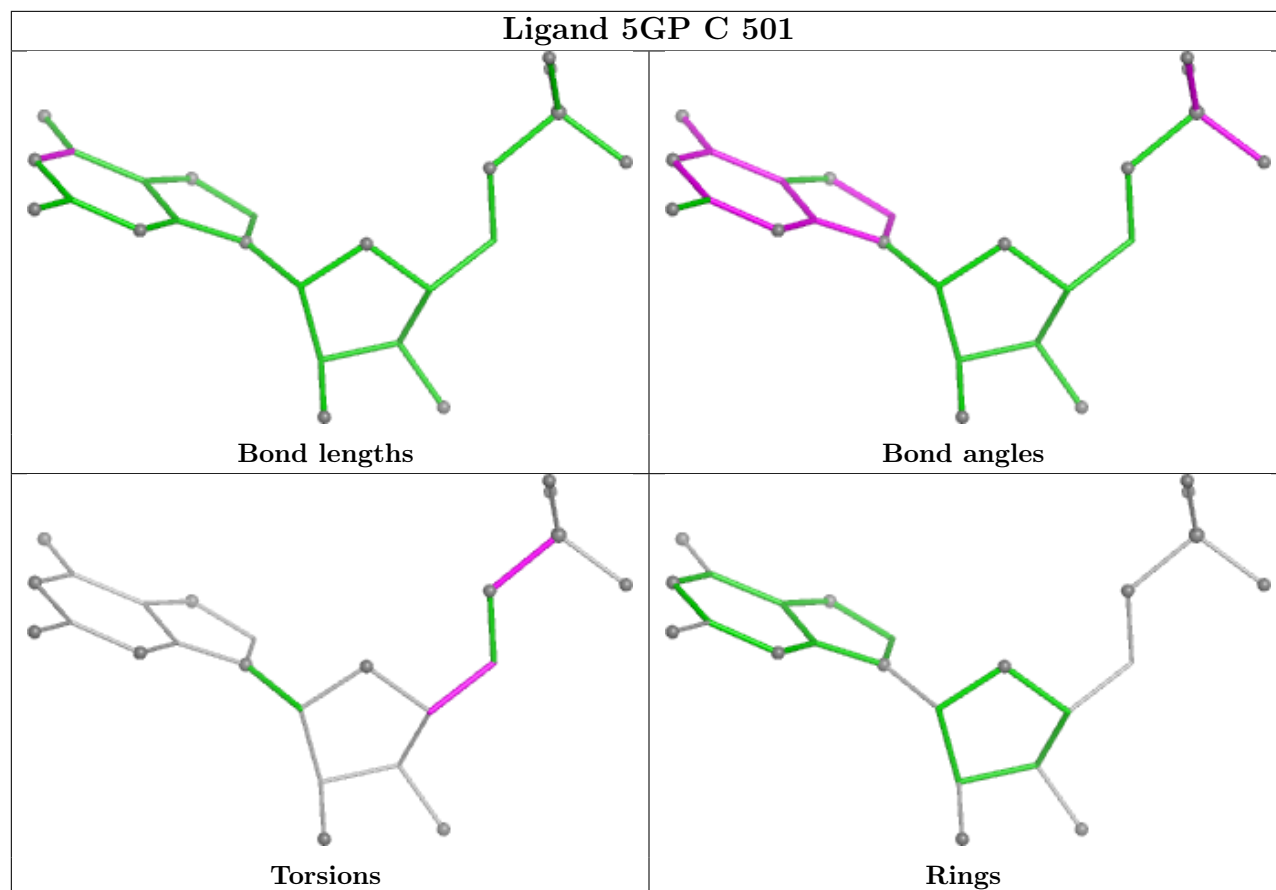
Ligand 5GP A 501



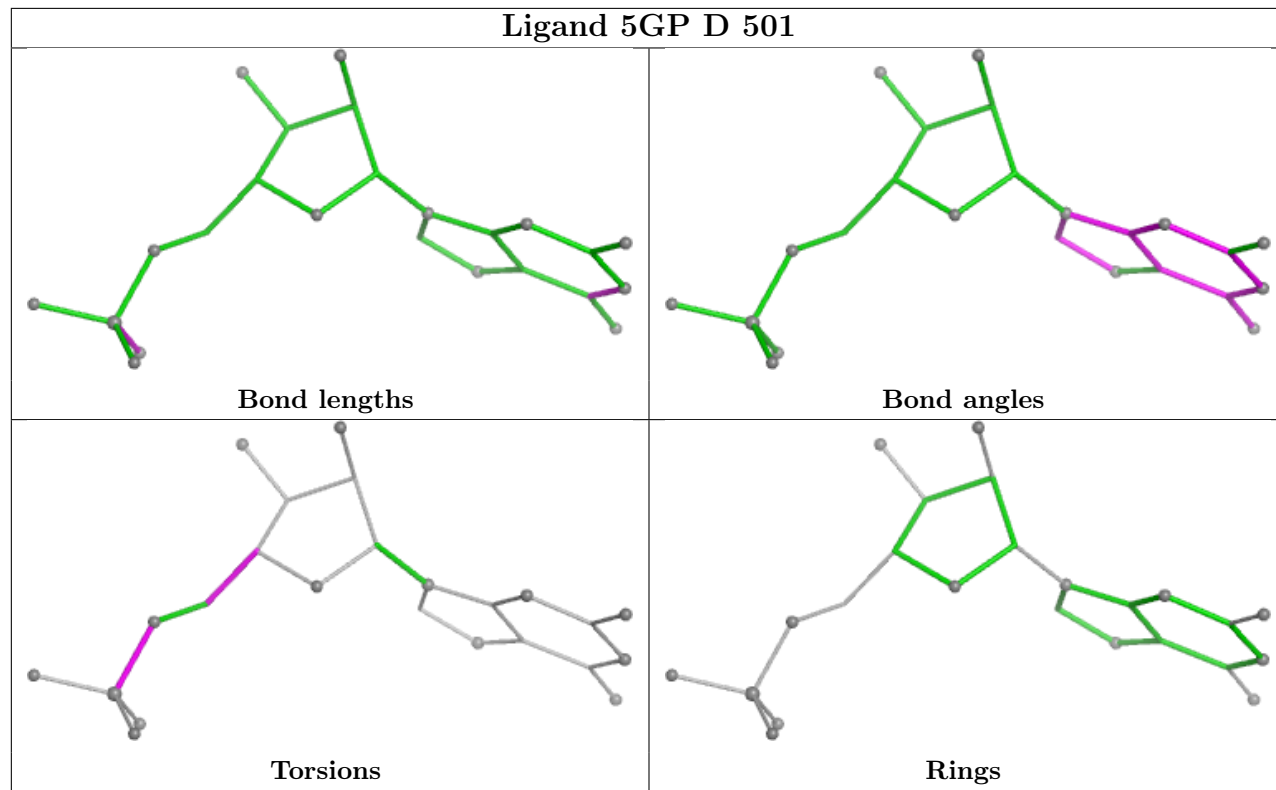
Ligand 5GP G 501



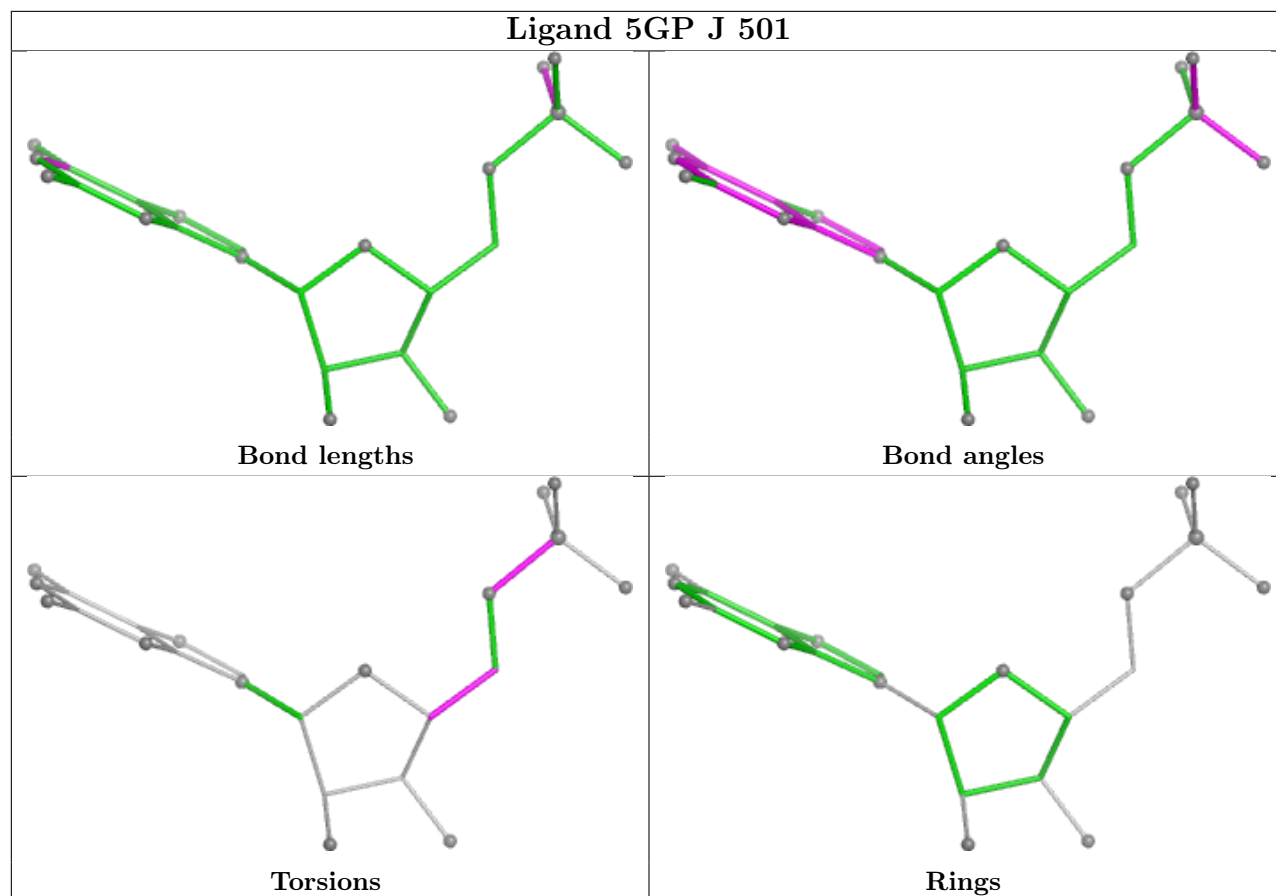
Ligand 5GP C 501



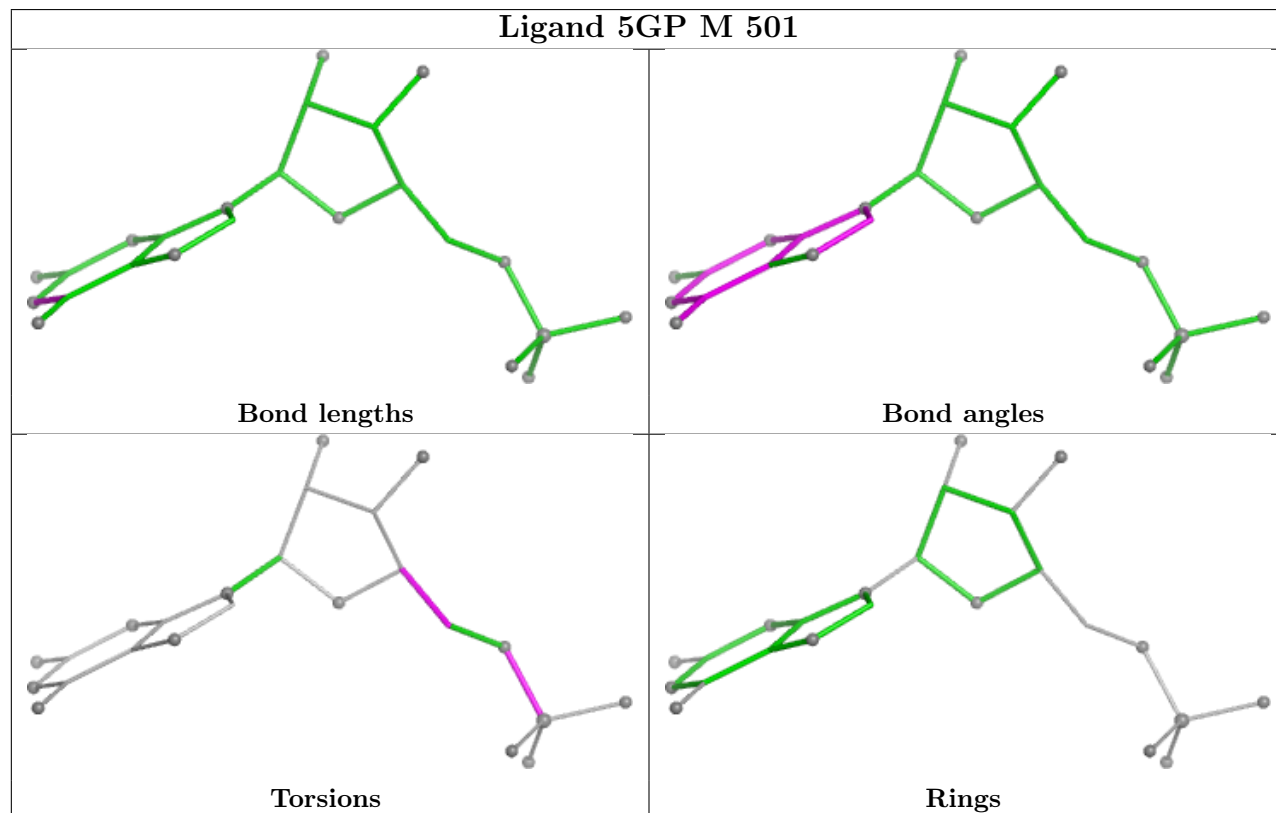
Ligand 5GP D 501

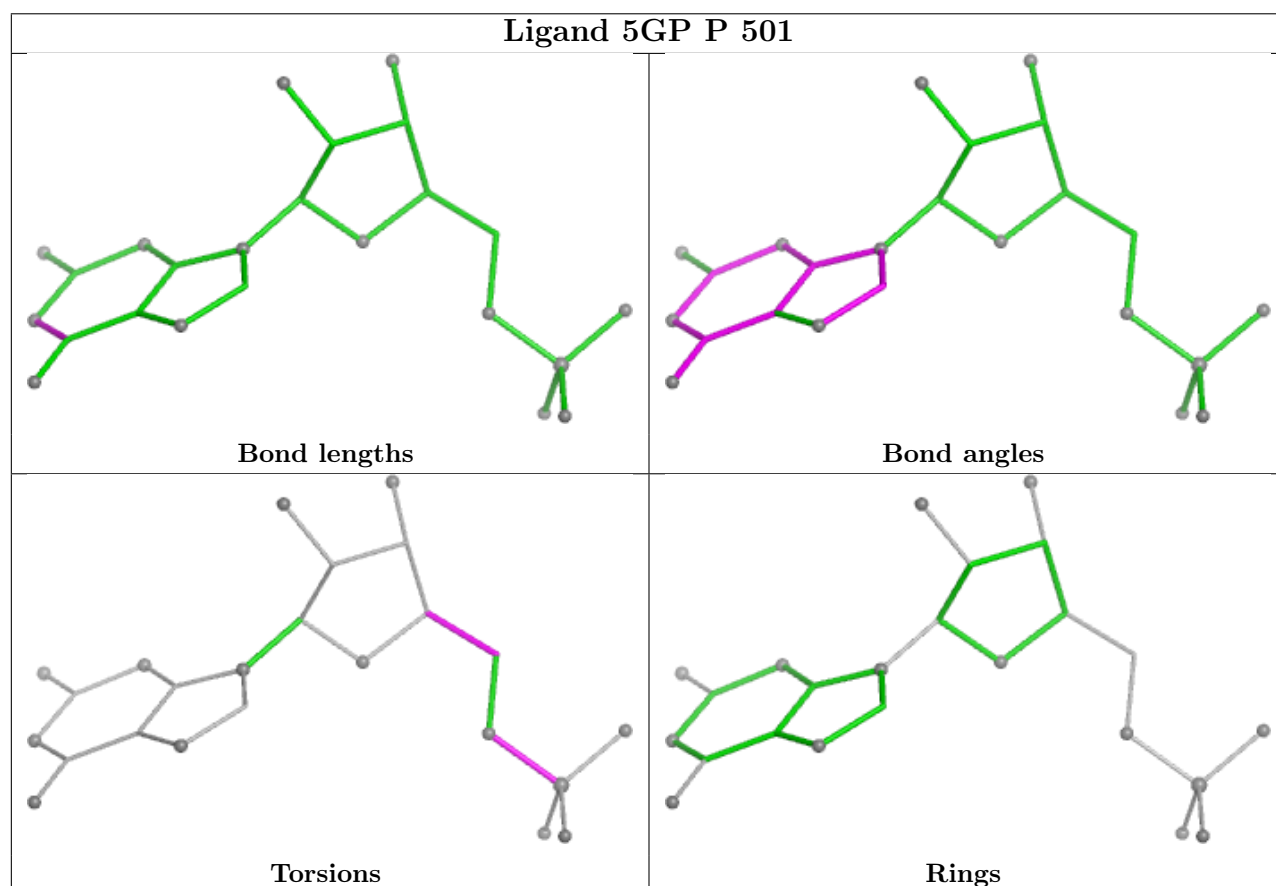
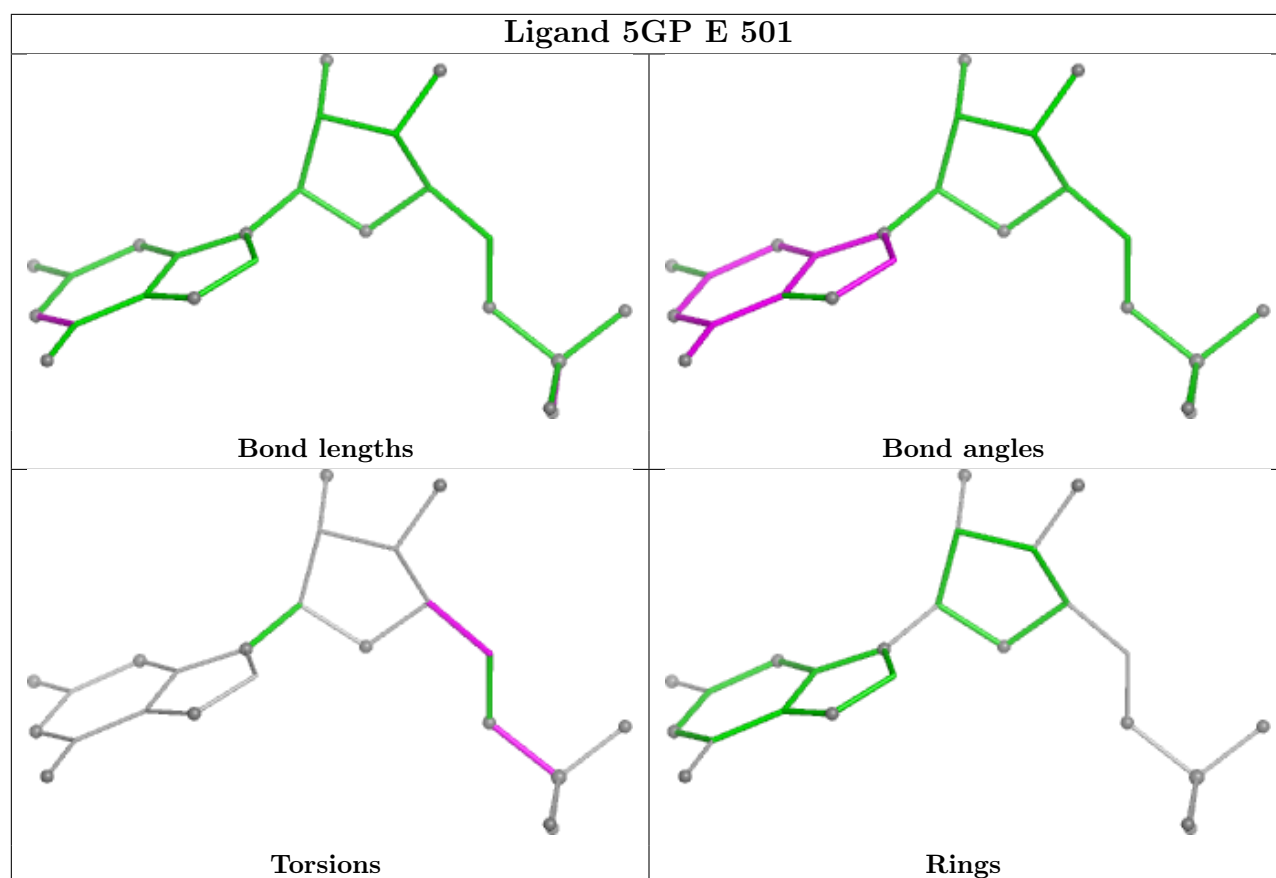


Ligand 5GP J 501

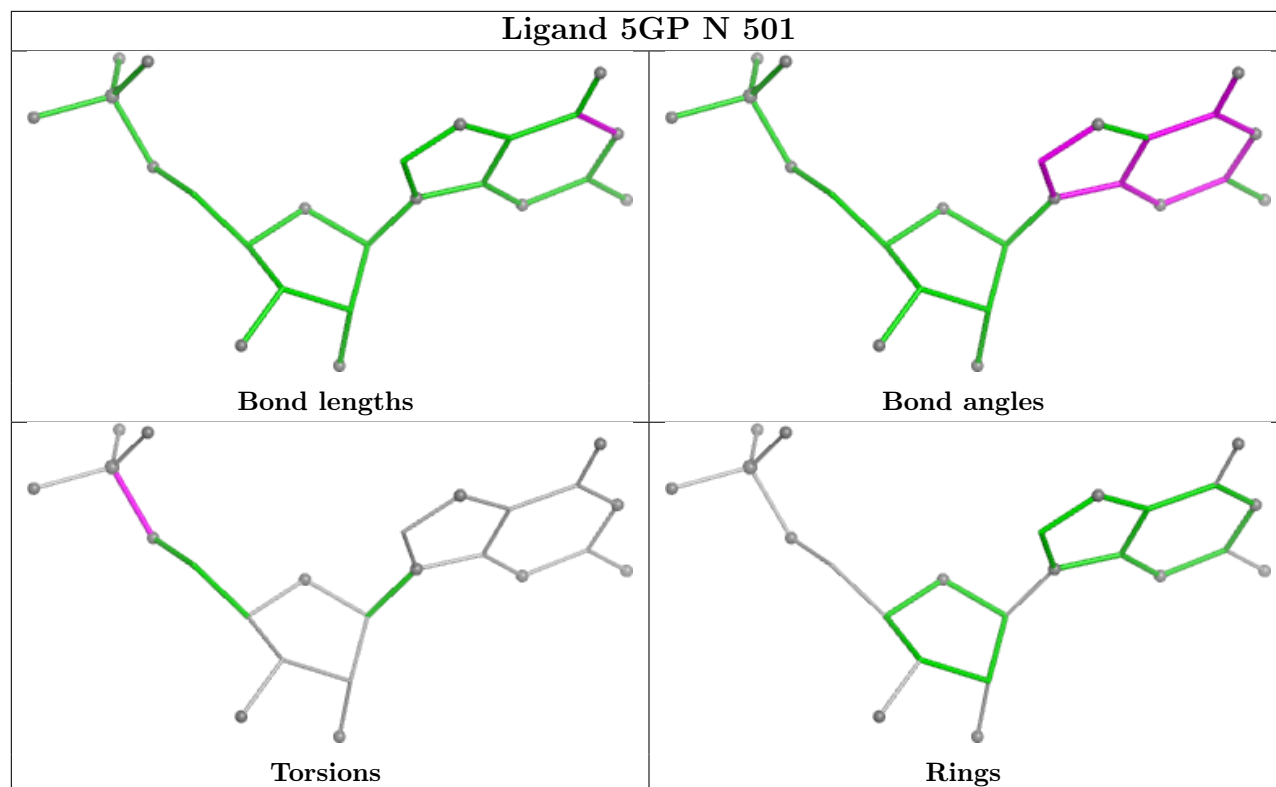


Ligand 5GP M 501

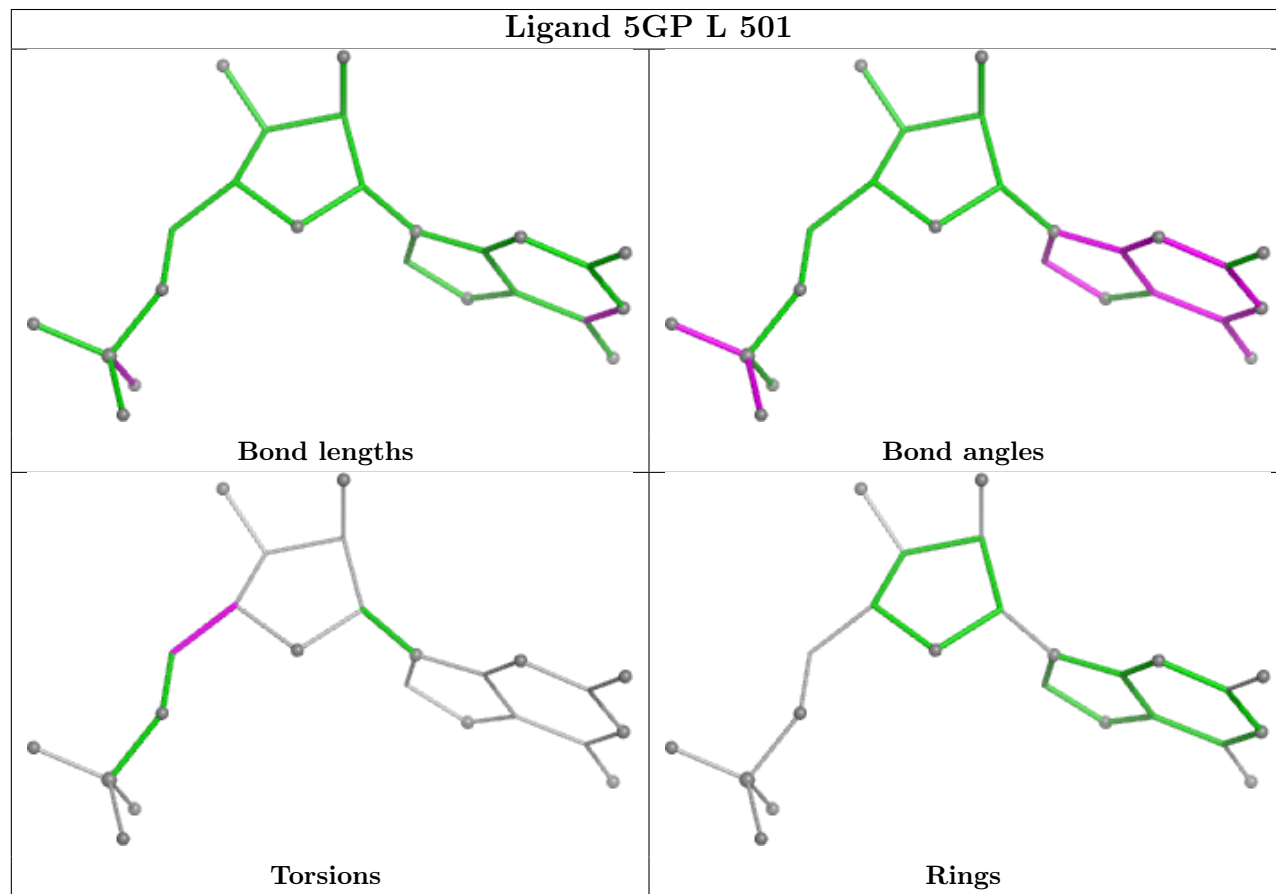




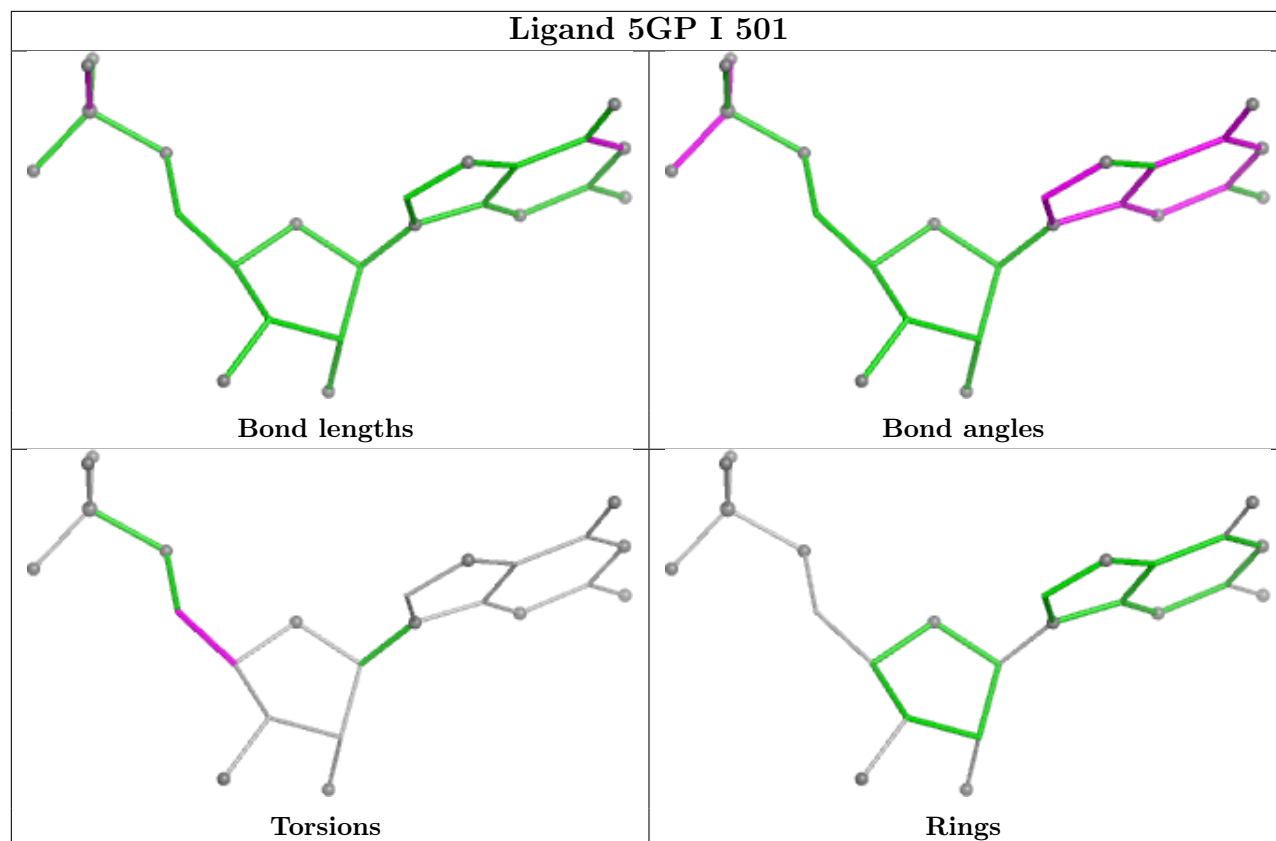
Ligand 5GP N 501



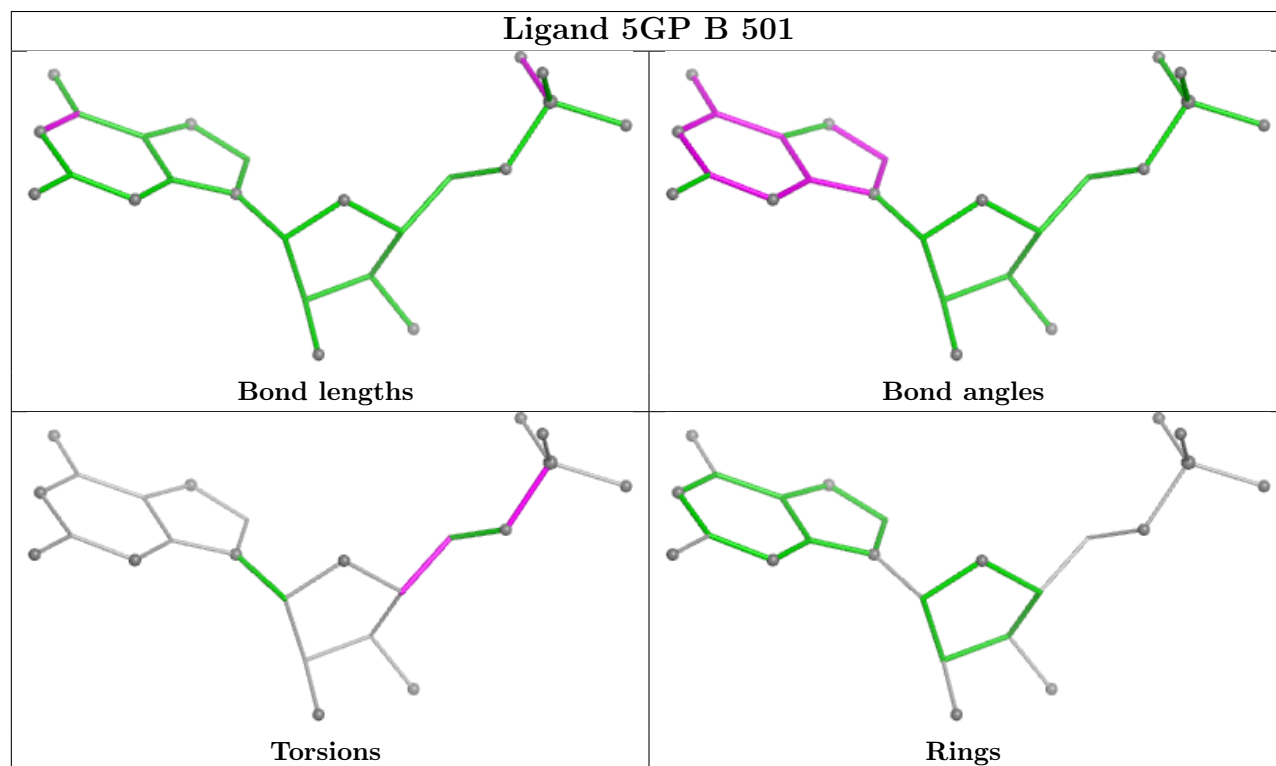
Ligand 5GP L 501

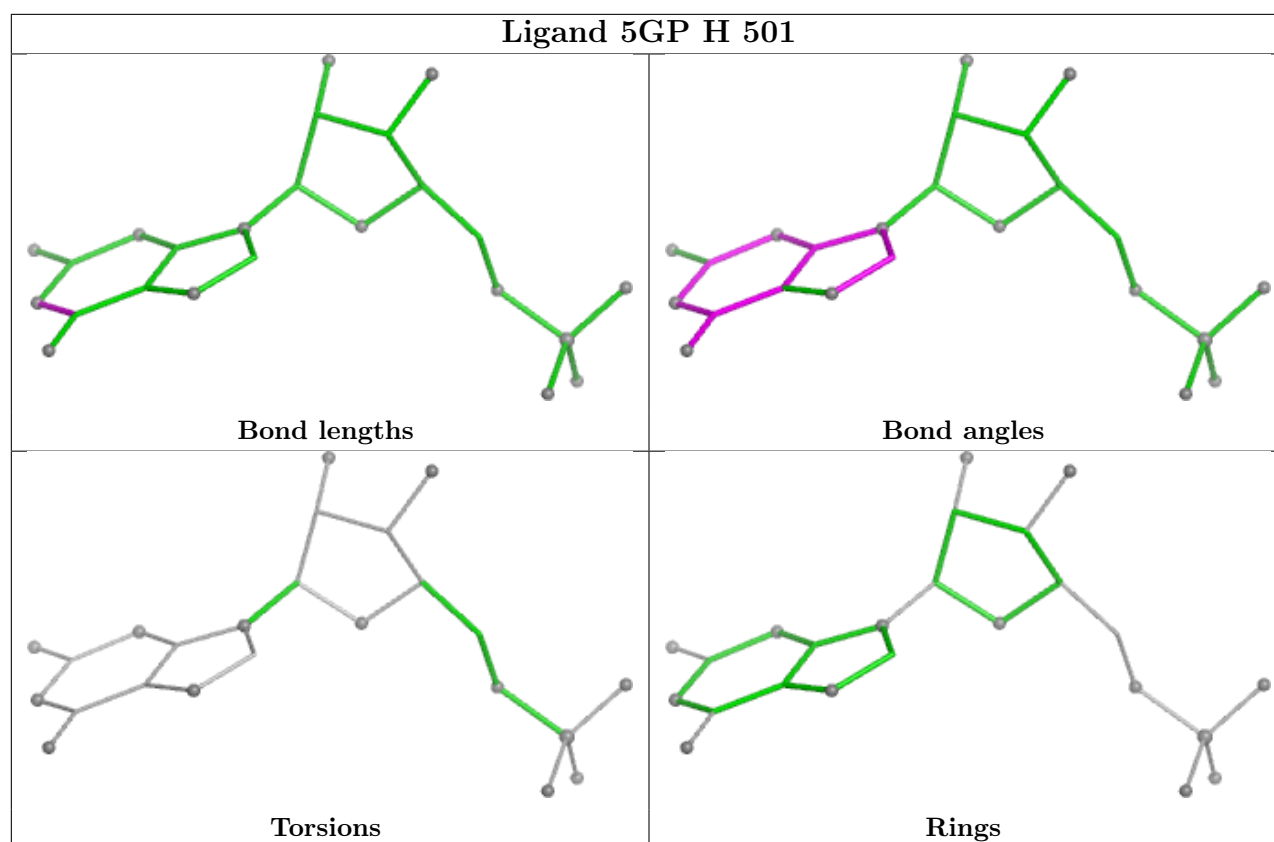


Ligand 5GP I 501



Ligand 5GP B 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	473/496 (95%)	0.79	32 (6%)	23	20	33, 47, 78, 105	0
1	B	447/496 (90%)	0.89	38 (8%)	16	14	38, 51, 83, 104	0
1	C	446/496 (89%)	0.81	22 (4%)	35	31	34, 53, 75, 95	0
1	D	468/496 (94%)	0.72	27 (5%)	29	25	35, 48, 64, 91	0
1	E	468/496 (94%)	0.88	24 (5%)	33	29	37, 55, 71, 91	0
1	F	440/496 (88%)	1.10	56 (12%)	8	6	42, 61, 90, 107	0
1	G	424/496 (85%)	1.23	55 (12%)	7	6	48, 68, 88, 103	0
1	H	468/496 (94%)	1.00	38 (8%)	18	15	39, 54, 77, 96	0
1	I	466/496 (93%)	1.00	40 (8%)	16	14	43, 57, 73, 98	1 (0%)
1	J	440/496 (88%)	1.15	53 (12%)	9	7	40, 61, 84, 97	1 (0%)
1	K	450/496 (90%)	1.04	52 (11%)	9	8	42, 56, 86, 103	0
1	L	465/496 (93%)	0.88	31 (6%)	24	21	40, 57, 77, 88	0
1	M	471/496 (94%)	0.87	37 (7%)	18	16	35, 53, 80, 94	0
1	N	461/496 (92%)	0.88	41 (8%)	15	13	33, 56, 79, 107	0
1	O	455/496 (91%)	0.91	42 (9%)	14	13	37, 55, 80, 95	0
1	P	465/496 (93%)	0.87	30 (6%)	25	22	39, 54, 73, 86	0
All	All	7307/7936 (92%)	0.94	618 (8%)	16	14	33, 56, 80, 107	2 (0%)

All (618) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	460	VAL	5.0
1	L	274	GLY	5.0
1	K	148	ALA	4.9
1	K	299	PRO	4.8
1	F	299	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	M	274	GLY	4.5
1	B	380	PRO	4.5
1	H	469	PHE	4.4
1	O	389	SER	4.4
1	L	152	ASP	4.3
1	N	114	ALA	4.3
1	H	274	GLY	4.2
1	K	151	ARG	4.2
1	E	274	GLY	4.2
1	G	123	ALA	4.2
1	H	468	GLY	4.1
1	P	470	ALA	4.0
1	K	425	ALA	4.0
1	F	274	GLY	4.0
1	G	415	ILE	3.9
1	G	380	PRO	3.9
1	O	415	ILE	3.9
1	M	476	PRO	3.8
1	G	165	THR	3.8
1	P	475	LEU	3.8
1	L	2	VAL	3.8
1	K	426	ARG	3.7
1	B	130	GLY	3.7
1	K	300	GLY	3.7
1	F	393	VAL	3.7
1	I	163	VAL	3.7
1	J	470	ALA	3.6
1	J	466	ALA	3.6
1	K	378	ASP	3.6
1	N	242	LEU	3.5
1	P	466	ALA	3.5
1	A	179	ILE	3.5
1	H	144	VAL	3.5
1	A	173	LEU	3.5
1	M	171	PHE	3.5
1	A	155	LEU	3.5
1	P	273	ALA	3.5
1	O	77	ASP	3.4
1	N	2	VAL	3.4
1	N	378	ASP	3.4
1	H	165	THR	3.4
1	J	265	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	386	GLY	3.4
1	I	296	GLY	3.4
1	D	29	ALA	3.4
1	K	393	VAL	3.3
1	L	410	LEU	3.3
1	C	435	HIS	3.3
1	J	376	ARG	3.3
1	M	158	PHE	3.3
1	E	152	ASP	3.3
1	B	386	GLY	3.3
1	N	274	GLY	3.3
1	B	311	VAL	3.3
1	B	190	THR	3.3
1	A	470	ALA	3.3
1	C	234	ALA	3.3
1	G	57	ALA	3.3
1	K	29	ALA	3.2
1	N	388	ALA	3.2
1	K	403	PHE	3.2
1	A	169	GLU	3.2
1	F	280	GLU	3.2
1	O	181	VAL	3.2
1	B	273	ALA	3.2
1	M	11	ALA	3.2
1	H	252	GLN	3.2
1	B	389	SER	3.2
1	M	135	LEU	3.2
1	F	415	ILE	3.2
1	K	360	SER	3.2
1	B	29	ALA	3.1
1	J	394	ALA	3.1
1	M	395	ALA	3.1
1	B	384	SER	3.1
1	D	416	SER	3.1
1	J	469	PHE	3.1
1	P	157	ASP	3.1
1	H	475	LEU	3.1
1	G	120	ALA	3.1
1	N	466	ALA	3.1
1	N	476	PRO	3.1
1	G	243	LEU	3.1
1	M	153	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	180	ASP	3.1
1	J	468	GLY	3.1
1	C	273	ALA	3.1
1	A	156	SER	3.1
1	C	359	GLY	3.1
1	J	465	SER	3.0
1	M	156	SER	3.0
1	M	154	ALA	3.0
1	P	467	ALA	3.0
1	O	469	PHE	3.0
1	C	52	ASN	3.0
1	J	297	VAL	3.0
1	L	153	ILE	3.0
1	A	176	HIS	3.0
1	F	360	SER	3.0
1	K	12	TYR	3.0
1	I	441	ARG	3.0
1	G	32	PHE	3.0
1	H	233	GLN	3.0
1	K	298	GLY	3.0
1	O	2	VAL	2.9
1	P	153	ILE	2.9
1	A	165	THR	2.9
1	F	304	THR	2.9
1	A	467	ALA	2.9
1	F	154	ALA	2.9
1	I	154	ALA	2.9
1	O	388	ALA	2.9
1	F	327	ARG	2.9
1	B	422	LEU	2.9
1	K	250	GLY	2.9
1	P	299	PRO	2.9
1	E	150	VAL	2.9
1	K	105	PRO	2.9
1	P	469	PHE	2.9
1	F	384	SER	2.9
1	G	122	GLY	2.9
1	G	126	VAL	2.9
1	L	339	VAL	2.9
1	A	192	ALA	2.9
1	B	139	ALA	2.9
1	G	29	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	128	PHE	2.9
1	M	189	GLY	2.9
1	J	245	ILE	2.8
1	A	159	VAL	2.8
1	I	28	VAL	2.8
1	J	160	THR	2.8
1	N	178	PRO	2.8
1	N	57	ALA	2.8
1	B	116	LEU	2.8
1	G	116	LEU	2.8
1	H	23	PRO	2.8
1	F	371	ASP	2.8
1	O	413	GLU	2.8
1	E	385	TYR	2.8
1	H	296	GLY	2.8
1	F	52	ASN	2.8
1	J	52	ASN	2.8
1	G	96	VAL	2.8
1	G	132	PRO	2.8
1	N	424	PRO	2.8
1	O	194	VAL	2.8
1	F	372	LEU	2.8
1	P	155	LEU	2.8
1	P	265	LEU	2.8
1	D	199	GLY	2.8
1	J	274	GLY	2.8
1	F	136	VAL	2.8
1	K	109	VAL	2.8
1	O	261	ALA	2.8
1	C	426	ARG	2.8
1	K	280	GLU	2.8
1	F	180	ASP	2.8
1	J	250	GLY	2.7
1	F	228	VAL	2.7
1	J	125	VAL	2.7
1	B	137	THR	2.7
1	K	377	ASP	2.7
1	A	153	ILE	2.7
1	O	299	PRO	2.7
1	A	127	VAL	2.7
1	B	109	VAL	2.7
1	G	125	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	127	VAL	2.7
1	K	108	SER	2.7
1	O	416	SER	2.7
1	G	256	LEU	2.7
1	L	155	LEU	2.7
1	J	221	ALA	2.7
1	N	176	HIS	2.7
1	M	152	ASP	2.7
1	N	377	ASP	2.7
1	P	180	ASP	2.7
1	P	188	ASP	2.7
1	D	472	GLY	2.7
1	I	125	VAL	2.7
1	I	126	VAL	2.7
1	K	429	VAL	2.7
1	O	109	VAL	2.7
1	F	57	ALA	2.7
1	G	306	ARG	2.7
1	L	240	ALA	2.7
1	P	419	ARG	2.7
1	A	274	GLY	2.7
1	F	476	PRO	2.7
1	D	410	LEU	2.7
1	G	72	VAL	2.7
1	H	297	VAL	2.7
1	K	244	VAL	2.7
1	F	385	TYR	2.7
1	E	11	ALA	2.7
1	J	467	ALA	2.7
1	M	161	ALA	2.7
1	N	117	HIS	2.7
1	L	77	ASP	2.6
1	F	289	GLY	2.6
1	C	133	ILE	2.6
1	D	115	LEU	2.6
1	G	78	LEU	2.6
1	C	139	ALA	2.6
1	F	406	ALA	2.6
1	G	112	ALA	2.6
1	K	38	THR	2.6
1	K	466	ALA	2.6
1	J	312	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	235	LEU	2.6
1	K	475	LEU	2.6
1	E	170	VAL	2.6
1	G	163	VAL	2.6
1	K	39	VAL	2.6
1	I	26	SER	2.6
1	J	238	ALA	2.6
1	M	124	ALA	2.6
1	O	123	ALA	2.6
1	I	332	HIS	2.6
1	I	435	HIS	2.6
1	J	180	ASP	2.6
1	K	423	ASP	2.6
1	O	300	GLY	2.6
1	K	380	PRO	2.6
1	M	105	PRO	2.6
1	A	128	PHE	2.6
1	M	413	GLU	2.6
1	G	136	VAL	2.6
1	K	388	ALA	2.6
1	N	123	ALA	2.6
1	J	176	HIS	2.6
1	O	15	THR	2.6
1	O	176	HIS	2.6
1	O	385	TYR	2.6
1	E	472	GLY	2.6
1	H	24	GLY	2.6
1	O	414	GLY	2.6
1	I	267	LEU	2.6
1	K	422	LEU	2.6
1	O	163	VAL	2.6
1	F	238	ALA	2.6
1	F	122	GLY	2.5
1	F	378	ASP	2.5
1	P	143	GLY	2.5
1	H	128	PHE	2.5
1	G	135	LEU	2.5
1	H	155	LEU	2.5
1	N	372	LEU	2.5
1	A	425	ALA	2.5
1	H	426	ARG	2.5
1	H	47	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	361	TRP	2.5
1	G	195	LEU	2.5
1	H	191	LEU	2.5
1	E	393	VAL	2.5
1	H	163	VAL	2.5
1	M	203	ALA	2.5
1	J	385	TYR	2.5
1	K	385	TYR	2.5
1	G	414	GLY	2.5
1	F	374	PHE	2.5
1	O	403	PHE	2.5
1	F	339	VAL	2.5
1	H	244	VAL	2.5
1	I	144	VAL	2.5
1	K	2	VAL	2.5
1	J	62	ALA	2.5
1	O	114	ALA	2.5
1	O	139	ALA	2.5
1	H	187	PRO	2.5
1	N	474	PRO	2.5
1	A	359	GLY	2.5
1	B	383	GLU	2.5
1	B	157	ASP	2.5
1	B	188	ASP	2.5
1	N	381	TYR	2.5
1	E	153	ILE	2.5
1	D	469	PHE	2.5
1	K	276	VAL	2.5
1	M	52	ASN	2.5
1	A	154	ALA	2.5
1	C	192	ALA	2.5
1	J	425	ALA	2.5
1	B	416	SER	2.5
1	G	416	SER	2.5
1	B	105	PRO	2.4
1	G	187	PRO	2.4
1	H	179	ILE	2.4
1	N	475	LEU	2.4
1	G	76	GLN	2.4
1	C	4	PHE	2.4
1	K	469	PHE	2.4
1	N	340	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	28	VAL	2.4
1	D	477	ALA	2.4
1	G	182	ALA	2.4
1	G	212	ALA	2.4
1	I	29	ALA	2.4
1	K	154	ALA	2.4
1	K	302	MET	2.4
1	L	120	ALA	2.4
1	O	477	ALA	2.4
1	B	299	PRO	2.4
1	F	77	ASP	2.4
1	J	292	ILE	2.4
1	F	381	TYR	2.4
1	J	74	LEU	2.4
1	D	147	PHE	2.4
1	F	163	VAL	2.4
1	K	297	VAL	2.4
1	N	244	VAL	2.4
1	B	57	ALA	2.4
1	M	138	GLU	2.4
1	N	386	GLY	2.4
1	M	103	LEU	2.4
1	O	135	LEU	2.4
1	E	426	ARG	2.4
1	F	31	ARG	2.4
1	L	473	HIS	2.4
1	L	147	PHE	2.4
1	D	159	VAL	2.4
1	F	297	VAL	2.4
1	G	97	VAL	2.4
1	I	276	VAL	2.4
1	K	163	VAL	2.4
1	L	275	ASN	2.4
1	G	466	ALA	2.4
1	I	401	SER	2.4
1	A	296	GLY	2.4
1	F	300	GLY	2.4
1	H	359	GLY	2.4
1	A	172	ASP	2.4
1	B	373	LEU	2.4
1	G	377	ASP	2.4
1	H	470	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	200	ALA	2.4
1	J	424	PRO	2.3
1	M	162	PRO	2.3
1	C	274	GLY	2.3
1	D	164	GLY	2.3
1	E	189	GLY	2.3
1	F	58	GLY	2.3
1	N	300	GLY	2.3
1	J	426	ARG	2.3
1	B	176	HIS	2.3
1	H	188	ASP	2.3
1	E	297	VAL	2.3
1	J	109	VAL	2.3
1	G	11	ALA	2.3
1	B	189	GLY	2.3
1	D	130	GLY	2.3
1	A	435	HIS	2.3
1	E	435	HIS	2.3
1	O	195	LEU	2.3
1	A	27	ASP	2.3
1	J	266	ASP	2.3
1	N	411	PHE	2.3
1	F	127	VAL	2.3
1	I	136	VAL	2.3
1	M	136	VAL	2.3
1	J	253	ALA	2.3
1	L	470	ALA	2.3
1	O	120	ALA	2.3
1	G	190	THR	2.3
1	I	54	THR	2.3
1	P	441	ARG	2.3
1	F	239	GLY	2.3
1	J	427	GLY	2.3
1	K	427	GLY	2.3
1	O	130	GLY	2.3
1	O	252	GLN	2.3
1	P	274	GLY	2.3
1	G	121	HIS	2.3
1	A	150	VAL	2.3
1	C	413	GLU	2.3
1	C	51	ALA	2.3
1	H	29	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	324	ALA	2.3
1	I	324	ALA	2.3
1	D	149	ARG	2.3
1	F	405	ARG	2.3
1	H	164	GLY	2.3
1	I	359	GLY	2.3
1	B	115	LEU	2.3
1	G	242	LEU	2.3
1	H	103	LEU	2.3
1	O	179	ILE	2.3
1	K	77	ASP	2.3
1	N	374	PHE	2.3
1	F	39	VAL	2.3
1	G	39	VAL	2.3
1	G	101	VAL	2.3
1	G	393	VAL	2.3
1	I	48	VAL	2.3
1	J	339	VAL	2.3
1	C	385	TYR	2.3
1	F	426	ARG	2.3
1	F	301	ALA	2.2
1	G	225	ASN	2.2
1	G	288	ALA	2.2
1	I	182	ALA	2.2
1	J	114	ALA	2.2
1	L	139	ALA	2.2
1	N	55	ALA	2.2
1	P	177	ALA	2.2
1	P	385	TYR	2.3
1	A	472	GLY	2.2
1	B	364	GLY	2.2
1	D	409	GLY	2.2
1	F	328	GLN	2.2
1	M	414	GLY	2.2
1	E	404	ASP	2.2
1	I	158	PHE	2.2
1	K	32	PHE	2.2
1	G	194	VAL	2.2
1	G	210	VAL	2.2
1	O	356	VAL	2.2
1	A	466	ALA	2.2
1	B	114	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	279	ALA	2.2
1	M	192	ALA	2.2
1	K	303	CYS	2.2
1	M	176	HIS	2.2
1	N	331	GLY	2.2
1	P	415	ILE	2.2
1	F	361	TRP	2.2
1	K	149	ARG	2.2
1	L	151	ARG	2.2
1	P	146	ARG	2.2
1	E	128	PHE	2.2
1	L	171	PHE	2.2
1	M	147	PHE	2.2
1	A	170	VAL	2.2
1	H	333	VAL	2.2
1	K	342	PRO	2.2
1	M	127	VAL	2.2
1	B	55	ALA	2.2
1	G	62	ALA	2.2
1	J	123	ALA	2.2
1	J	395	ALA	2.2
1	O	466	ALA	2.2
1	B	305	THR	2.2
1	D	417	THR	2.2
1	M	160	THR	2.2
1	C	115	LEU	2.2
1	H	189	GLY	2.2
1	J	115	LEU	2.2
1	J	189	GLY	2.2
1	L	271	LEU	2.2
1	I	436	ILE	2.2
1	J	80	ILE	2.2
1	M	415	ILE	2.2
1	E	416	SER	2.2
1	L	389	SER	2.2
1	I	404	ASP	2.2
1	B	158	PHE	2.2
1	L	403	PHE	2.2
1	D	163	VAL	2.2
1	I	150	VAL	2.2
1	G	273	ALA	2.2
1	H	273	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	55	ALA	2.2
1	O	51	ALA	2.2
1	O	230	ALA	2.2
1	I	385	TYR	2.2
1	N	198	THR	2.2
1	O	196	THR	2.2
1	A	143	GLY	2.2
1	C	422	LEU	2.2
1	J	285	LEU	2.2
1	N	103	LEU	2.2
1	N	135	LEU	2.2
1	J	358	ILE	2.2
1	O	156	SER	2.2
1	A	180	ASP	2.2
1	E	413	GLU	2.2
1	K	152	ASP	2.2
1	J	327	ARG	2.2
1	A	393	VAL	2.1
1	J	194	VAL	2.1
1	M	101	VAL	2.1
1	F	53	MET	2.1
1	H	464	GLN	2.1
1	I	212	ALA	2.1
1	J	353	ALA	2.1
1	L	57	ALA	2.1
1	L	123	ALA	2.1
1	O	57	ALA	2.1
1	C	305	THR	2.1
1	F	115	LEU	2.1
1	I	102	THR	2.1
1	M	130	GLY	2.1
1	M	155	LEU	2.1
1	N	359	GLY	2.1
1	G	292	ILE	2.1
1	B	327	ARG	2.1
1	G	412	GLU	2.1
1	N	156	SER	2.1
1	P	340	ARG	2.1
1	I	27	ASP	2.1
1	I	128	PHE	2.1
1	L	109	VAL	2.1
1	N	53	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	238	ALA	2.1
1	A	386	GLY	2.1
1	E	122	GLY	2.1
1	F	155	LEU	2.1
1	H	472	GLY	2.1
1	I	58	GLY	2.1
1	I	195	LEU	2.1
1	K	338	GLY	2.1
1	P	282	THR	2.1
1	D	153	ILE	2.1
1	H	292	ILE	2.1
1	I	205	ILE	2.1
1	F	6	ASP	2.1
1	K	404	ASP	2.1
1	L	371	ASP	2.1
1	B	403	PHE	2.1
1	D	393	VAL	2.1
1	G	244	VAL	2.1
1	J	48	VAL	2.1
1	M	183	VAL	2.1
1	P	276	VAL	2.1
1	G	177	ALA	2.1
1	H	219	ALA	2.1
1	L	154	ALA	2.1
1	L	466	ALA	2.1
1	M	323	ALA	2.1
1	P	82	ALA	2.1
1	A	309	THR	2.1
1	C	414	GLY	2.1
1	F	7	GLY	2.1
1	K	373	LEU	2.1
1	L	78	LEU	2.1
1	L	164	GLY	2.1
1	N	122	GLY	2.1
1	B	376	ARG	2.1
1	N	419	ARG	2.1
1	F	358	ILE	2.1
1	D	141	CYS	2.1
1	E	384	SER	2.1
1	L	402	SER	2.1
1	L	380	PRO	2.1
1	N	380	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	362	PHE	2.1
1	J	222	VAL	2.1
1	P	56	VAL	2.1
1	C	29	ALA	2.1
1	F	103	LEU	2.1
1	M	475	LEU	2.1
1	P	140	ASN	2.1
1	D	414	GLY	2.1
1	G	274	GLY	2.1
1	I	352	GLY	2.1
1	O	298	GLY	2.1
1	O	386	GLY	2.1
1	C	383	GLU	2.1
1	E	383	GLU	2.1
1	I	417	THR	2.1
1	J	282	THR	2.1
1	H	245	ILE	2.1
1	E	12	TYR	2.1
1	G	404	ASP	2.1
1	L	180	ASP	2.1
1	K	110	SER	2.1
1	N	389	SER	2.1
1	P	132	PRO	2.1
1	D	171	PHE	2.0
1	F	32	PHE	2.0
1	O	136	VAL	2.0
1	C	419	ARG	2.0
1	E	149	ARG	2.0
1	H	406	ALA	2.0
1	J	57	ALA	2.0
1	J	273	ALA	2.0
1	N	240	ALA	2.0
1	D	106	GLU	2.0
1	F	133	ILE	2.0
1	B	371	ASP	2.0
1	M	6	ASP	2.0
1	O	100	PRO	2.0
1	O	178	PRO	2.0
1	D	251	HIS	2.0
1	A	194	VAL	2.0
1	B	65	VAL	2.0
1	C	374	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	150	VAL	2.0
1	E	277	VAL	2.0
1	H	460	VAL	2.0
1	K	339	VAL	2.0
1	N	158	PHE	2.0
1	B	372	LEU	2.0
1	B	388	ALA	2.0
1	E	329	LEU	2.0
1	F	346	ALA	2.0
1	I	351	ALA	2.0
1	K	106	GLU	2.0
1	N	116	LEU	2.0
1	B	274	GLY	2.0
1	F	472	GLY	2.0
1	I	130	GLY	2.0
1	N	70	GLY	2.0
1	G	245	ILE	2.0
1	I	133	ILE	2.0
1	P	54	THR	2.0
1	P	137	THR	2.0
1	D	308	MET	2.0
1	F	10	PRO	2.0
1	K	53	MET	2.0
1	D	385	TYR	2.0
1	F	251	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

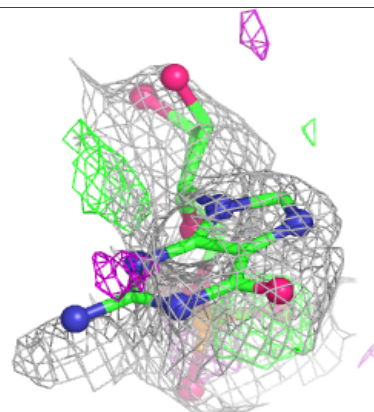
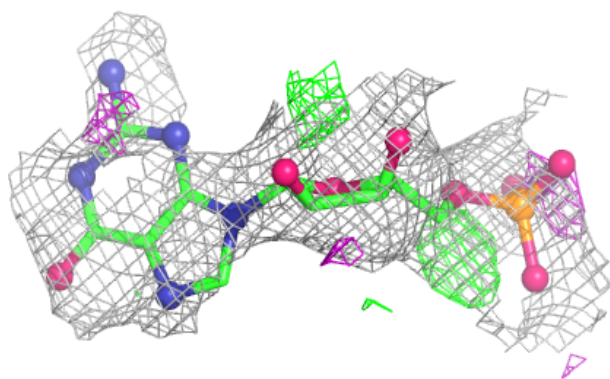
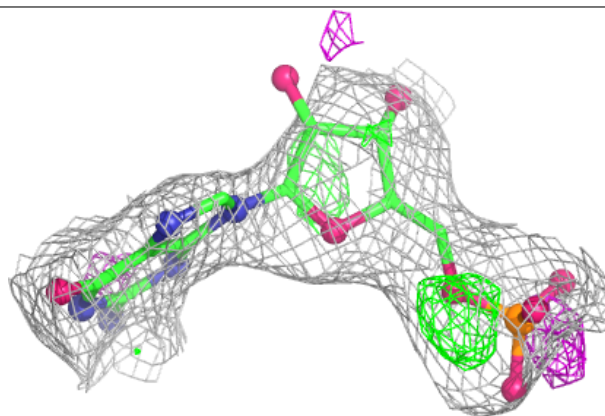
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	5GP	F	501	24/24	0.67	0.17	61,79,87,92	0
2	5GP	G	501	24/24	0.76	0.14	56,68,76,80	0
2	5GP	I	501	24/24	0.82	0.12	41,56,62,67	0
2	5GP	K	501	24/24	0.83	0.13	53,66,82,85	0
2	5GP	A	501	24/24	0.86	0.13	34,48,53,54	0
2	5GP	C	501	24/24	0.86	0.11	43,50,57,64	0
2	5GP	N	501	24/24	0.87	0.11	45,56,65,69	0
2	5GP	M	501	24/24	0.88	0.11	38,46,54,59	0
2	5GP	P	501	24/24	0.88	0.12	47,53,60,64	0
2	5GP	L	501	24/24	0.89	0.11	44,59,66,68	0
2	5GP	J	501	24/24	0.89	0.10	46,53,61,62	0
2	5GP	D	501	24/24	0.90	0.11	34,43,49,58	0
2	5GP	O	501	24/24	0.91	0.09	41,54,62,66	0
2	5GP	H	501	24/24	0.91	0.11	37,50,54,59	0
2	5GP	E	501	24/24	0.92	0.10	28,48,55,64	0
2	5GP	B	501	24/24	0.92	0.10	38,55,64,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

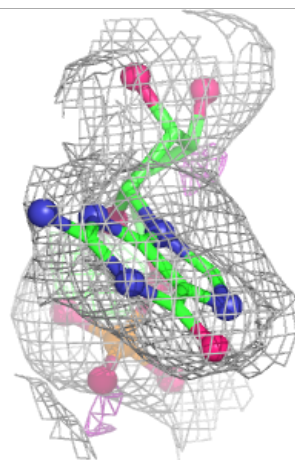
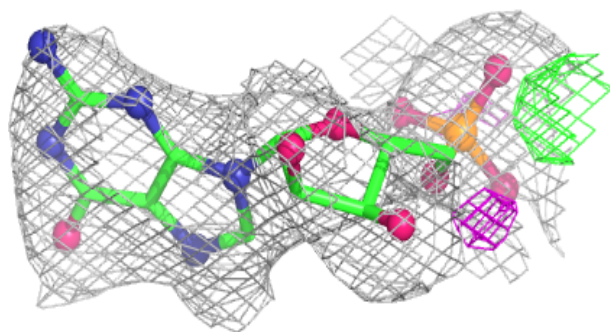
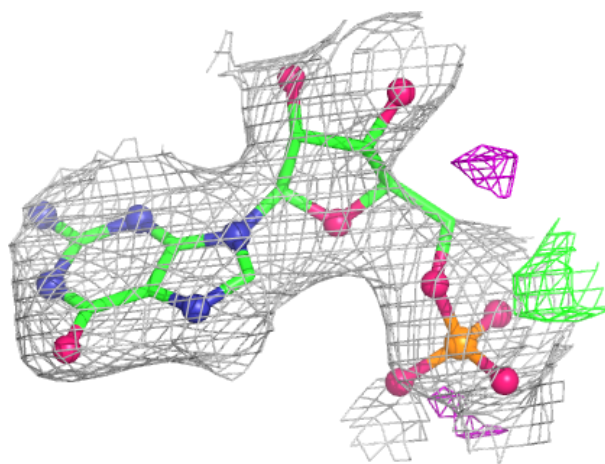
Electron density around 5GP F 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



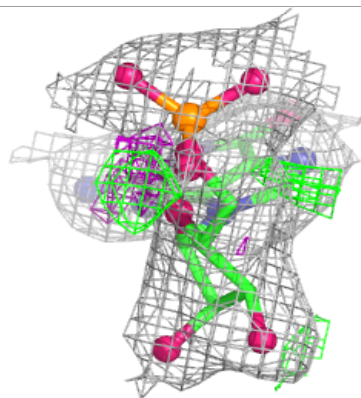
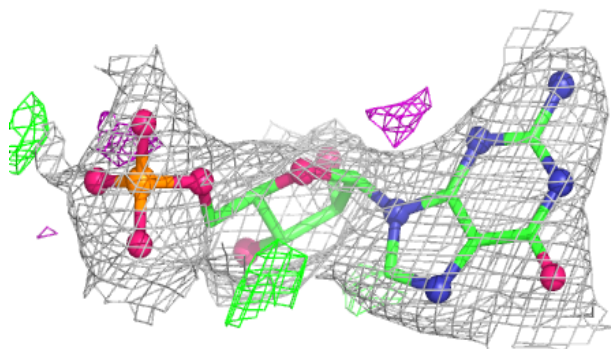
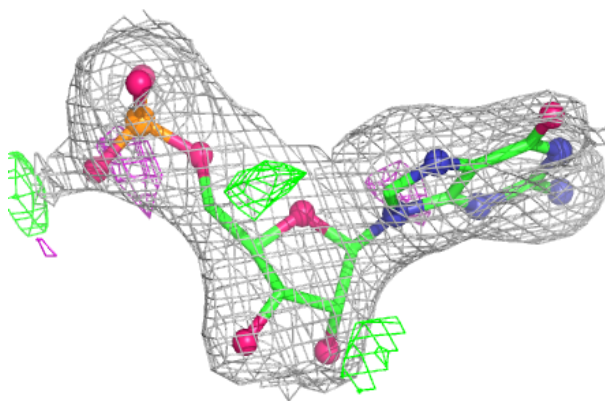
Electron density around 5GP G 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

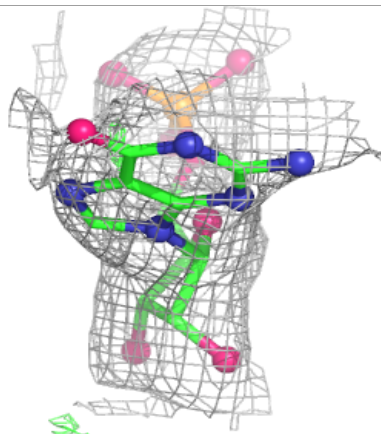
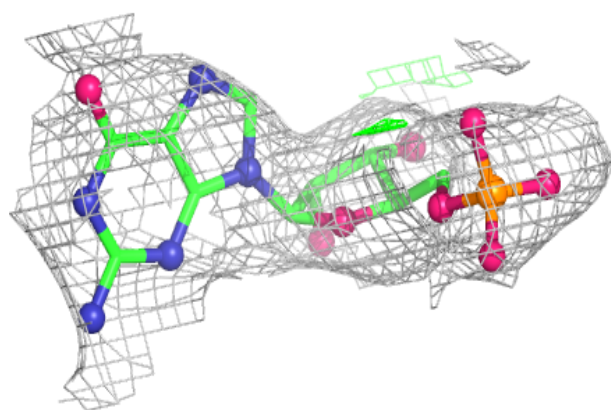
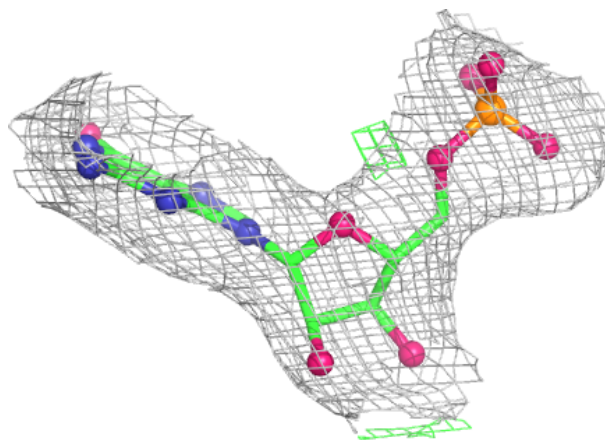


Electron density around 5GP I 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

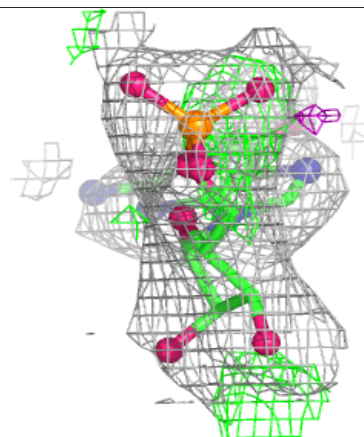
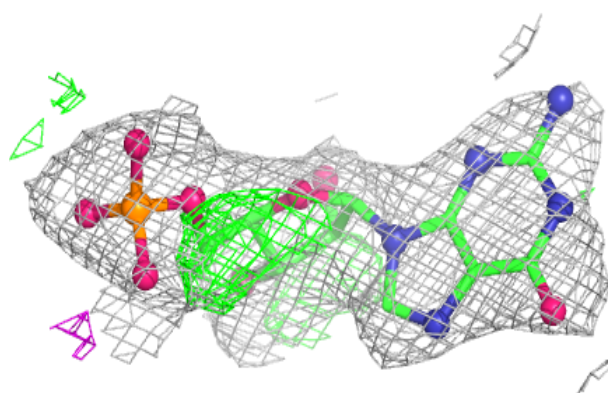
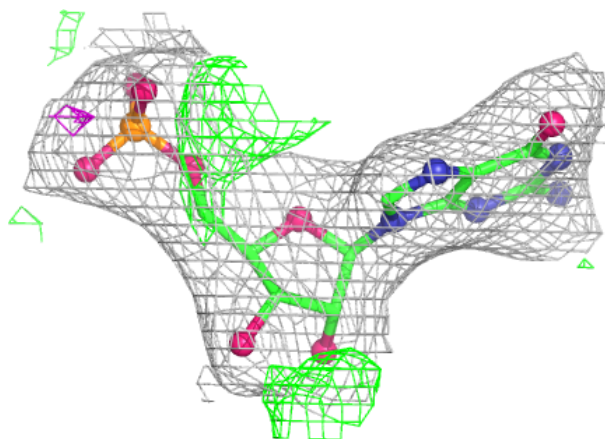
**Electron density around 5GP K 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



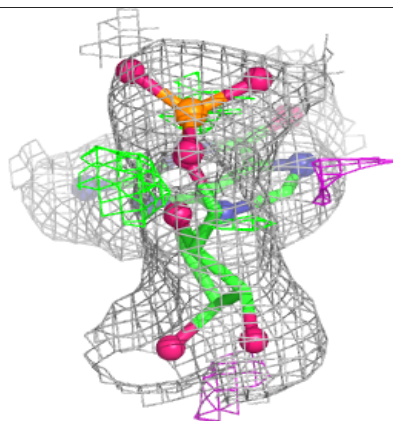
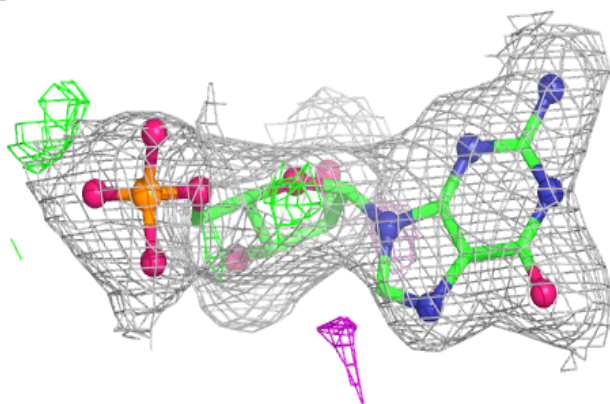
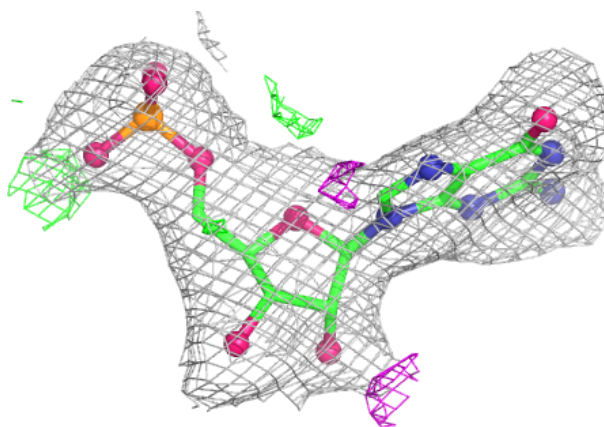
Electron density around 5GP A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

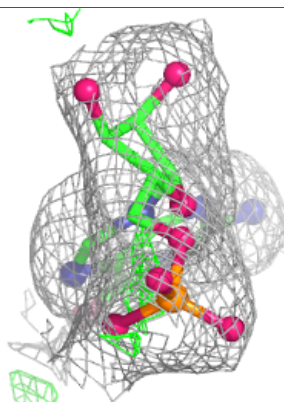
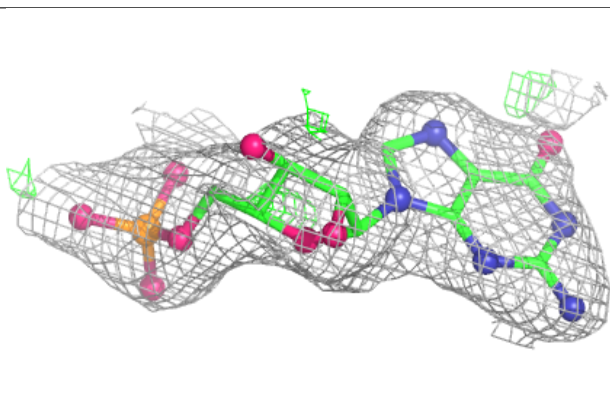
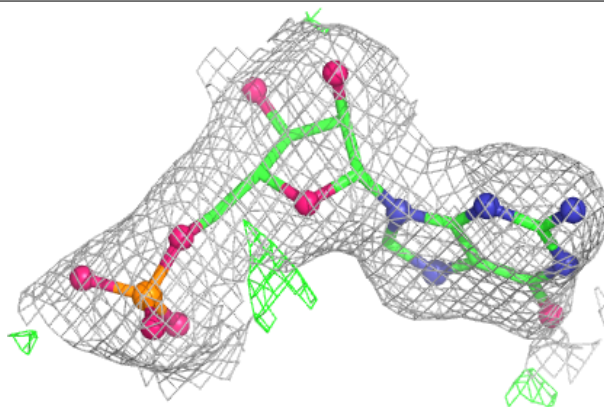


Electron density around 5GP C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

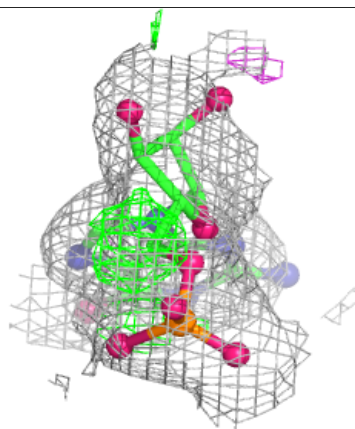
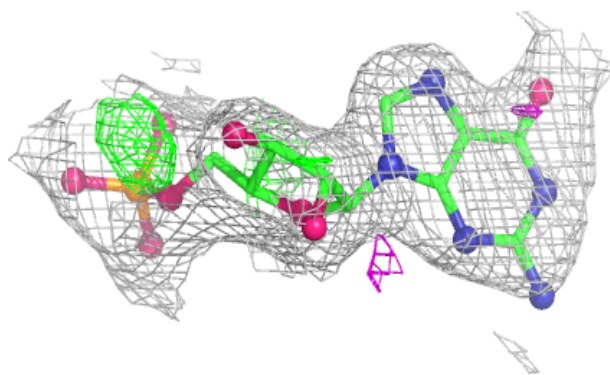
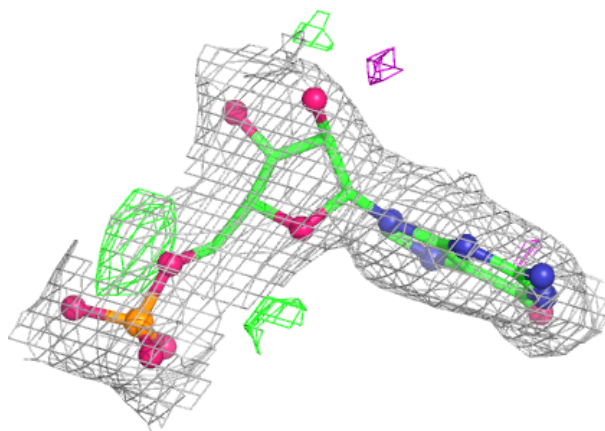
**Electron density around 5GP N 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



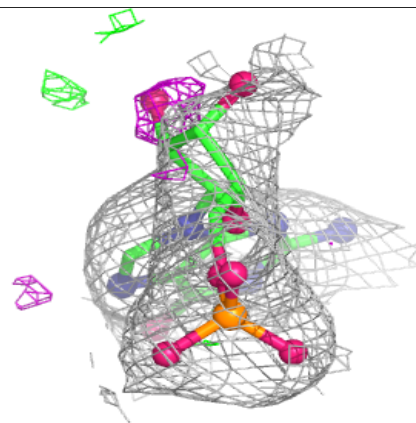
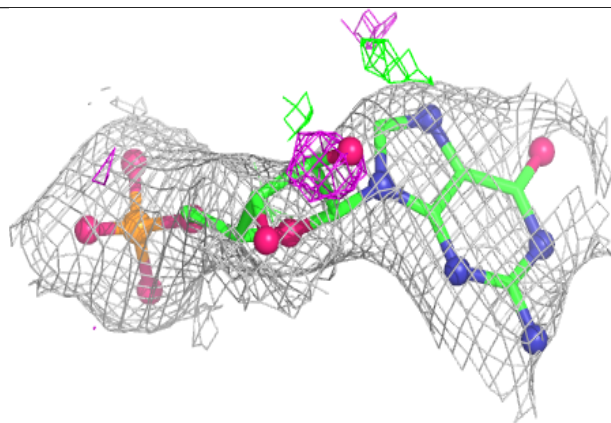
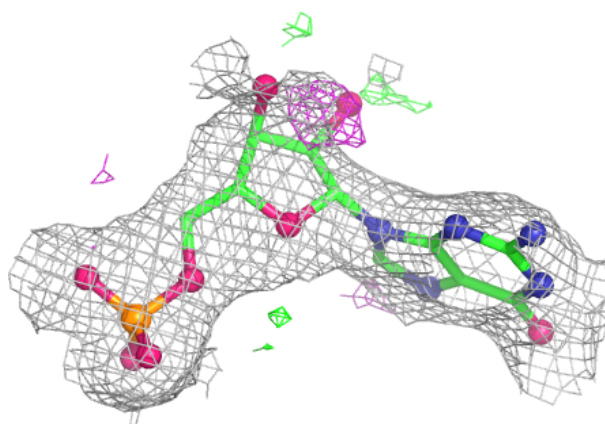
Electron density around 5GP M 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



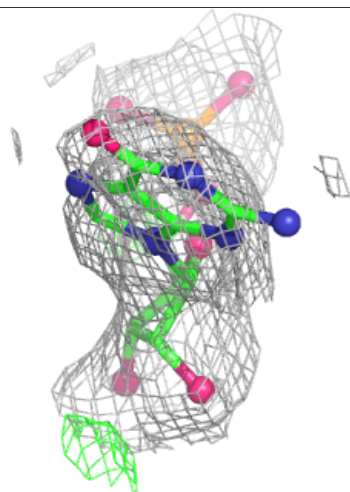
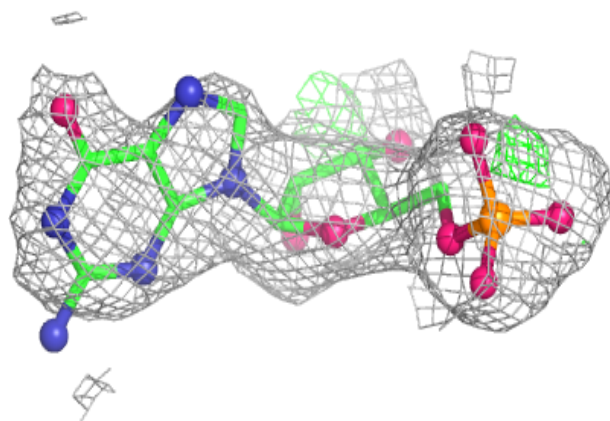
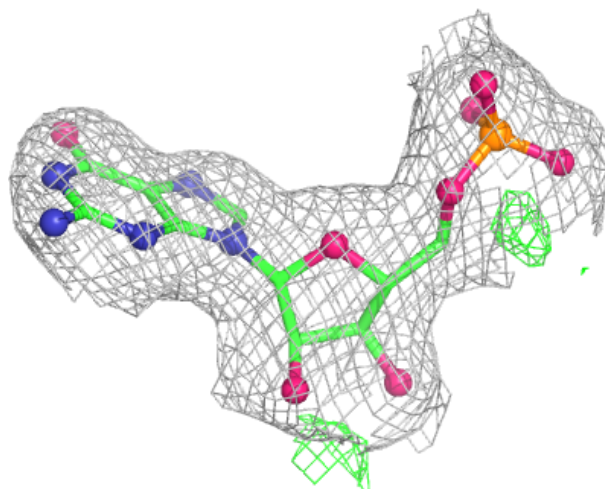
Electron density around 5GP P 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



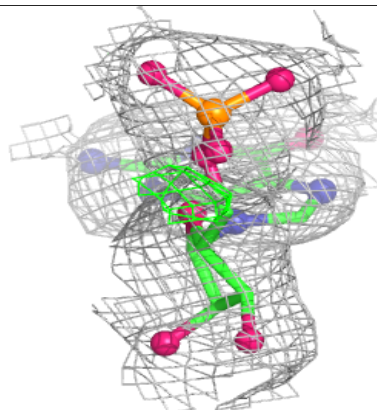
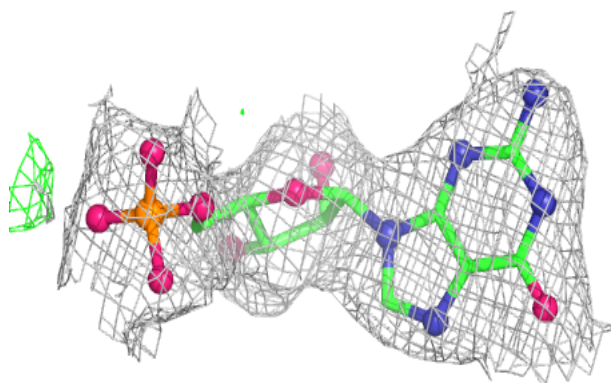
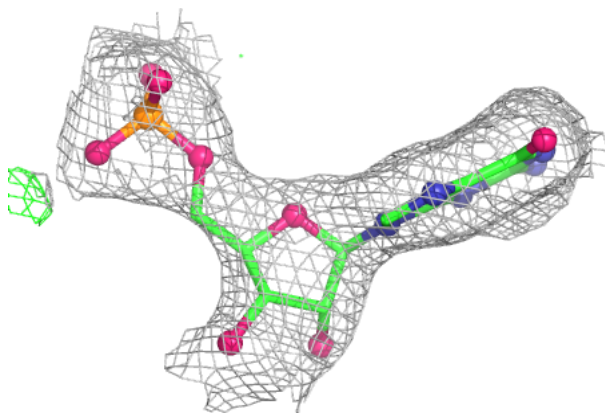
Electron density around 5GP L 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

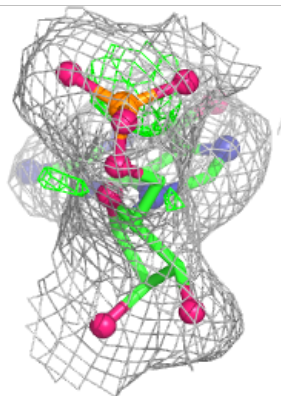
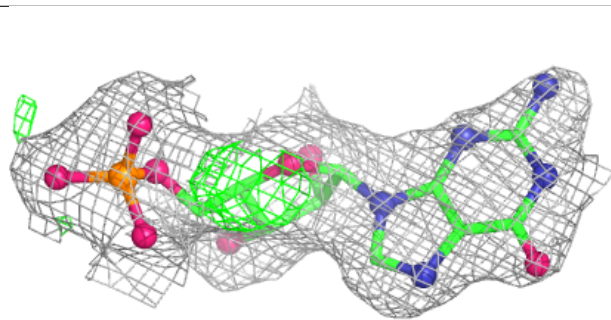
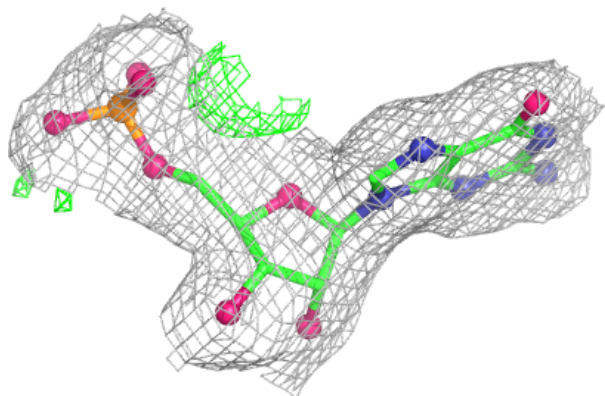


Electron density around 5GP J 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

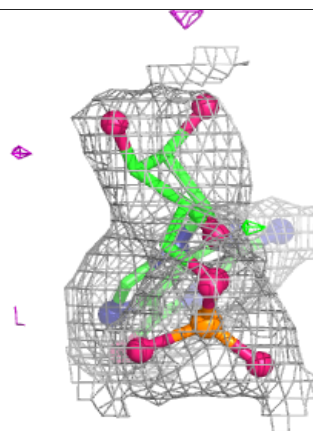
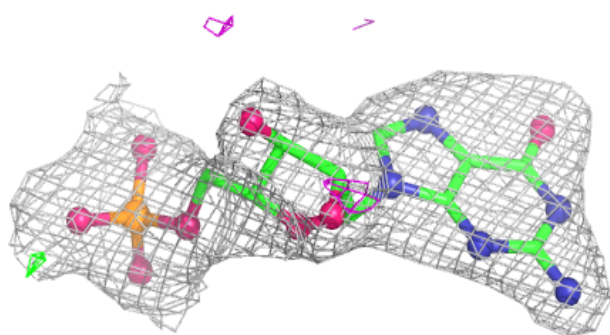
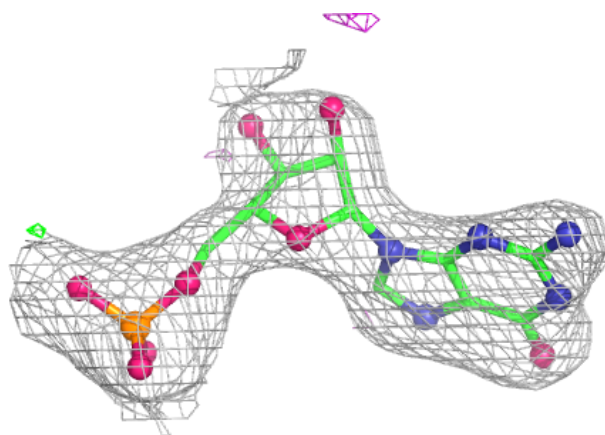
**Electron density around 5GP D 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



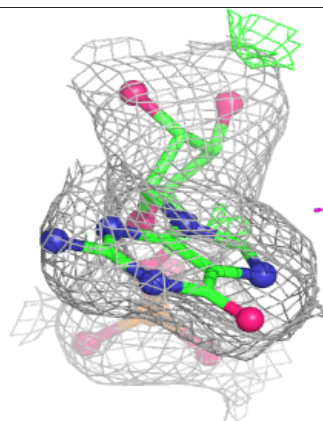
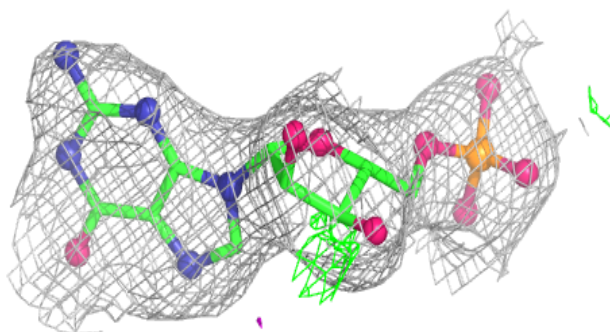
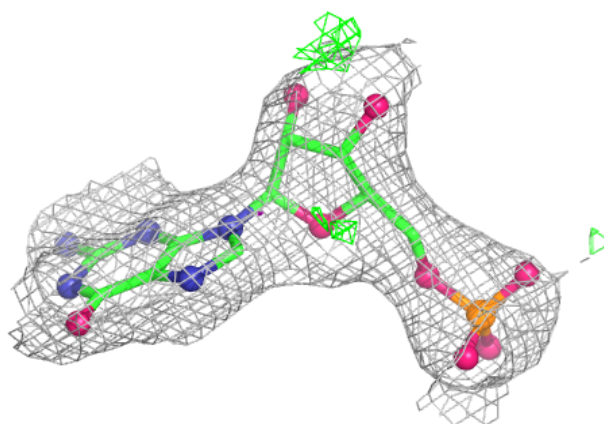
Electron density around 5GP O 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

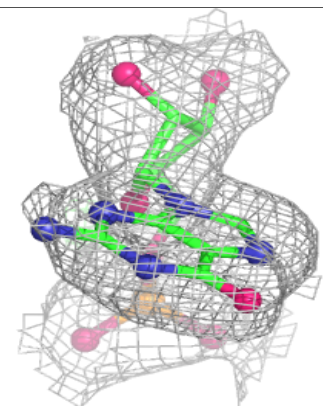
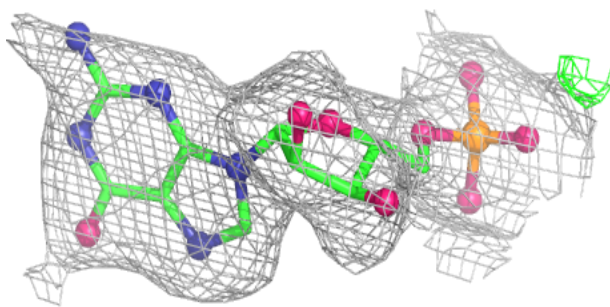
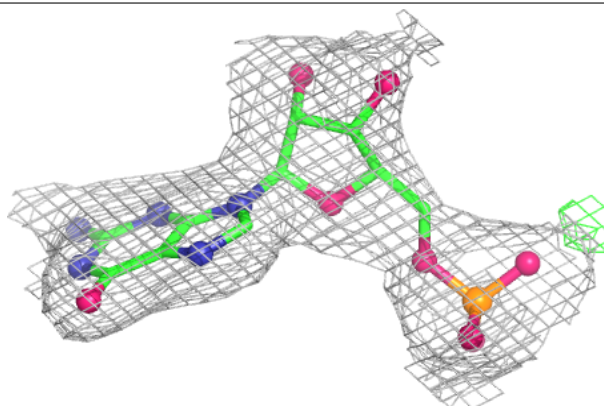


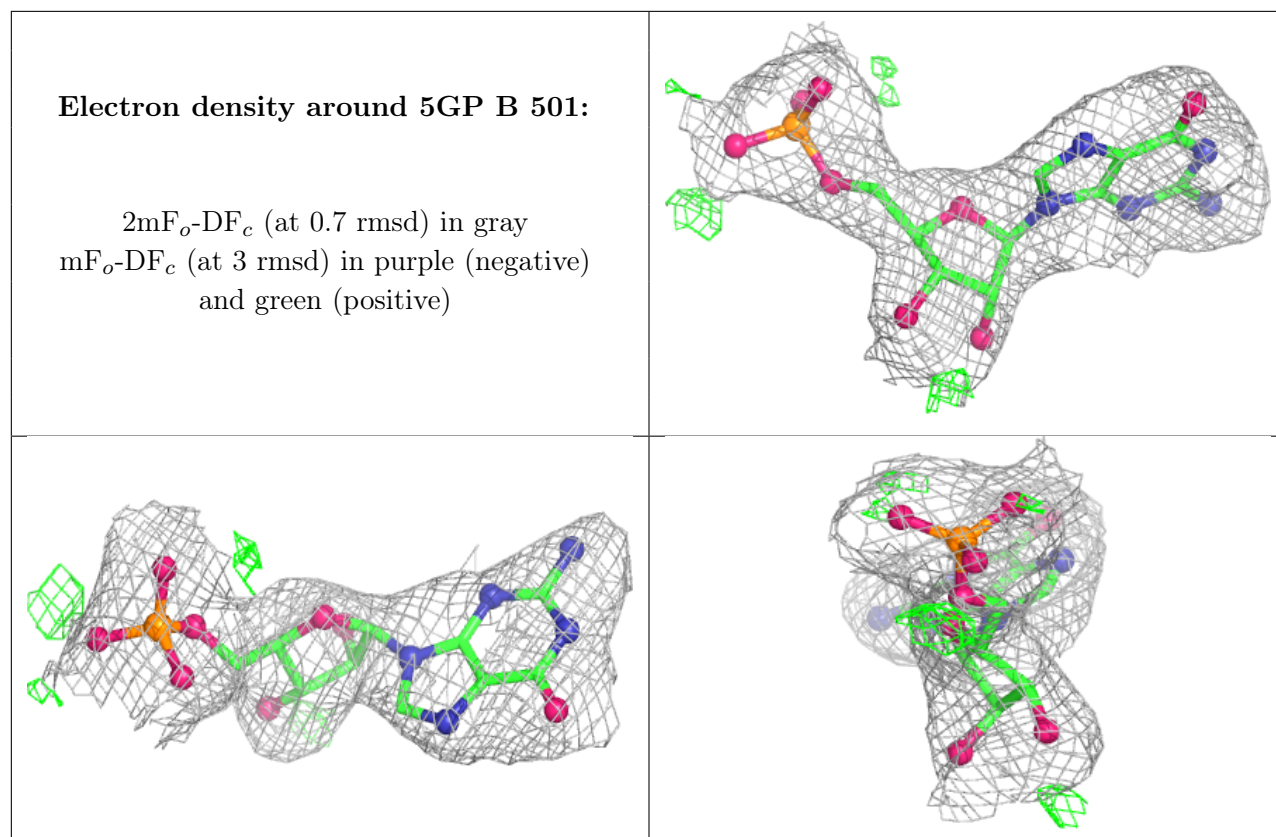
Electron density around 5GP H 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 5GP E 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.