



Full wwPDB X-ray Structure Validation Report i

Apr 20, 2022 – 10:16 am BST

PDB ID : 7R50
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 i symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

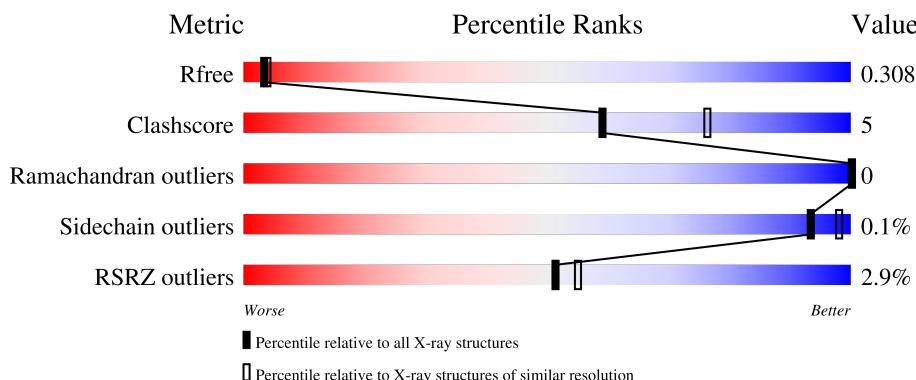
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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.



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Mol	Chain	Length	Quality of chain			
1	F	496	4%	74%	14%	11%
1	G	496	7%	74%	11%	15%
1	H	496	2%	82%	12%	6%
1	I	496	3%	83%	11%	6%
1	J	496	3%	76%	12%	11%
1	K	496	4%	79%	12%	9%
1	L	496	1%	83%	11%	6%
1	M	496	3%	85%	9%	5%
1	N	496	4%	85%	8%	7%
1	O	496	2%	81%	11%	8%
1	P	496	1%	81%	12%	6%

2 Entry composition i

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 Inosine-5-monophosphate dehydrogenase guaB1.

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

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	-	insertion	UNP I7GA39
A	480	THR	-	expression tag	UNP I7GA39
A	481	ALA	-	expression tag	UNP I7GA39
A	482	ALA	-	expression tag	UNP I7GA39
A	483	ALA	-	expression tag	UNP I7GA39
A	484	LYS	-	expression tag	UNP I7GA39
A	485	GLU	-	expression tag	UNP I7GA39
A	486	ASP	-	expression tag	UNP I7GA39
A	487	LEU	-	expression tag	UNP I7GA39
A	488	GLU	-	expression tag	UNP I7GA39
A	489	HIS	-	expression tag	UNP I7GA39
A	490	HIS	-	expression tag	UNP I7GA39
A	491	HIS	-	expression tag	UNP I7GA39
A	492	HIS	-	expression tag	UNP I7GA39
A	493	HIS	-	expression tag	UNP I7GA39
A	494	HIS	-	expression tag	UNP I7GA39
A	495	HIS	-	expression tag	UNP I7GA39
A	496	HIS	-	expression tag	UNP I7GA39
B	2	VAL	-	insertion	UNP I7GA39
B	480	THR	-	expression tag	UNP I7GA39
B	481	ALA	-	expression tag	UNP I7GA39
B	482	ALA	-	expression tag	UNP I7GA39
B	483	ALA	-	expression tag	UNP I7GA39
B	484	LYS	-	expression tag	UNP I7GA39
B	485	GLU	-	expression tag	UNP I7GA39
B	486	ASP	-	expression tag	UNP I7GA39
B	487	LEU	-	expression tag	UNP I7GA39
B	488	GLU	-	expression tag	UNP I7GA39
B	489	HIS	-	expression tag	UNP I7GA39
B	490	HIS	-	expression tag	UNP I7GA39
B	491	HIS	-	expression tag	UNP I7GA39
B	492	HIS	-	expression tag	UNP I7GA39
B	493	HIS	-	expression tag	UNP I7GA39
B	494	HIS	-	expression tag	UNP I7GA39
B	495	HIS	-	expression tag	UNP I7GA39
B	496	HIS	-	expression tag	UNP I7GA39
C	2	VAL	-	insertion	UNP I7GA39
C	480	THR	-	expression tag	UNP I7GA39
C	481	ALA	-	expression tag	UNP I7GA39
C	482	ALA	-	expression tag	UNP I7GA39
C	483	ALA	-	expression tag	UNP I7GA39
C	484	LYS	-	expression tag	UNP I7GA39

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Chain	Residue	Modelled	Actual	Comment	Reference
C	485	GLU	-	expression tag	UNP I7GA39
C	486	ASP	-	expression tag	UNP I7GA39
C	487	LEU	-	expression tag	UNP I7GA39
C	488	GLU	-	expression tag	UNP I7GA39
C	489	HIS	-	expression tag	UNP I7GA39
C	490	HIS	-	expression tag	UNP I7GA39
C	491	HIS	-	expression tag	UNP I7GA39
C	492	HIS	-	expression tag	UNP I7GA39
C	493	HIS	-	expression tag	UNP I7GA39
C	494	HIS	-	expression tag	UNP I7GA39
C	495	HIS	-	expression tag	UNP I7GA39
C	496	HIS	-	expression tag	UNP I7GA39
D	2	VAL	-	insertion	UNP I7GA39
D	480	THR	-	expression tag	UNP I7GA39
D	481	ALA	-	expression tag	UNP I7GA39
D	482	ALA	-	expression tag	UNP I7GA39
D	483	ALA	-	expression tag	UNP I7GA39
D	484	LYS	-	expression tag	UNP I7GA39
D	485	GLU	-	expression tag	UNP I7GA39
D	486	ASP	-	expression tag	UNP I7GA39
D	487	LEU	-	expression tag	UNP I7GA39
D	488	GLU	-	expression tag	UNP I7GA39
D	489	HIS	-	expression tag	UNP I7GA39
D	490	HIS	-	expression tag	UNP I7GA39
D	491	HIS	-	expression tag	UNP I7GA39
D	492	HIS	-	expression tag	UNP I7GA39
D	493	HIS	-	expression tag	UNP I7GA39
D	494	HIS	-	expression tag	UNP I7GA39
D	495	HIS	-	expression tag	UNP I7GA39
D	496	HIS	-	expression tag	UNP I7GA39
E	2	VAL	-	insertion	UNP I7GA39
E	480	THR	-	expression tag	UNP I7GA39
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E	482	ALA	-	expression tag	UNP I7GA39
E	483	ALA	-	expression tag	UNP I7GA39
E	484	LYS	-	expression tag	UNP I7GA39
E	485	GLU	-	expression tag	UNP I7GA39
E	486	ASP	-	expression tag	UNP I7GA39
E	487	LEU	-	expression tag	UNP I7GA39
E	488	GLU	-	expression tag	UNP I7GA39
E	489	HIS	-	expression tag	UNP I7GA39
E	490	HIS	-	expression tag	UNP I7GA39

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Chain	Residue	Modelled	Actual	Comment	Reference
E	491	HIS	-	expression tag	UNP I7GA39
E	492	HIS	-	expression tag	UNP I7GA39
E	493	HIS	-	expression tag	UNP I7GA39
E	494	HIS	-	expression tag	UNP I7GA39
E	495	HIS	-	expression tag	UNP I7GA39
E	496	HIS	-	expression tag	UNP I7GA39
F	2	VAL	-	insertion	UNP I7GA39
F	480	THR	-	expression tag	UNP I7GA39
F	481	ALA	-	expression tag	UNP I7GA39
F	482	ALA	-	expression tag	UNP I7GA39
F	483	ALA	-	expression tag	UNP I7GA39
F	484	LYS	-	expression tag	UNP I7GA39
F	485	GLU	-	expression tag	UNP I7GA39
F	486	ASP	-	expression tag	UNP I7GA39
F	487	LEU	-	expression tag	UNP I7GA39
F	488	GLU	-	expression tag	UNP I7GA39
F	489	HIS	-	expression tag	UNP I7GA39
F	490	HIS	-	expression tag	UNP I7GA39
F	491	HIS	-	expression tag	UNP I7GA39
F	492	HIS	-	expression tag	UNP I7GA39
F	493	HIS	-	expression tag	UNP I7GA39
F	494	HIS	-	expression tag	UNP I7GA39
F	495	HIS	-	expression tag	UNP I7GA39
F	496	HIS	-	expression tag	UNP I7GA39
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G	481	ALA	-	expression tag	UNP I7GA39
G	482	ALA	-	expression tag	UNP I7GA39
G	483	ALA	-	expression tag	UNP I7GA39
G	484	LYS	-	expression tag	UNP I7GA39
G	485	GLU	-	expression tag	UNP I7GA39
G	486	ASP	-	expression tag	UNP I7GA39
G	487	LEU	-	expression tag	UNP I7GA39
G	488	GLU	-	expression tag	UNP I7GA39
G	489	HIS	-	expression tag	UNP I7GA39
G	490	HIS	-	expression tag	UNP I7GA39
G	491	HIS	-	expression tag	UNP I7GA39
G	492	HIS	-	expression tag	UNP I7GA39
G	493	HIS	-	expression tag	UNP I7GA39
G	494	HIS	-	expression tag	UNP I7GA39
G	495	HIS	-	expression tag	UNP I7GA39
G	496	HIS	-	expression tag	UNP I7GA39

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Chain	Residue	Modelled	Actual	Comment	Reference
H	2	VAL	-	insertion	UNP I7GA39
H	480	THR	-	expression tag	UNP I7GA39
H	481	ALA	-	expression tag	UNP I7GA39
H	482	ALA	-	expression tag	UNP I7GA39
H	483	ALA	-	expression tag	UNP I7GA39
H	484	LYS	-	expression tag	UNP I7GA39
H	485	GLU	-	expression tag	UNP I7GA39
H	486	ASP	-	expression tag	UNP I7GA39
H	487	LEU	-	expression tag	UNP I7GA39
H	488	GLU	-	expression tag	UNP I7GA39
H	489	HIS	-	expression tag	UNP I7GA39
H	490	HIS	-	expression tag	UNP I7GA39
H	491	HIS	-	expression tag	UNP I7GA39
H	492	HIS	-	expression tag	UNP I7GA39
H	493	HIS	-	expression tag	UNP I7GA39
H	494	HIS	-	expression tag	UNP I7GA39
H	495	HIS	-	expression tag	UNP I7GA39
H	496	HIS	-	expression tag	UNP I7GA39
I	2	VAL	-	insertion	UNP I7GA39
I	480	THR	-	expression tag	UNP I7GA39
I	481	ALA	-	expression tag	UNP I7GA39
I	482	ALA	-	expression tag	UNP I7GA39
I	483	ALA	-	expression tag	UNP I7GA39
I	484	LYS	-	expression tag	UNP I7GA39
I	485	GLU	-	expression tag	UNP I7GA39
I	486	ASP	-	expression tag	UNP I7GA39
I	487	LEU	-	expression tag	UNP I7GA39
I	488	GLU	-	expression tag	UNP I7GA39
I	489	HIS	-	expression tag	UNP I7GA39
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I	492	HIS	-	expression tag	UNP I7GA39
I	493	HIS	-	expression tag	UNP I7GA39
I	494	HIS	-	expression tag	UNP I7GA39
I	495	HIS	-	expression tag	UNP I7GA39
I	496	HIS	-	expression tag	UNP I7GA39
J	2	VAL	-	insertion	UNP I7GA39
J	480	THR	-	expression tag	UNP I7GA39
J	481	ALA	-	expression tag	UNP I7GA39
J	482	ALA	-	expression tag	UNP I7GA39
J	483	ALA	-	expression tag	UNP I7GA39
J	484	LYS	-	expression tag	UNP I7GA39

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Chain	Residue	Modelled	Actual	Comment	Reference
J	485	GLU	-	expression tag	UNP I7GA39
J	486	ASP	-	expression tag	UNP I7GA39
J	487	LEU	-	expression tag	UNP I7GA39
J	488	GLU	-	expression tag	UNP I7GA39
J	489	HIS	-	expression tag	UNP I7GA39
J	490	HIS	-	expression tag	UNP I7GA39
J	491	HIS	-	expression tag	UNP I7GA39
J	492	HIS	-	expression tag	UNP I7GA39
J	493	HIS	-	expression tag	UNP I7GA39
J	494	HIS	-	expression tag	UNP I7GA39
J	495	HIS	-	expression tag	UNP I7GA39
J	496	HIS	-	expression tag	UNP I7GA39
K	2	VAL	-	insertion	UNP I7GA39
K	480	THR	-	expression tag	UNP I7GA39
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K	482	ALA	-	expression tag	UNP I7GA39
K	483	ALA	-	expression tag	UNP I7GA39
K	484	LYS	-	expression tag	UNP I7GA39
K	485	GLU	-	expression tag	UNP I7GA39
K	486	ASP	-	expression tag	UNP I7GA39
K	487	LEU	-	expression tag	UNP I7GA39
K	488	GLU	-	expression tag	UNP I7GA39
K	489	HIS	-	expression tag	UNP I7GA39
K	490	HIS	-	expression tag	UNP I7GA39
K	491	HIS	-	expression tag	UNP I7GA39
K	492	HIS	-	expression tag	UNP I7GA39
K	493	HIS	-	expression tag	UNP I7GA39
K	494	HIS	-	expression tag	UNP I7GA39
K	495	HIS	-	expression tag	UNP I7GA39
K	496	HIS	-	expression tag	UNP I7GA39
L	2	VAL	-	insertion	UNP I7GA39
L	480	THR	-	expression tag	UNP I7GA39
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L	484	LYS	-	expression tag	UNP I7GA39
L	485	GLU	-	expression tag	UNP I7GA39
L	486	ASP	-	expression tag	UNP I7GA39
L	487	LEU	-	expression tag	UNP I7GA39
L	488	GLU	-	expression tag	UNP I7GA39
L	489	HIS	-	expression tag	UNP I7GA39
L	490	HIS	-	expression tag	UNP I7GA39

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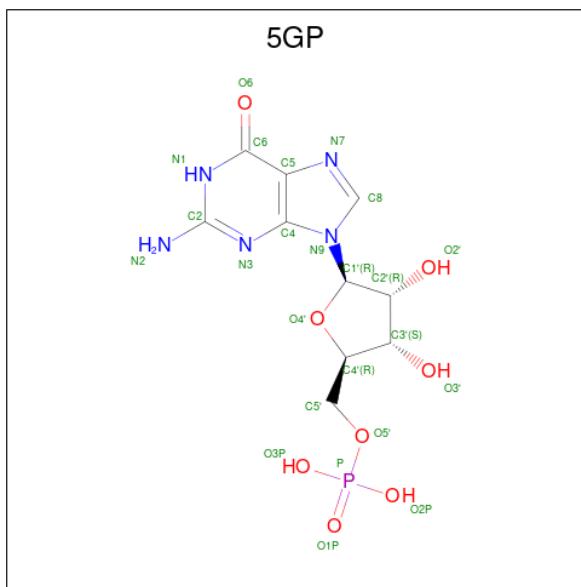
Chain	Residue	Modelled	Actual	Comment	Reference
L	491	HIS	-	expression tag	UNP I7GA39
L	492	HIS	-	expression tag	UNP I7GA39
L	493	HIS	-	expression tag	UNP I7GA39
L	494	HIS	-	expression tag	UNP I7GA39
L	495	HIS	-	expression tag	UNP I7GA39
L	496	HIS	-	expression tag	UNP I7GA39
M	2	VAL	-	insertion	UNP I7GA39
M	480	THR	-	expression tag	UNP I7GA39
M	481	ALA	-	expression tag	UNP I7GA39
M	482	ALA	-	expression tag	UNP I7GA39
M	483	ALA	-	expression tag	UNP I7GA39
M	484	LYS	-	expression tag	UNP I7GA39
M	485	GLU	-	expression tag	UNP I7GA39
M	486	ASP	-	expression tag	UNP I7GA39
M	487	LEU	-	expression tag	UNP I7GA39
M	488	GLU	-	expression tag	UNP I7GA39
M	489	HIS	-	expression tag	UNP I7GA39
M	490	HIS	-	expression tag	UNP I7GA39
M	491	HIS	-	expression tag	UNP I7GA39
M	492	HIS	-	expression tag	UNP I7GA39
M	493	HIS	-	expression tag	UNP I7GA39
M	494	HIS	-	expression tag	UNP I7GA39
M	495	HIS	-	expression tag	UNP I7GA39
M	496	HIS	-	expression tag	UNP I7GA39
N	2	VAL	-	insertion	UNP I7GA39
N	480	THR	-	expression tag	UNP I7GA39
N	481	ALA	-	expression tag	UNP I7GA39
N	482	ALA	-	expression tag	UNP I7GA39
N	483	ALA	-	expression tag	UNP I7GA39
N	484	LYS	-	expression tag	UNP I7GA39
N	485	GLU	-	expression tag	UNP I7GA39
N	486	ASP	-	expression tag	UNP I7GA39
N	487	LEU	-	expression tag	UNP I7GA39
N	488	GLU	-	expression tag	UNP I7GA39
N	489	HIS	-	expression tag	UNP I7GA39
N	490	HIS	-	expression tag	UNP I7GA39
N	491	HIS	-	expression tag	UNP I7GA39
N	492	HIS	-	expression tag	UNP I7GA39
N	493	HIS	-	expression tag	UNP I7GA39
N	494	HIS	-	expression tag	UNP I7GA39
N	495	HIS	-	expression tag	UNP I7GA39
N	496	HIS	-	expression tag	UNP I7GA39

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Chain	Residue	Modelled	Actual	Comment	Reference
O	2	VAL	-	insertion	UNP I7GA39
O	480	THR	-	expression tag	UNP I7GA39
O	481	ALA	-	expression tag	UNP I7GA39
O	482	ALA	-	expression tag	UNP I7GA39
O	483	ALA	-	expression tag	UNP I7GA39
O	484	LYS	-	expression tag	UNP I7GA39
O	485	GLU	-	expression tag	UNP I7GA39
O	486	ASP	-	expression tag	UNP I7GA39
O	487	LEU	-	expression tag	UNP I7GA39
O	488	GLU	-	expression tag	UNP I7GA39
O	489	HIS	-	expression tag	UNP I7GA39
O	490	HIS	-	expression tag	UNP I7GA39
O	491	HIS	-	expression tag	UNP I7GA39
O	492	HIS	-	expression tag	UNP I7GA39
O	493	HIS	-	expression tag	UNP I7GA39
O	494	HIS	-	expression tag	UNP I7GA39
O	495	HIS	-	expression tag	UNP I7GA39
O	496	HIS	-	expression tag	UNP I7GA39
P	2	VAL	-	insertion	UNP I7GA39
P	480	THR	-	expression tag	UNP I7GA39
P	481	ALA	-	expression tag	UNP I7GA39
P	482	ALA	-	expression tag	UNP I7GA39
P	483	ALA	-	expression tag	UNP I7GA39
P	484	LYS	-	expression tag	UNP I7GA39
P	485	GLU	-	expression tag	UNP I7GA39
P	486	ASP	-	expression tag	UNP I7GA39
P	487	LEU	-	expression tag	UNP I7GA39
P	488	GLU	-	expression tag	UNP I7GA39
P	489	HIS	-	expression tag	UNP I7GA39
P	490	HIS	-	expression tag	UNP I7GA39
P	491	HIS	-	expression tag	UNP I7GA39
P	492	HIS	-	expression tag	UNP I7GA39
P	493	HIS	-	expression tag	UNP I7GA39
P	494	HIS	-	expression tag	UNP I7GA39
P	495	HIS	-	expression tag	UNP I7GA39
P	496	HIS	-	expression tag	UNP I7GA39

- Molecule 2 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: C₁₀H₁₄N₅O₈P) (labeled as "Ligand of Interest" by depositor).



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

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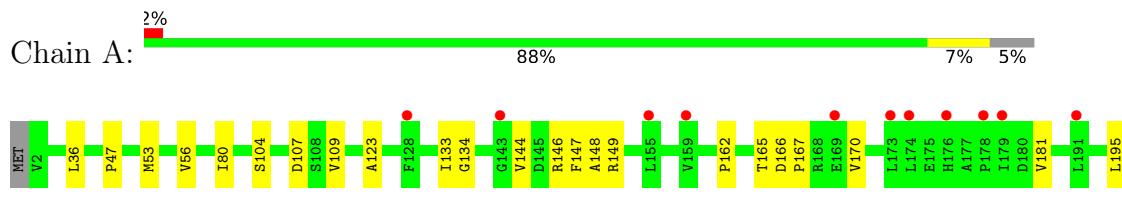
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	O	1	24	10	5	8	1	0	0
2	P	1	24	10	5	8	1	0	0

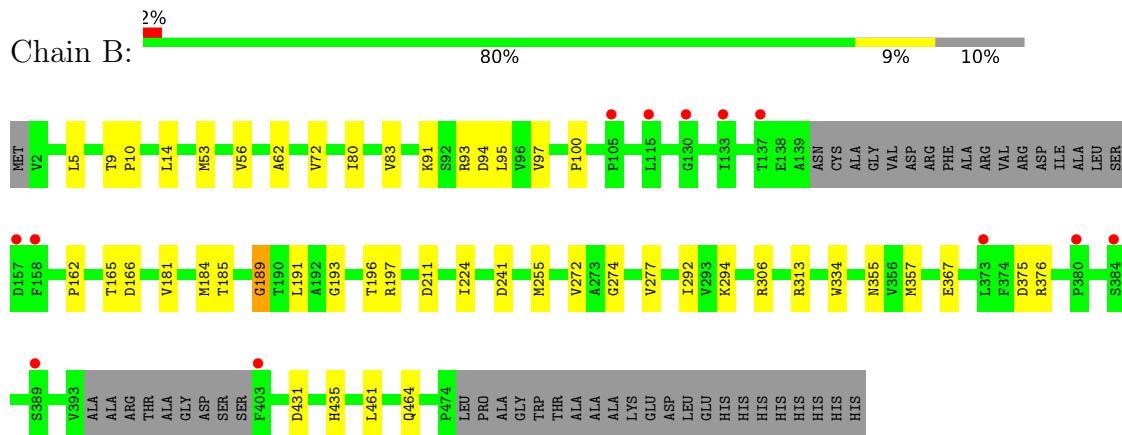
3 Residue-property plots

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.

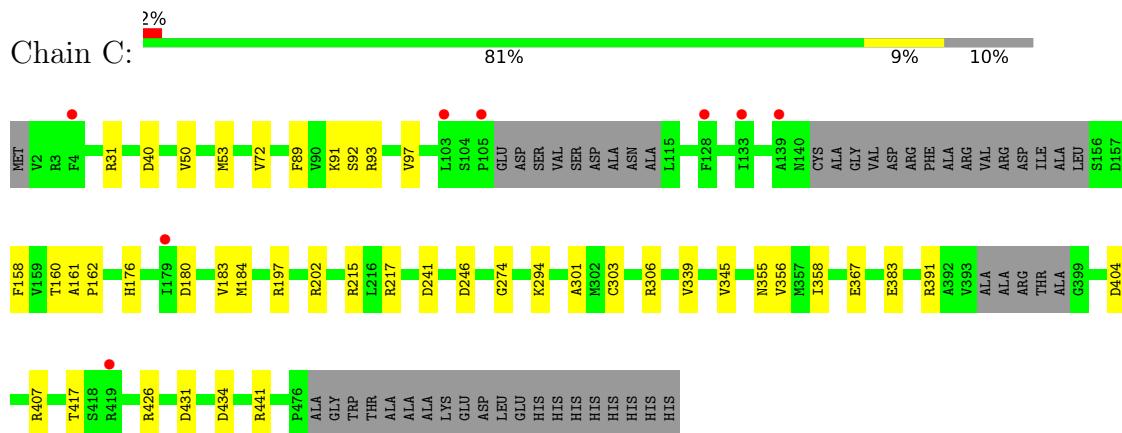
- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1



- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

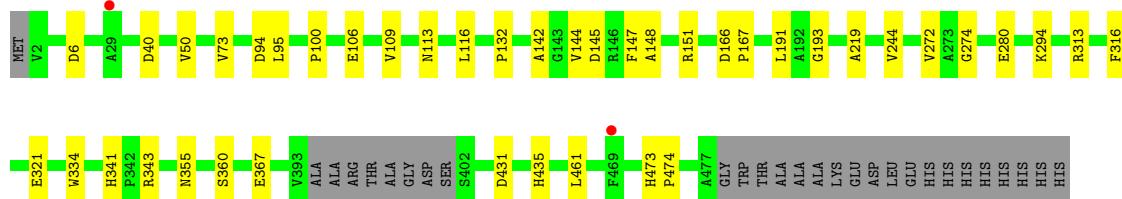


- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1



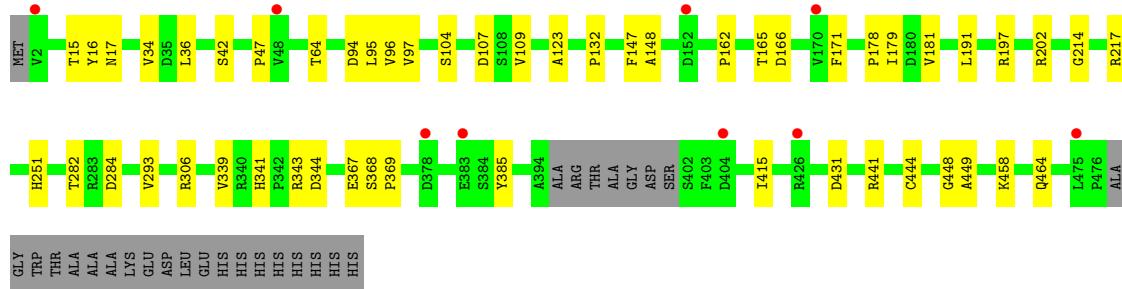
- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain D: 



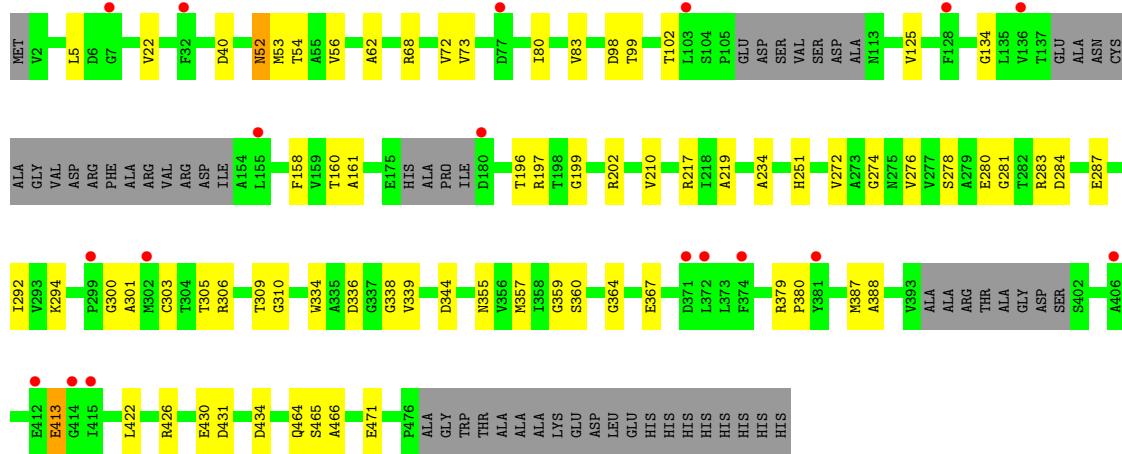
- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain E:  2%



- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

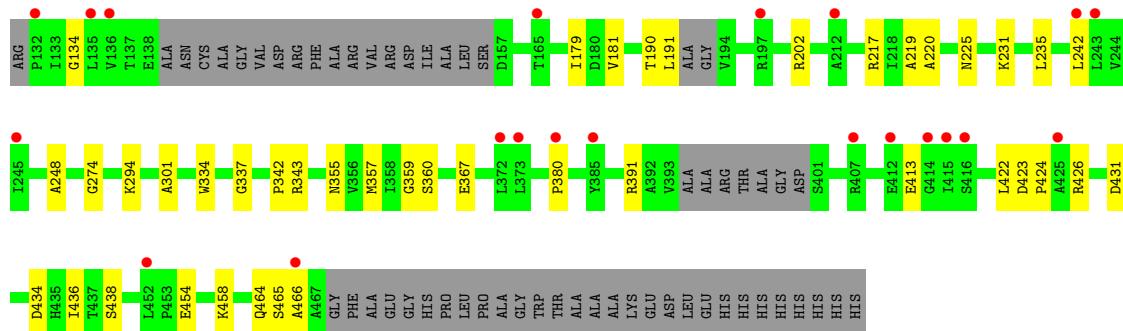
Chain F:  4%



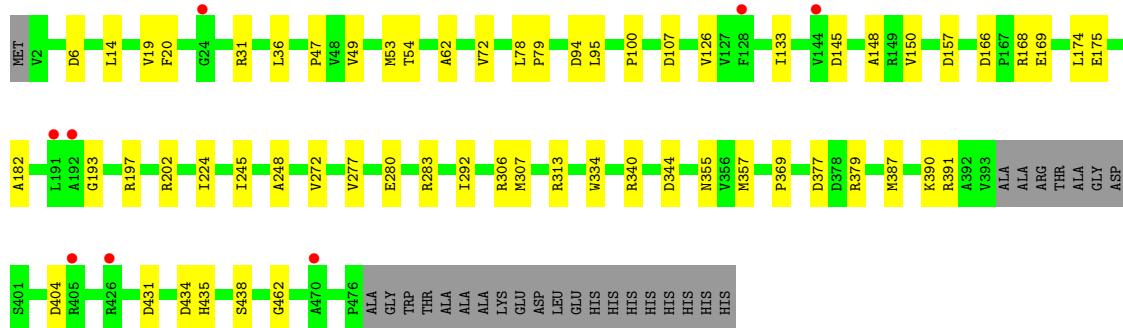
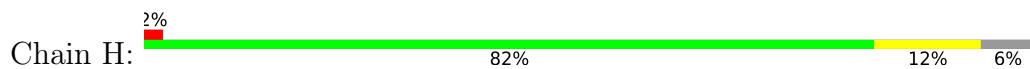
- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

Chain G:  7%

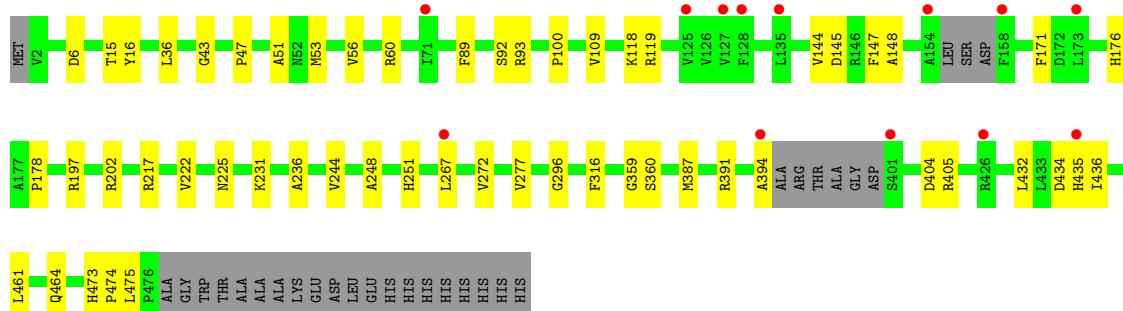
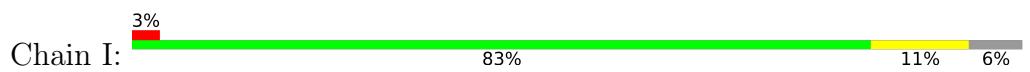




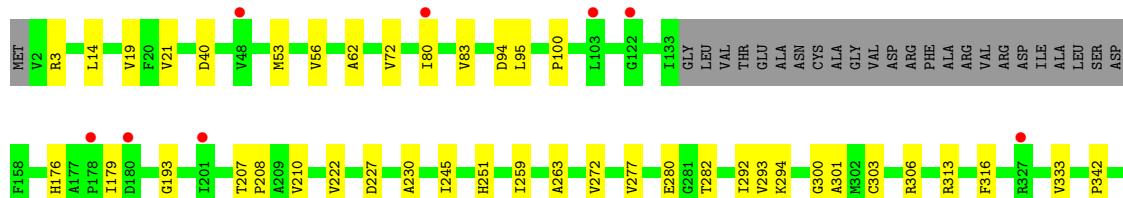
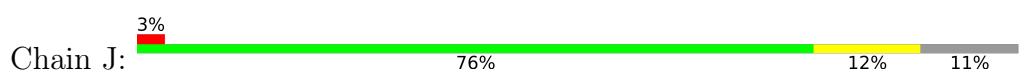
- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

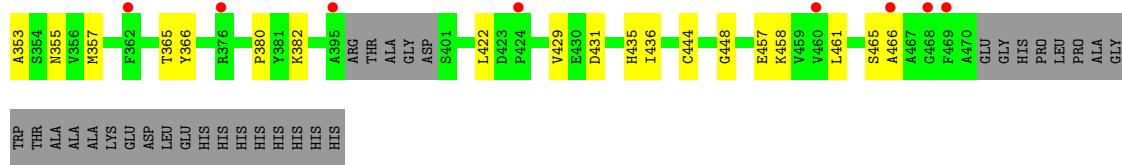


- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

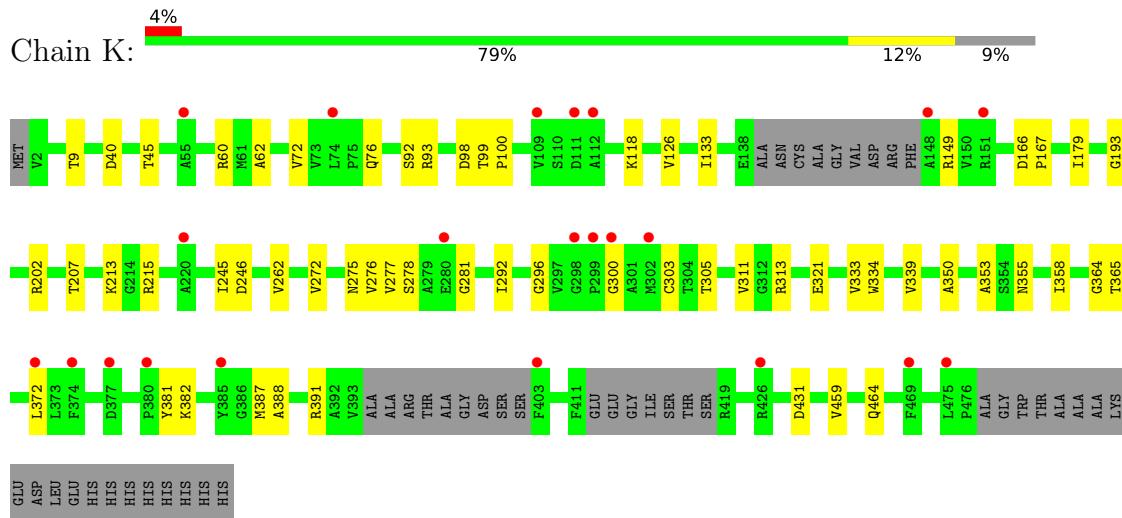


- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1

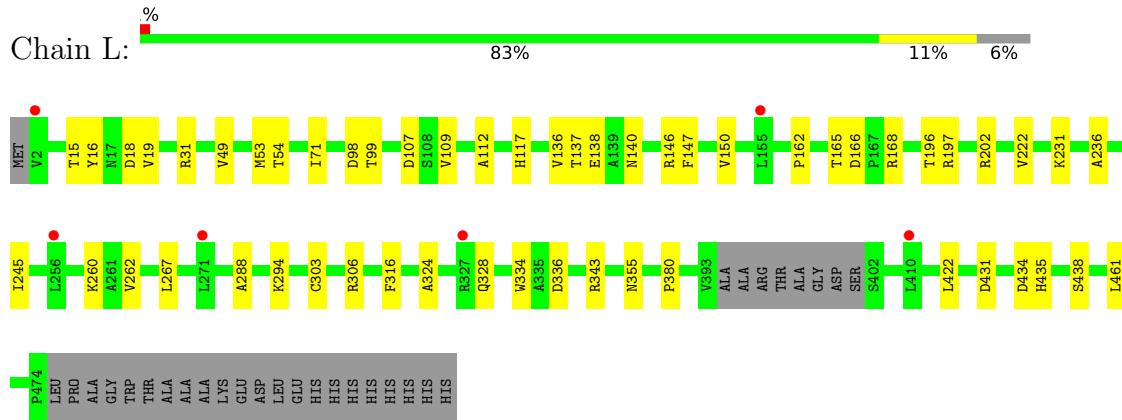




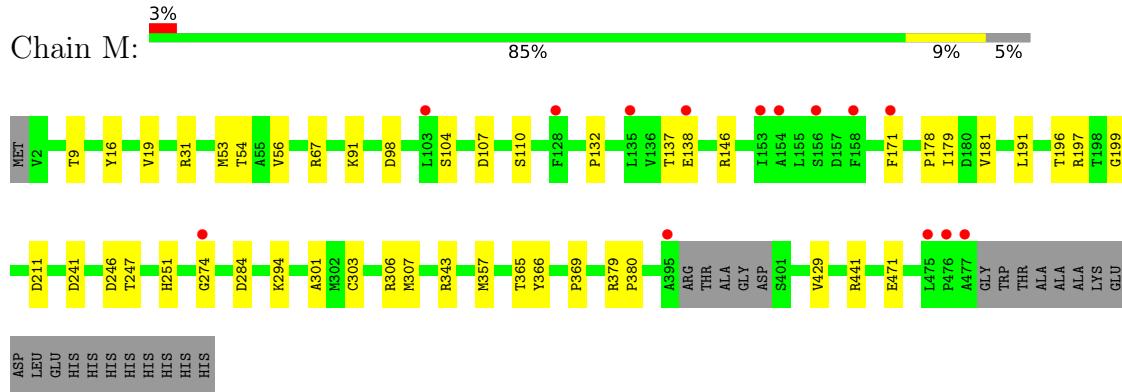
- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1



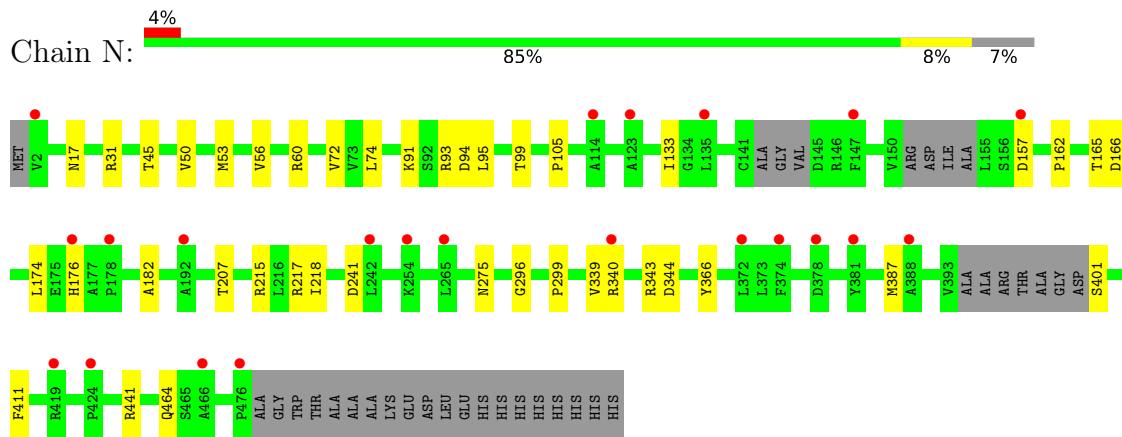
- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1



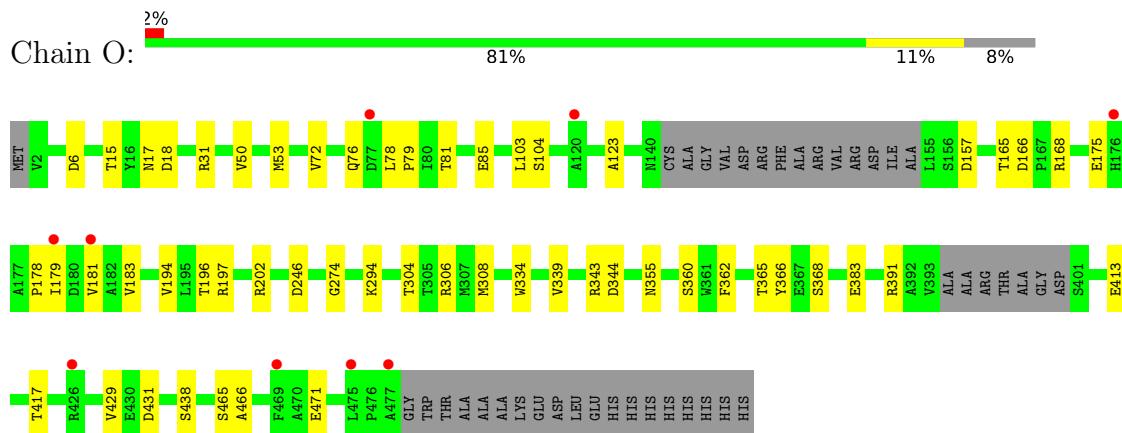
- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1



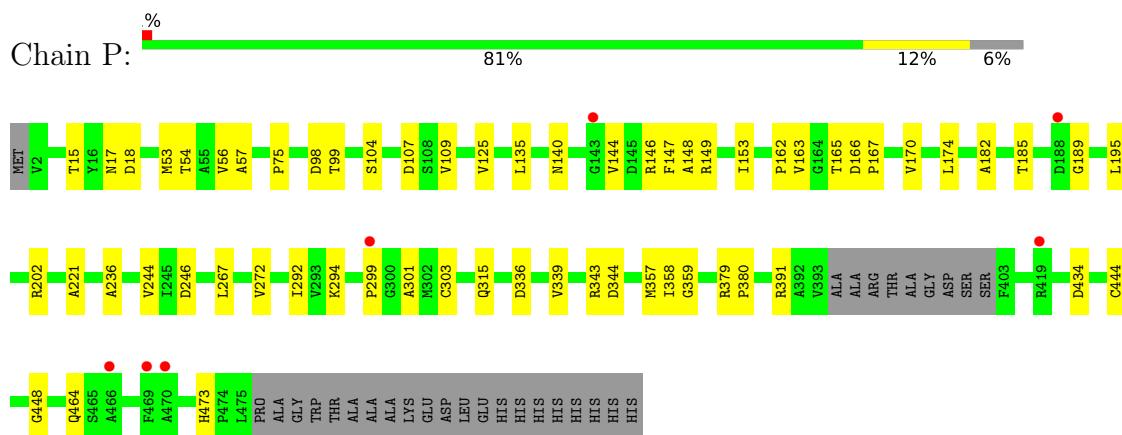
- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1



- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1



- Molecule 1: Inosine-5-monophosphate dehydrogenase guaB1



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ 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 (4.95%)	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)	(Not available) , (Not available)	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.21	0/3460	0.41	0/4717
1	B	0.23	0/3283	0.46	0/4474
1	C	0.21	0/3289	0.42	0/4478
1	D	0.22	0/3446	0.44	1/4696 (0.0%)
1	E	0.21	0/3447	0.41	0/4697
1	F	0.22	0/3218	0.43	0/4381
1	G	0.21	0/3063	0.43	0/4176
1	H	0.21	0/3433	0.42	0/4678
1	I	0.21	0/3431	0.42	0/4673
1	J	0.24	0/3206	0.45	1/4372 (0.0%)
1	K	0.22	0/3270	0.45	0/4462
1	L	0.21	0/3401	0.42	0/4637
1	M	0.21	0/3433	0.42	0/4683
1	N	0.21	0/3405	0.42	0/4635
1	O	0.22	0/3334	0.41	0/4544
1	P	0.21	0/3425	0.43	1/4665 (0.0%)
All	All	0.22	0/53544	0.43	3/72968 (0.0%)

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	LEU	CA-CB-CG	8.43	134.68	115.30
1	P	189	GLY	N-CA-C	5.47	126.79	113.10
1	J	210	VAL	N-CA-C	5.10	124.76	111.00

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 [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3403	0	3371	21	0
1	B	3230	0	3204	28	1
1	C	3235	0	3222	27	0
1	D	3389	0	3370	26	1
1	E	3390	0	3372	32	0
1	F	3168	0	3163	44	0
1	G	3017	0	2977	36	0
1	H	3378	0	3358	41	0
1	I	3375	0	3358	38	0
1	J	3154	0	3119	39	0
1	K	3216	0	3177	36	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	37	1
1	P	3369	0	3360	39	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	2	0
2	G	24	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	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	494	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 (494) 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
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:O2P	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:53:MET:HE2	2:N:501:5GP:H8	1.75	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:O2P	2.31	0.63
1:B:91:LYS:NZ	1:B:241:ASP:OD2	2.30	0.62
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: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:O2P	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O1P	2.35	0.58
1:K:202:ARG:NH2	1:K:431:ASP:OD1	2.33	0.58
1:F:54:THR:H	1:F:387:MET:HE3	1.68	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:O1P	2.39	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
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:162:PRO:O	1:N:165:THR:OG1	2.25	0.54
1:P:53:MET:HE2	2:P:501:5GP:H8	1.88	0.54
1:G:360:SER:N	2:G:501:5GP:O3P	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:162:PRO:O	1:A:165:THR:OG1	2.22	0.52
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: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:80:ILE:HA	1:J:83:VAL:HG12	1.92	0.52
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:J:366:TYR:O	1:J:382:LYS:NZ	2.42	0.52
1:A:360:SER:N	2:A:501:5GP:O3P	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:E:341:HIS:HB2	1:E:343:ARG:HG2	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:N:31:ARG:HB2	1:N:441:ARG:HB3	1.94	0.48
1:N:45:THR:OG1	1:N:207:THR:O	2.28	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: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: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:M:91:LYS:NZ	1:M:211:ASP:OD2	2.35	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:294:LYS:HD2	1:M:357:MET:HE1	1.96	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: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
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: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: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:M:91:LYS:NZ	1:M:241:ASP:OD2	2.46	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:HB8	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:O2P	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: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:H:166:ASP:C	1:H:168:ARG:H	2.19	0.43
1:N:93:ARG:NE	1:N:99:THR:OG1	2.52	0.43
1:G:225:ASN:O	1:G:231:LYS:NZ	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:P:294:LYS:HD2	1:P:357:MET:HE1	2.02	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: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:O1P	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O3P	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:O2P	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:O1P	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:O2P	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:E:448:GLY:O	1:E:458:LYS:NZ	2.50	0.40
1:H:334:TRP:CD1	1:H:355:ASN:HB2	2.56	0.40
1:J:227:ASP:OD1	1:J:230:ALA:N	2.46	0.40
1:J:300:GLY:HA2	2:J:501:5GP:O2P	2.21	0.40
1:M:178:PRO:HG2	1:M:179:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:224:ILE:HG21	1:B:255:MET:HE2	2.02	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/372 (93%)	346 (100%)	0	100	100
1	B	331/372 (89%)	330 (100%)	1 (0%)	92	97
1	C	333/372 (90%)	333 (100%)	0	100	100
1	D	348/372 (94%)	348 (100%)	0	100	100
1	E	348/372 (94%)	348 (100%)	0	100	100
1	F	324/372 (87%)	322 (99%)	2 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	305/372 (82%)	305 (100%)	0	100	100
1	H	347/372 (93%)	347 (100%)	0	100	100
1	I	346/372 (93%)	345 (100%)	1 (0%)	92	97
1	J	321/372 (86%)	321 (100%)	0	100	100
1	K	323/372 (87%)	322 (100%)	1 (0%)	92	97
1	L	341/372 (92%)	340 (100%)	1 (0%)	92	97
1	M	343/372 (92%)	343 (100%)	0	100	100
1	N	346/372 (93%)	346 (100%)	0	100	100
1	O	337/372 (91%)	337 (100%)	0	100	100
1	P	344/372 (92%)	344 (100%)	0	100	100
All	All	5383/5952 (90%)	5377 (100%)	6 (0%)	93	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	93	ARG
1	F	52	ASN
1	F	413	GLU
1	I	251	HIS
1	K	381	TYR
1	L	146	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	M	501	-	22,26,26	0.64	0	27,40,40	0.68	0
2	5GP	G	501	-	22,26,26	0.63	0	27,40,40	0.78	0
2	5GP	J	501	-	22,26,26	0.87	1 (4%)	27,40,40	0.75	1 (3%)
2	5GP	D	501	-	22,26,26	0.85	1 (4%)	27,40,40	0.70	0
2	5GP	L	501	-	22,26,26	0.87	1 (4%)	27,40,40	0.73	1 (3%)
2	5GP	H	501	-	22,26,26	0.64	0	27,40,40	0.69	0
2	5GP	C	501	-	22,26,26	0.87	1 (4%)	27,40,40	0.75	1 (3%)
2	5GP	K	501	-	22,26,26	0.90	1 (4%)	27,40,40	0.71	0
2	5GP	N	501	-	22,26,26	0.64	0	27,40,40	0.70	0
2	5GP	E	501	-	22,26,26	0.85	1 (4%)	27,40,40	0.69	0
2	5GP	A	501	-	22,26,26	0.88	1 (4%)	27,40,40	0.76	0
2	5GP	F	501	-	22,26,26	0.86	1 (4%)	27,40,40	0.75	0
2	5GP	B	501	-	22,26,26	0.86	1 (4%)	27,40,40	0.69	0
2	5GP	O	501	-	22,26,26	0.87	1 (4%)	27,40,40	0.74	1 (3%)
2	5GP	I	501	-	22,26,26	0.88	1 (4%)	27,40,40	0.80	1 (3%)
2	5GP	P	501	-	22,26,26	0.67	0	27,40,40	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5GP	M	501	-	-	5/6/26/26	0/3/3/3
2	5GP	G	501	-	-	5/6/26/26	0/3/3/3
2	5GP	J	501	-	-	5/6/26/26	0/3/3/3
2	5GP	D	501	-	-	5/6/26/26	0/3/3/3
2	5GP	L	501	-	-	1/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5GP	H	501	-	-	0/6/26/26	0/3/3/3
2	5GP	C	501	-	-	5/6/26/26	0/3/3/3
2	5GP	K	501	-	-	5/6/26/26	0/3/3/3
2	5GP	N	501	-	-	3/6/26/26	0/3/3/3
2	5GP	E	501	-	-	3/6/26/26	0/3/3/3
2	5GP	A	501	-	-	0/6/26/26	0/3/3/3
2	5GP	F	501	-	-	0/6/26/26	0/3/3/3
2	5GP	B	501	-	-	5/6/26/26	0/3/3/3
2	5GP	O	501	-	-	1/6/26/26	0/3/3/3
2	5GP	I	501	-	-	1/6/26/26	0/3/3/3
2	5GP	P	501	-	-	5/6/26/26	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	501	5GP	P-O1P	2.90	1.59	1.50
2	C	501	5GP	P-O1P	2.84	1.59	1.50
2	L	501	5GP	P-O1P	2.83	1.59	1.50
2	O	501	5GP	P-O1P	2.83	1.59	1.50
2	J	501	5GP	P-O1P	2.83	1.59	1.50
2	I	501	5GP	P-O1P	2.71	1.59	1.50
2	F	501	5GP	P-O1P	2.70	1.59	1.50
2	B	501	5GP	P-O1P	2.66	1.59	1.50
2	E	501	5GP	P-O1P	2.65	1.59	1.50
2	A	501	5GP	P-O1P	2.64	1.59	1.50
2	D	501	5GP	P-O1P	2.63	1.59	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	501	5GP	O3P-P-O2P	2.39	116.76	107.64
2	O	501	5GP	O3P-P-O2P	2.28	116.35	107.64
2	C	501	5GP	O3P-P-O2P	2.24	116.19	107.64
2	J	501	5GP	O3P-P-O2P	2.18	115.95	107.64
2	L	501	5GP	O3P-P-O2P	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-O1P
2	B	501	5GP	C5'-O5'-P-O2P
2	B	501	5GP	C5'-O5'-P-O3P
2	B	501	5GP	C3'-C4'-C5'-O5'
2	C	501	5GP	C5'-O5'-P-O1P
2	C	501	5GP	C5'-O5'-P-O2P
2	C	501	5GP	C3'-C4'-C5'-O5'
2	D	501	5GP	C5'-O5'-P-O1P
2	D	501	5GP	C5'-O5'-P-O2P
2	D	501	5GP	C5'-O5'-P-O3P
2	D	501	5GP	C3'-C4'-C5'-O5'
2	G	501	5GP	C5'-O5'-P-O1P
2	G	501	5GP	C5'-O5'-P-O2P
2	G	501	5GP	C5'-O5'-P-O3P
2	J	501	5GP	C5'-O5'-P-O2P
2	J	501	5GP	C5'-O5'-P-O3P
2	J	501	5GP	C3'-C4'-C5'-O5'
2	K	501	5GP	C5'-O5'-P-O1P
2	K	501	5GP	C5'-O5'-P-O2P
2	M	501	5GP	C5'-O5'-P-O1P
2	M	501	5GP	C5'-O5'-P-O2P
2	M	501	5GP	C5'-O5'-P-O3P
2	M	501	5GP	C3'-C4'-C5'-O5'
2	N	501	5GP	C5'-O5'-P-O2P
2	N	501	5GP	C5'-O5'-P-O3P
2	P	501	5GP	C5'-O5'-P-O1P
2	P	501	5GP	C5'-O5'-P-O2P
2	P	501	5GP	C5'-O5'-P-O3P
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'
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-O1P
2	N	501	5GP	C5'-O5'-P-O1P

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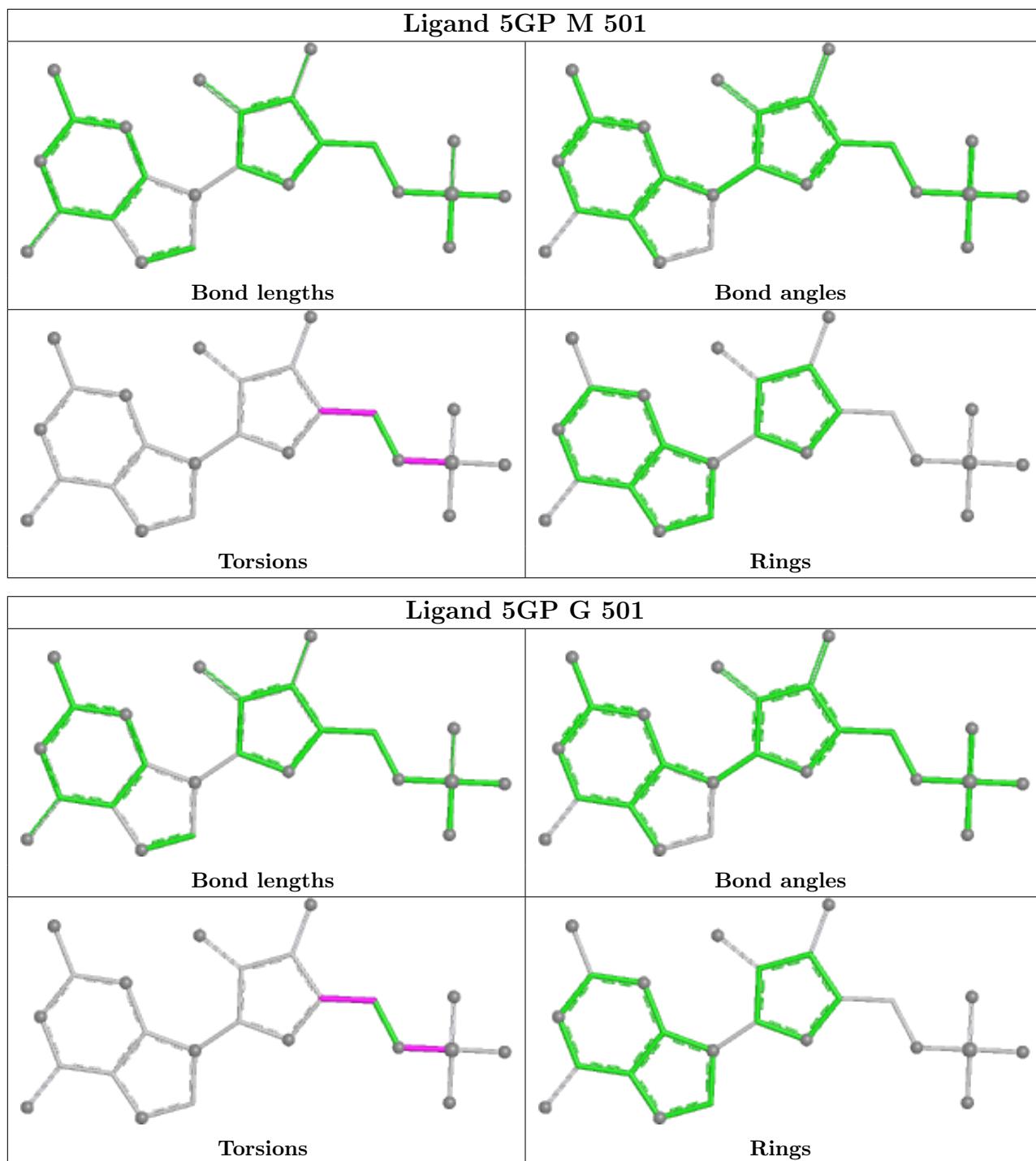
Mol	Chain	Res	Type	Atoms
2	O	501	5GP	C5'-O5'-P-O1P
2	C	501	5GP	C5'-O5'-P-O3P
2	E	501	5GP	C5'-O5'-P-O2P
2	K	501	5GP	C5'-O5'-P-O3P
2	I	501	5GP	C3'-C4'-C5'-O5'
2	L	501	5GP	C3'-C4'-C5'-O5'

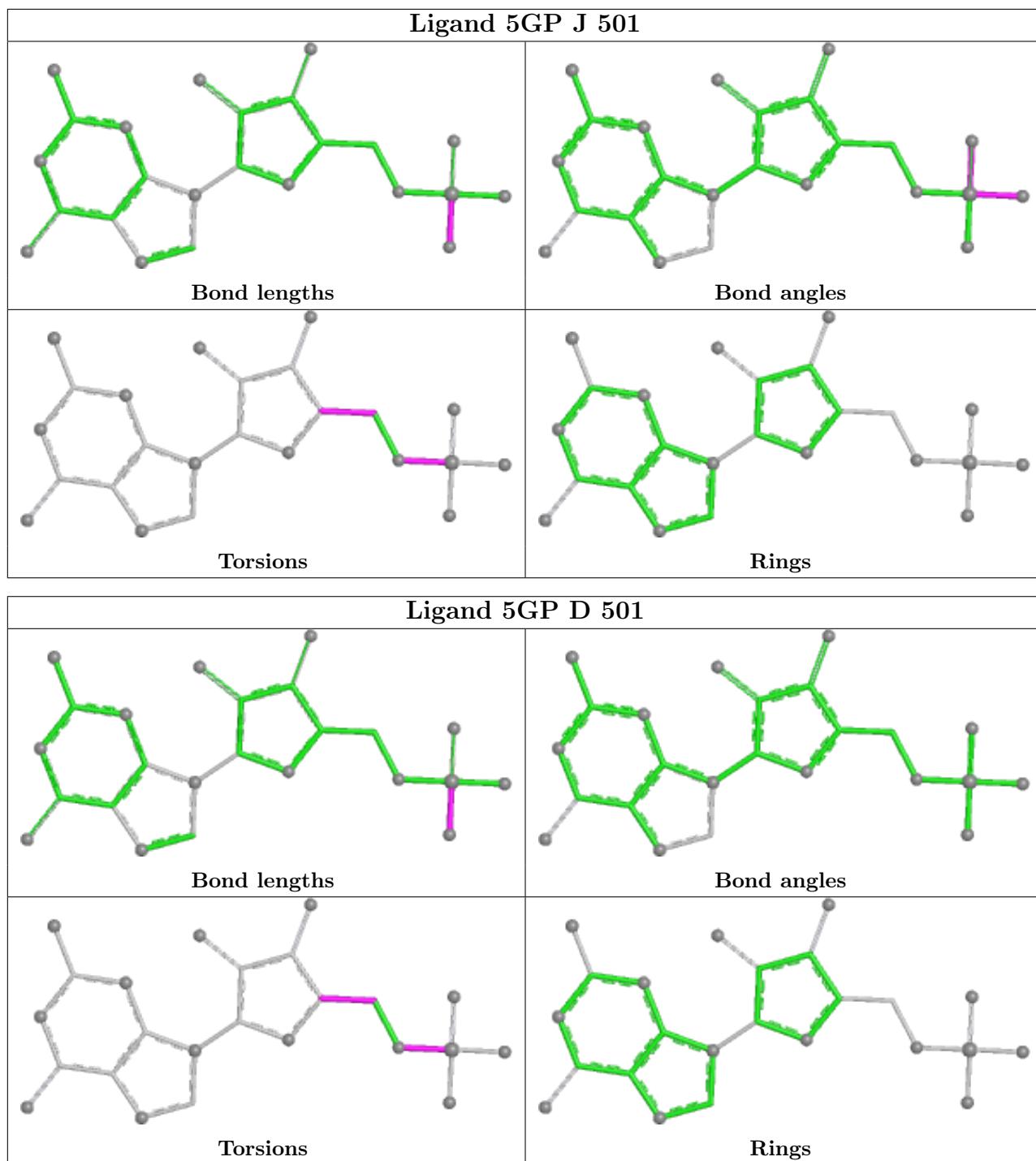
There are no ring outliers.

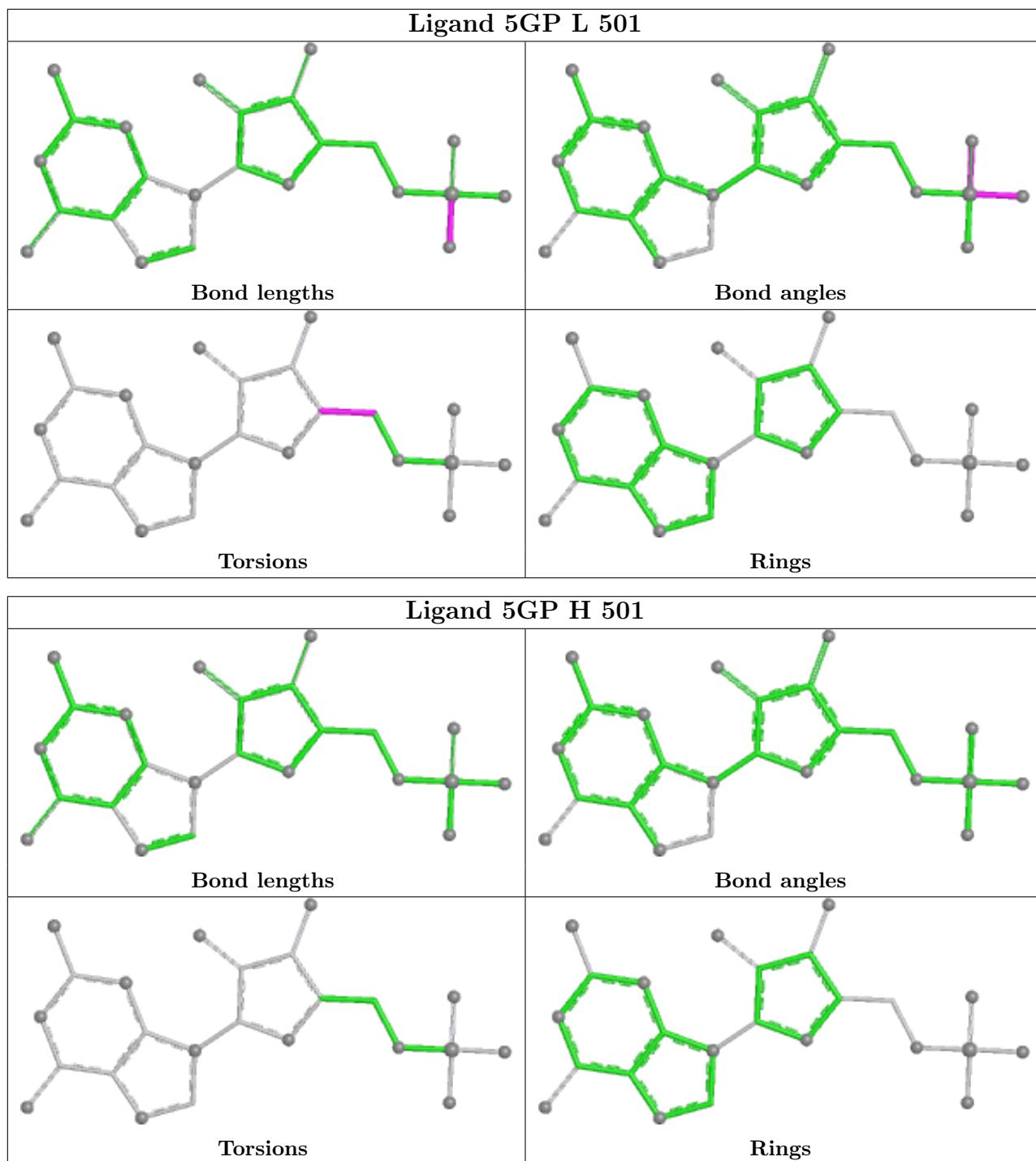
13 monomers are involved in 34 short contacts:

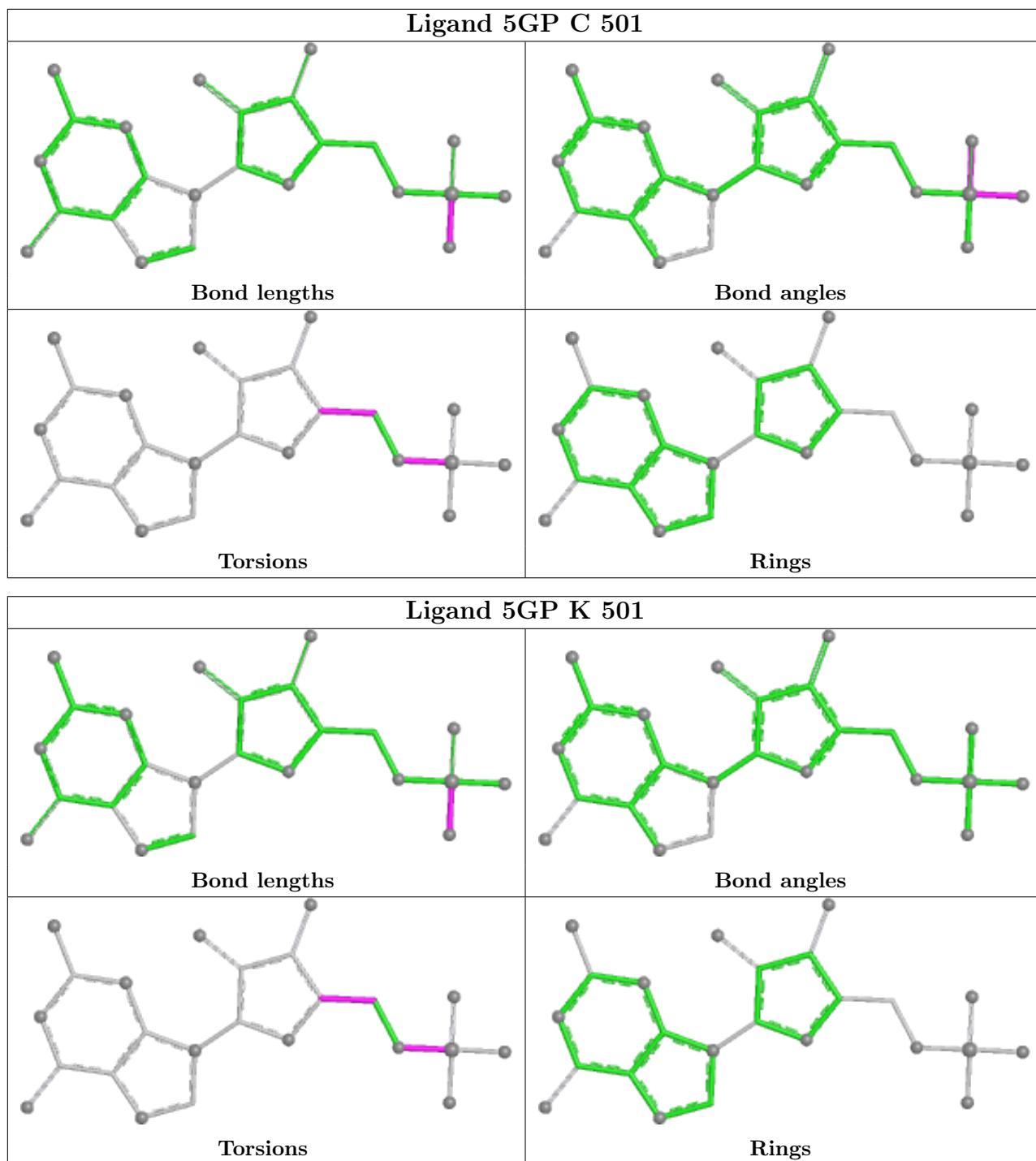
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	501	5GP	3	0
2	G	501	5GP	4	0
2	J	501	5GP	3	0
2	D	501	5GP	1	0
2	L	501	5GP	2	0
2	C	501	5GP	3	0
2	K	501	5GP	5	0
2	N	501	5GP	1	0
2	A	501	5GP	2	0
2	F	501	5GP	2	0
2	O	501	5GP	2	0
2	I	501	5GP	2	0
2	P	501	5GP	4	0

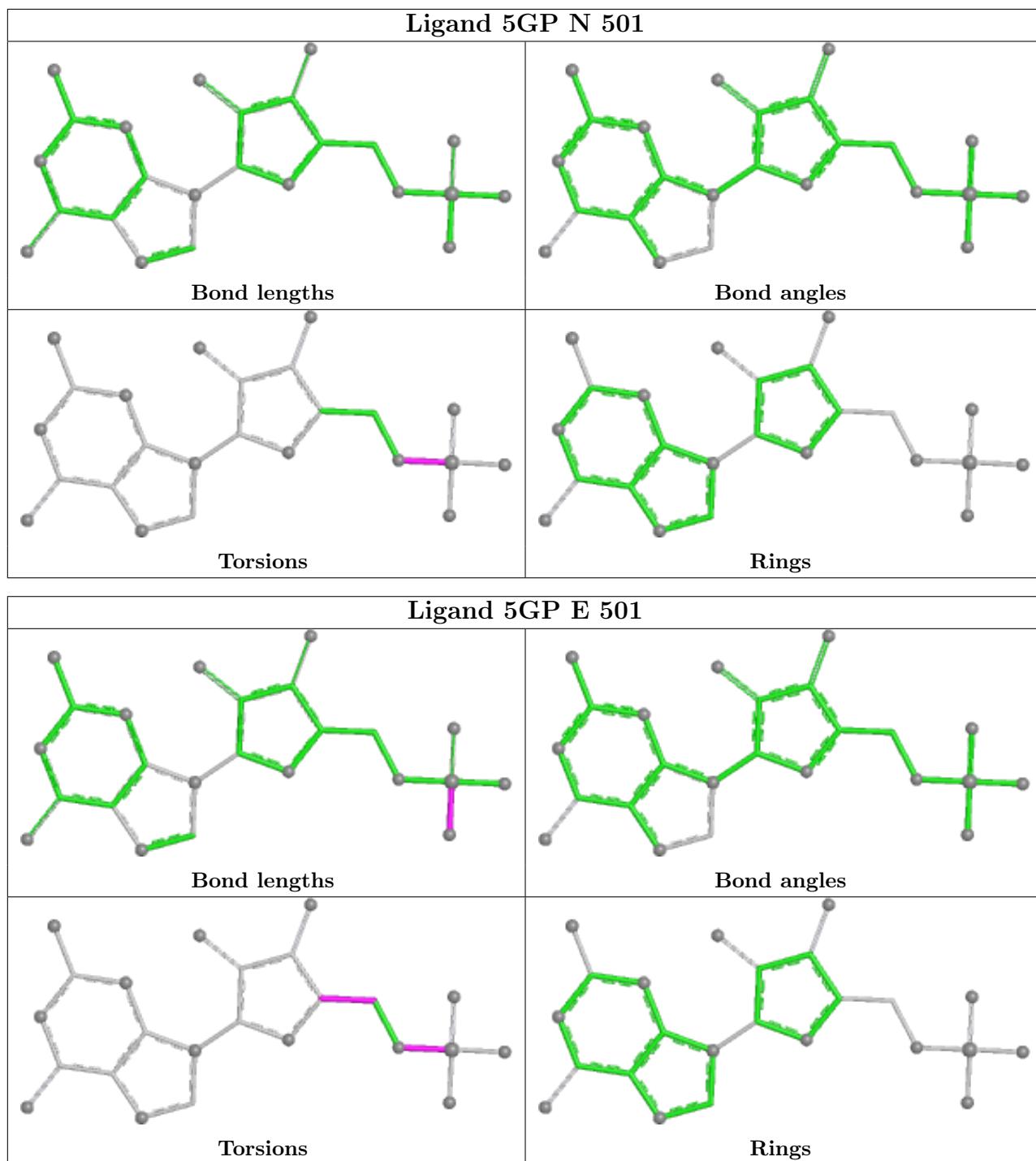
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

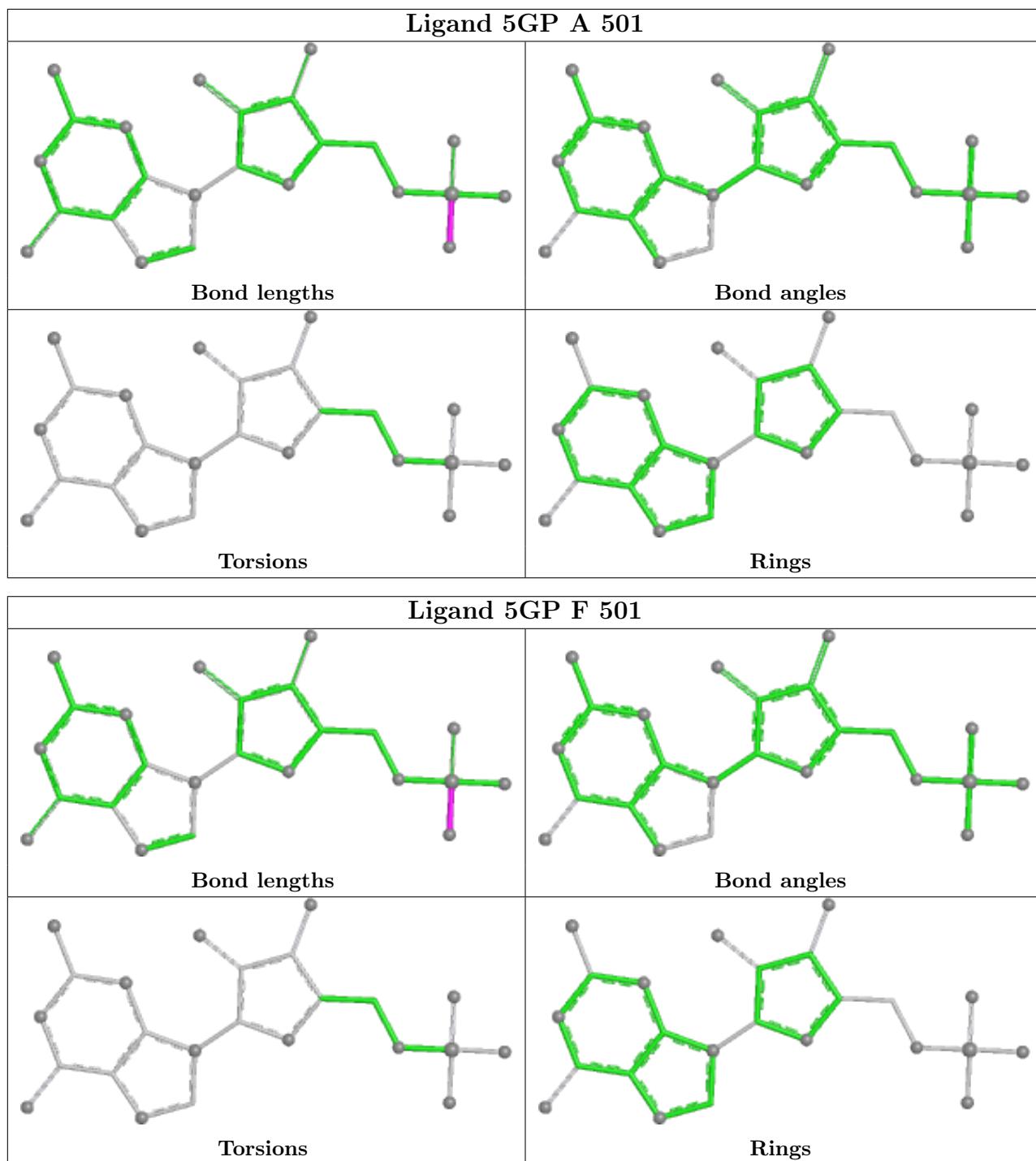


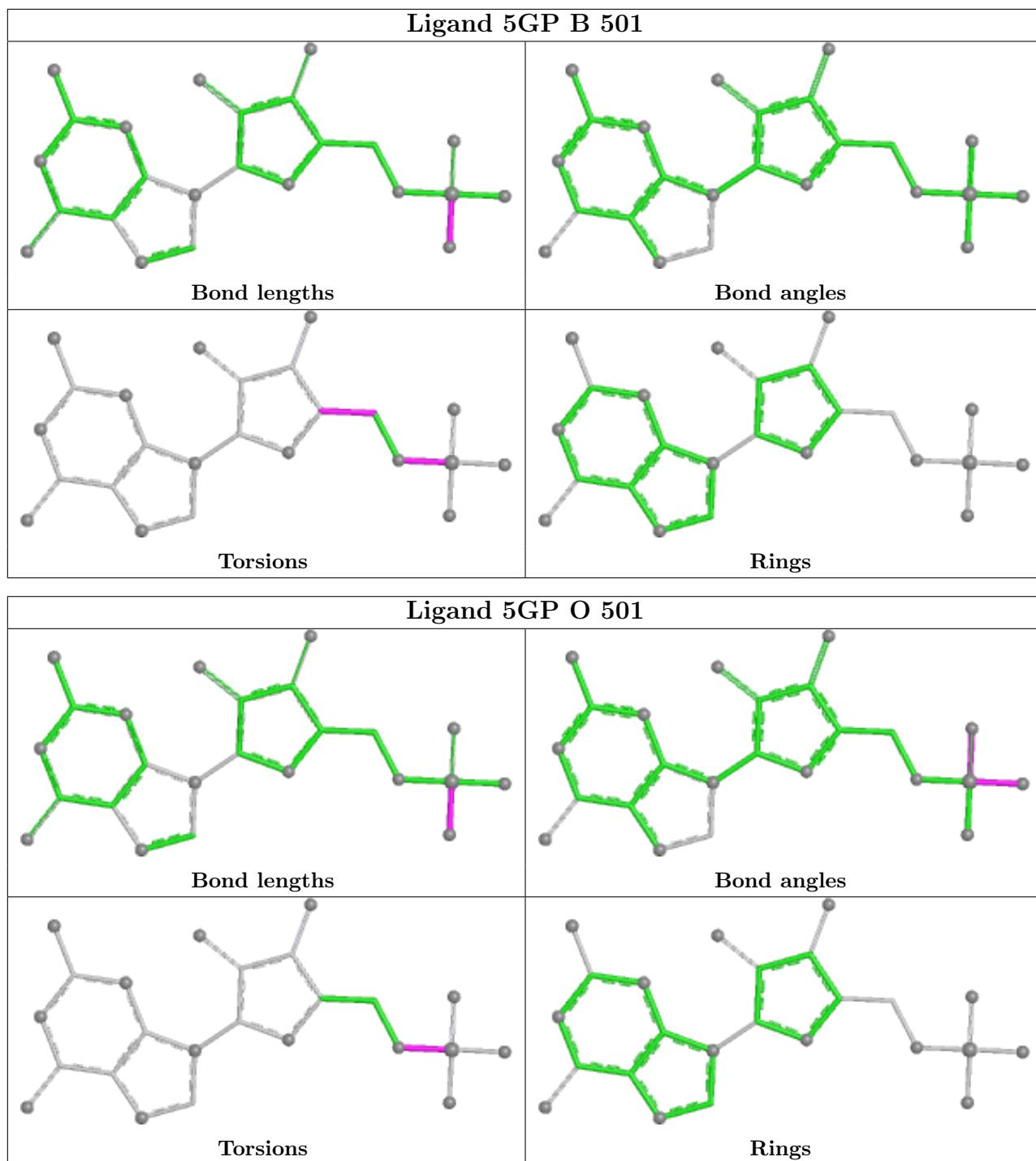


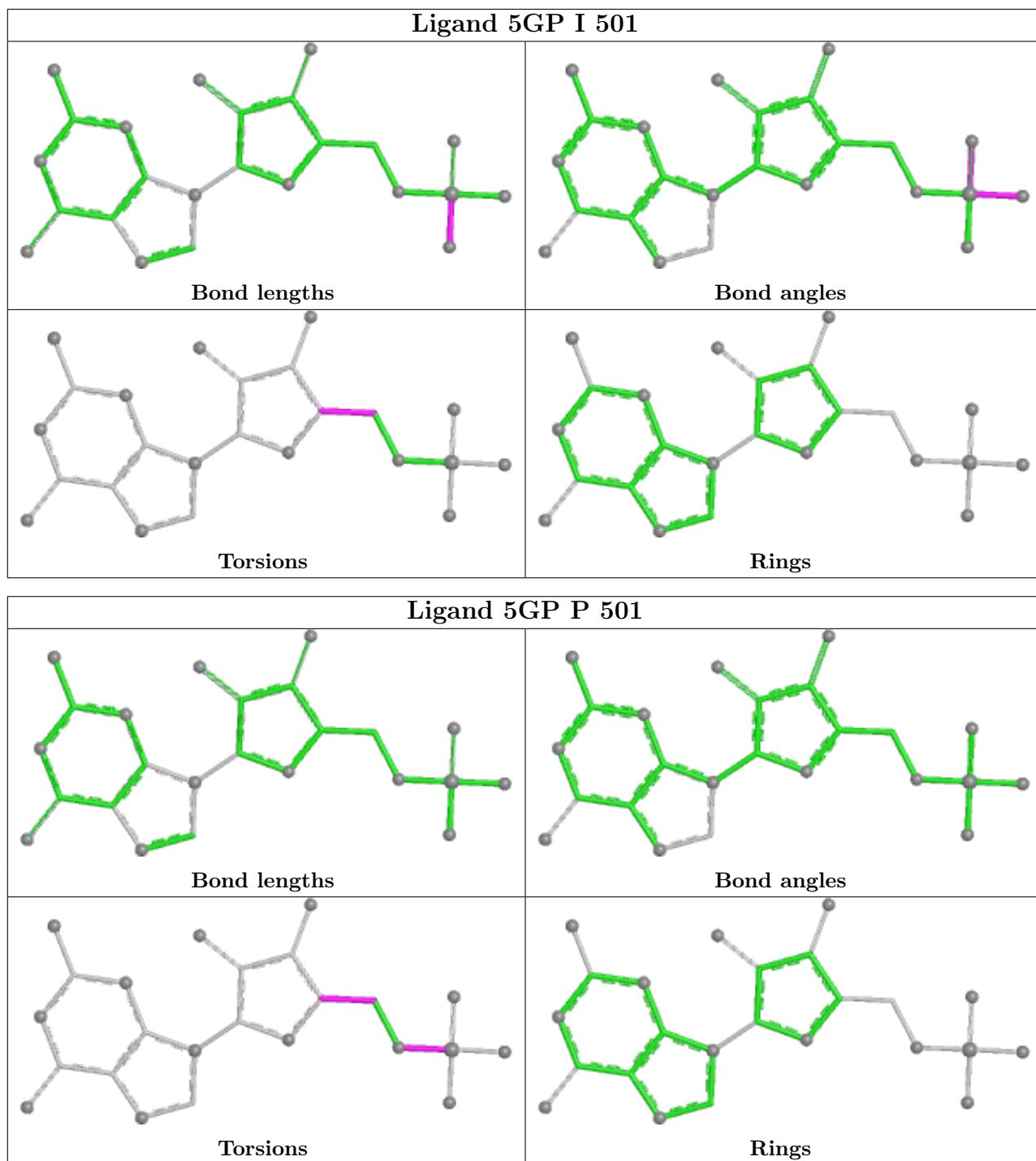












5.7 Other polymers i

There are no such residues in this entry.

5.8 Polymer linkage issues i

There are no chain breaks in this entry.

6 Fit of model and data [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	473/496 (95%)	0.04	11 (2%)	60	63	33, 47, 78, 105	0
1	B	447/496 (90%)	0.15	12 (2%)	54	58	38, 51, 83, 104	0
1	C	446/496 (89%)	0.00	8 (1%)	68	71	34, 53, 75, 95	0
1	D	468/496 (94%)	-0.09	2 (0%)	92	93	35, 48, 64, 91	0
1	E	468/496 (94%)	0.06	9 (1%)	66	69	37, 55, 71, 91	0
1	F	440/496 (88%)	0.24	18 (4%)	37	40	42, 61, 90, 107	0
1	G	424/496 (85%)	0.45	37 (8%)	10	10	48, 68, 88, 103	0
1	H	468/496 (94%)	0.08	8 (1%)	70	72	39, 54, 77, 96	0
1	I	466/496 (93%)	0.13	13 (2%)	53	56	43, 57, 73, 98	1 (0%)
1	J	440/496 (88%)	0.22	16 (3%)	42	46	40, 61, 84, 97	1 (0%)
1	K	450/496 (90%)	0.20	22 (4%)	29	31	42, 56, 86, 103	0
1	L	465/496 (93%)	0.03	6 (1%)	77	79	40, 57, 77, 88	0
1	M	471/496 (94%)	0.05	14 (2%)	50	53	35, 53, 80, 94	0
1	N	461/496 (92%)	0.14	22 (4%)	30	32	33, 56, 79, 107	0
1	O	455/496 (91%)	0.09	9 (1%)	65	68	37, 55, 80, 95	0
1	P	465/496 (93%)	-0.02	7 (1%)	73	75	39, 54, 73, 86	0
All	All	7307/7936 (92%)	0.11	214 (2%)	51	55	33, 56, 80, 107	2 (0%)

All (214) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	123	ALA	6.0
1	G	135	LEU	5.6
1	K	299	PRO	5.6
1	I	401	SER	5.1
1	A	176	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	380	PRO	4.9
1	G	380	PRO	4.8
1	G	125	VAL	4.5
1	F	414	GLY	4.3
1	G	415	ILE	4.3
1	H	128	PHE	4.2
1	G	414	GLY	4.2
1	N	419	ARG	4.1
1	A	128	PHE	4.1
1	F	299	PRO	4.0
1	B	137	THR	3.9
1	G	126	VAL	3.9
1	F	372	LEU	3.8
1	G	136	VAL	3.8
1	L	2	VAL	3.8
1	H	144	VAL	3.7
1	M	103	LEU	3.7
1	K	380	PRO	3.7
1	A	143	GLY	3.7
1	N	114	ALA	3.7
1	G	72	VAL	3.7
1	G	120	ALA	3.7
1	K	302	MET	3.6
1	K	112	ALA	3.6
1	A	179	ILE	3.6
1	F	136	VAL	3.6
1	M	395	ALA	3.6
1	G	132	PRO	3.5
1	K	148	ALA	3.5
1	E	2	VAL	3.5
1	J	460	VAL	3.5
1	G	165	THR	3.4
1	K	469	PHE	3.4
1	E	475	LEU	3.4
1	N	378	ASP	3.4
1	J	466	ALA	3.4
1	M	476	PRO	3.3
1	P	470	ALA	3.3
1	A	155	LEU	3.3
1	M	153	ILE	3.3
1	F	155	LEU	3.3
1	M	128	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	O	77	ASP	3.2
1	G	197	ARG	3.2
1	P	419	ARG	3.1
1	G	78	LEU	3.1
1	M	477	ALA	3.1
1	A	173	LEU	3.1
1	C	103	LEU	3.1
1	N	176	HIS	3.1
1	K	109	VAL	3.0
1	J	80	ILE	3.0
1	H	470	ALA	3.0
1	J	103	LEU	3.0
1	M	135	LEU	3.0
1	I	173	LEU	2.9
1	K	475	LEU	2.9
1	G	57	ALA	2.9
1	F	374	PHE	2.9
1	J	376	ARG	2.8
1	I	125	VAL	2.8
1	E	383	GLU	2.8
1	I	128	PHE	2.8
1	D	29	ALA	2.8
1	I	154	ALA	2.8
1	F	7	GLY	2.8
1	L	327	ARG	2.8
1	P	299	PRO	2.8
1	F	412	GLU	2.8
1	N	242	LEU	2.8
1	K	385	TYR	2.7
1	G	3	ARG	2.7
1	O	426	ARG	2.7
1	G	121	HIS	2.7
1	B	130	GLY	2.7
1	K	374	PHE	2.7
1	L	155	LEU	2.7
1	I	127	VAL	2.7
1	P	188	ASP	2.7
1	K	300	GLY	2.7
1	M	138	GLU	2.7
1	I	394	ALA	2.7
1	G	122	GLY	2.7
1	B	158	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	N	135	LEU	2.7
1	F	371	ASP	2.7
1	N	192	ALA	2.6
1	P	469	PHE	2.6
1	C	133	ILE	2.6
1	C	419	ARG	2.6
1	G	425	ALA	2.6
1	F	302	MET	2.6
1	M	274	GLY	2.6
1	N	374	PHE	2.6
1	O	176	HIS	2.6
1	B	105	PRO	2.5
1	E	152	ASP	2.5
1	O	477	ALA	2.5
1	K	151	ARG	2.5
1	J	362	PHE	2.5
1	J	395	ALA	2.5
1	N	123	ALA	2.5
1	A	174	LEU	2.5
1	K	403	PHE	2.5
1	M	158	PHE	2.5
1	I	426	ARG	2.5
1	A	178	PRO	2.5
1	C	105	PRO	2.5
1	N	388	ALA	2.5
1	L	410	LEU	2.5
1	K	426	ARG	2.5
1	N	178	PRO	2.5
1	N	157	ASP	2.5
1	G	373	LEU	2.5
1	N	2	VAL	2.4
1	B	384	SER	2.4
1	G	385	TYR	2.4
1	G	4	PHE	2.4
1	B	403	PHE	2.4
1	N	340	ARG	2.4
1	O	120	ALA	2.4
1	E	48	VAL	2.4
1	G	212	ALA	2.4
1	J	469	PHE	2.4
1	M	475	LEU	2.4
1	N	265	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	381	TYR	2.4
1	H	192	ALA	2.4
1	M	154	ALA	2.4
1	E	170	VAL	2.3
1	I	435	HIS	2.3
1	F	415	ILE	2.3
1	F	32	PHE	2.3
1	K	377	ASP	2.3
1	G	243	LEU	2.3
1	I	135	LEU	2.3
1	L	271	LEU	2.3
1	O	181	VAL	2.3
1	J	201	ILE	2.3
1	F	406	ALA	2.3
1	P	466	ALA	2.3
1	O	469	PHE	2.3
1	C	139	ALA	2.3
1	J	327	ARG	2.3
1	J	468	GLY	2.3
1	A	191	LEU	2.3
1	B	115	LEU	2.3
1	K	280	GLU	2.3
1	E	426	ARG	2.3
1	J	122	GLY	2.3
1	N	476	PRO	2.2
1	F	77	ASP	2.2
1	B	133	ILE	2.2
1	K	220	ALA	2.2
1	G	29	ALA	2.2
1	I	71	ILE	2.2
1	B	373	LEU	2.2
1	K	298	GLY	2.2
1	G	74	LEU	2.2
1	G	116	LEU	2.2
1	H	191	LEU	2.2
1	J	178	PRO	2.2
1	N	424	PRO	2.2
1	A	169	GLU	2.2
1	G	245	ILE	2.2
1	E	378	ASP	2.2
1	J	180	ASP	2.2
1	C	4	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	407	ARG	2.2
1	H	426	ARG	2.2
1	N	372	LEU	2.2
1	O	475	LEU	2.2
1	G	466	ALA	2.1
1	M	171	PHE	2.1
1	F	381	TYR	2.1
1	C	128	PHE	2.1
1	D	469	PHE	2.1
1	G	76	GLN	2.1
1	B	389	SER	2.1
1	G	12	TYR	2.1
1	O	179	ILE	2.1
1	F	103	LEU	2.1
1	G	242	LEU	2.1
1	G	452	LEU	2.1
1	M	156	SER	2.1
1	E	404	ASP	2.1
1	K	372	LEU	2.1
1	A	159	VAL	2.1
1	C	179	ILE	2.1
1	G	416	SER	2.1
1	I	158	PHE	2.1
1	K	111	ASP	2.1
1	I	267	LEU	2.1
1	N	147	PHE	2.1
1	G	412	GLU	2.1
1	N	254	LYS	2.1
1	N	466	ALA	2.1
1	F	128	PHE	2.1
1	K	74	LEU	2.1
1	F	180	ASP	2.0
1	L	256	LEU	2.0
1	H	24	GLY	2.0
1	P	143	GLY	2.0
1	K	55	ALA	2.0
1	B	157	ASP	2.0
1	J	424	PRO	2.0
1	J	48	VAL	2.0
1	H	405	ARG	2.0
1	G	372	LEU	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

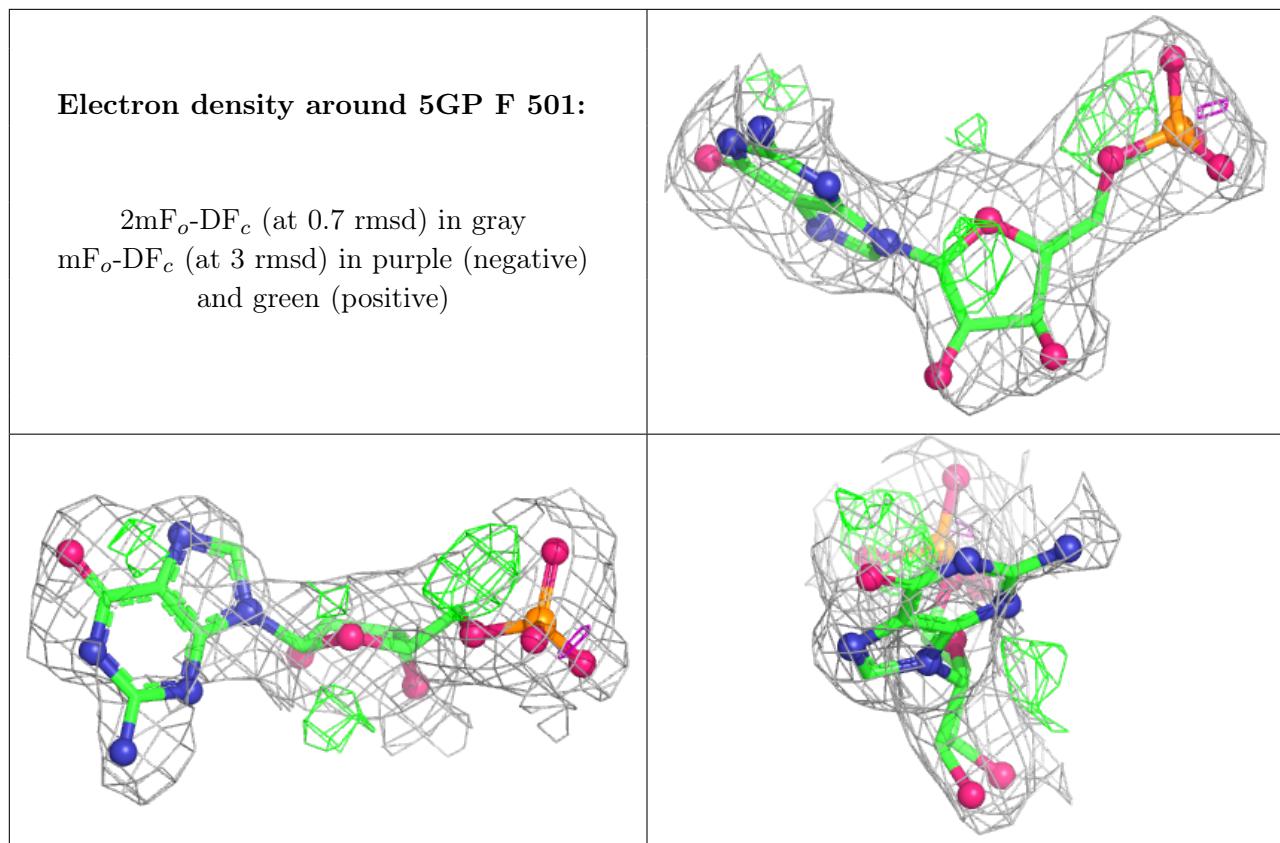
There are no monosaccharides in this entry.

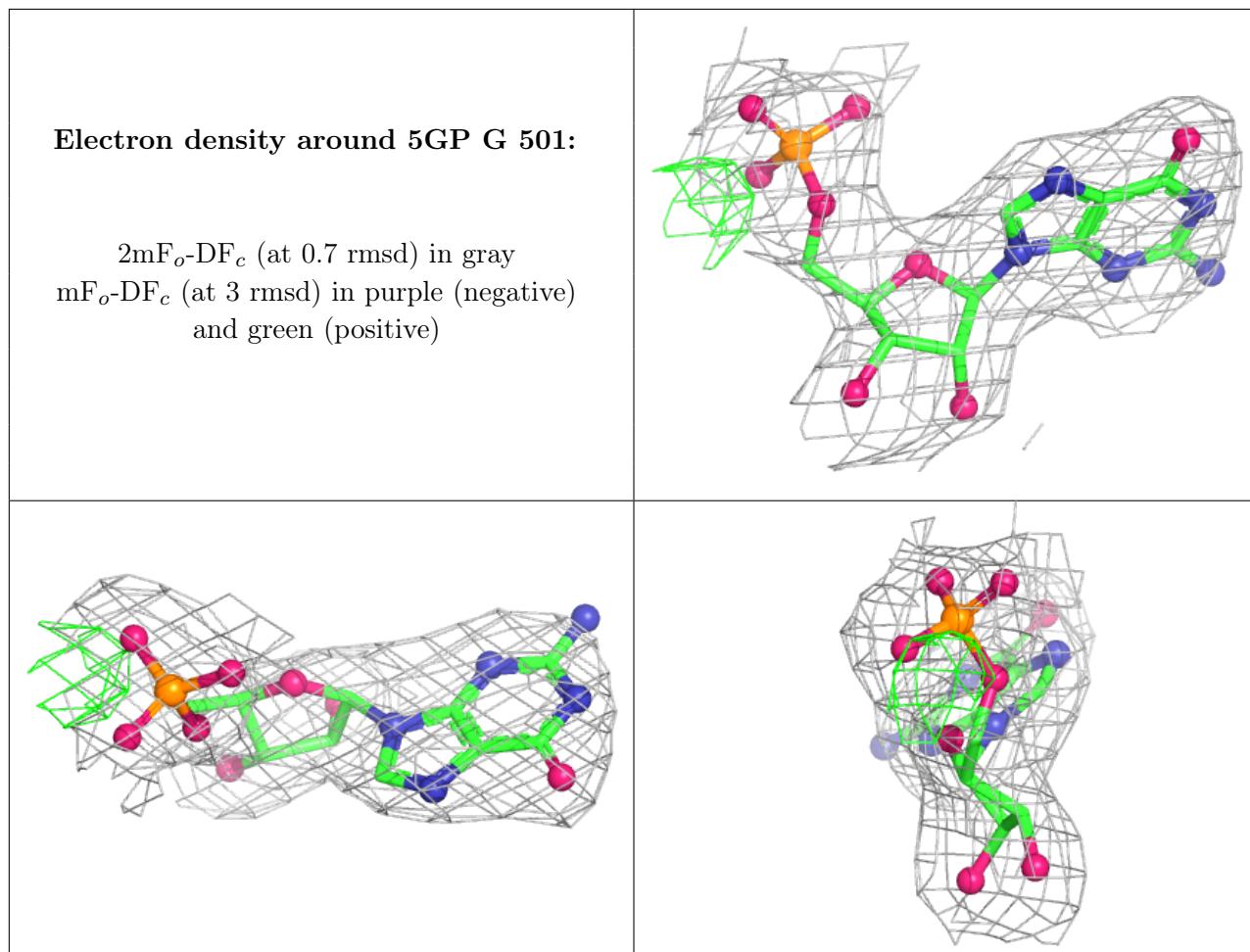
6.4 Ligands [\(i\)](#)

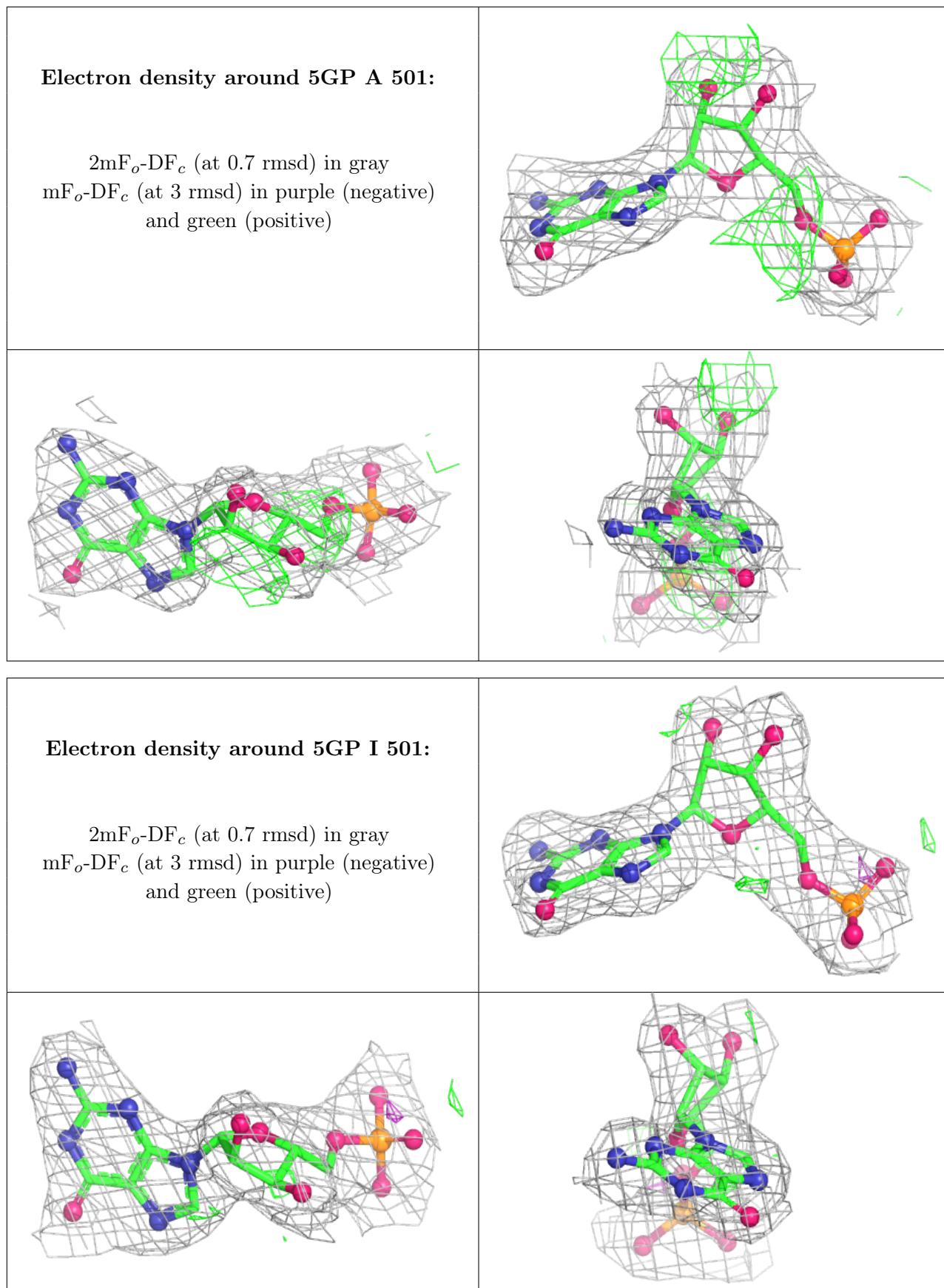
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

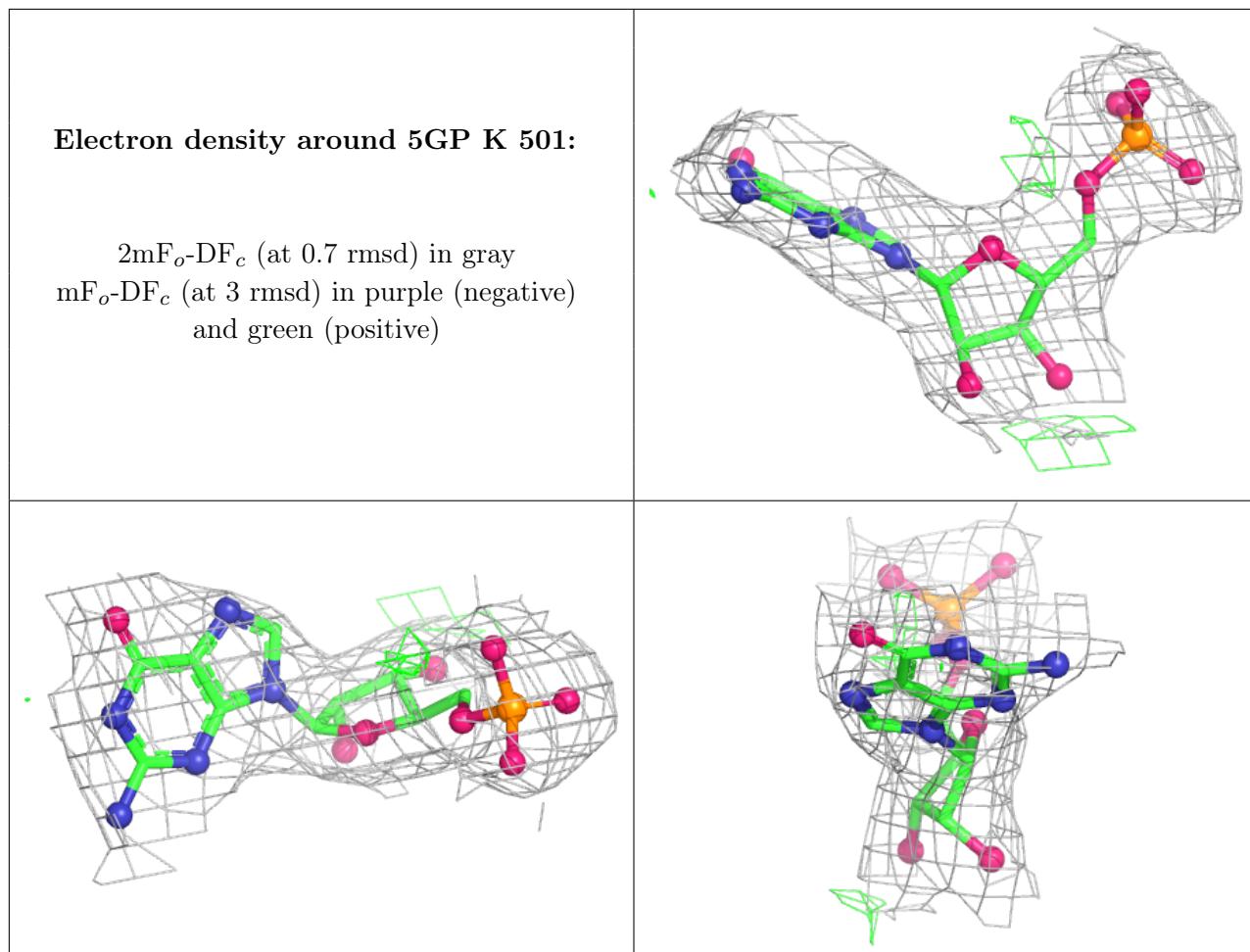
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	5GP	F	501	24/24	0.86	0.18	61,79,87,92	0
2	5GP	G	501	24/24	0.90	0.14	56,68,76,80	0
2	5GP	A	501	24/24	0.92	0.15	34,48,53,54	0
2	5GP	I	501	24/24	0.93	0.11	41,56,62,67	0
2	5GP	K	501	24/24	0.93	0.13	53,66,82,85	0
2	5GP	L	501	24/24	0.93	0.13	44,59,66,68	0
2	5GP	P	501	24/24	0.93	0.14	47,53,60,64	0
2	5GP	M	501	24/24	0.94	0.14	38,46,54,59	0
2	5GP	N	501	24/24	0.94	0.13	45,56,65,69	0
2	5GP	C	501	24/24	0.94	0.12	43,50,57,64	0
2	5GP	J	501	24/24	0.95	0.11	46,53,61,62	0
2	5GP	D	501	24/24	0.95	0.14	34,43,49,58	0
2	5GP	O	501	24/24	0.96	0.11	41,54,62,66	0
2	5GP	H	501	24/24	0.97	0.11	37,50,54,59	0
2	5GP	B	501	24/24	0.97	0.11	38,55,64,66	0
2	5GP	E	501	24/24	0.97	0.09	28,48,55,64	0

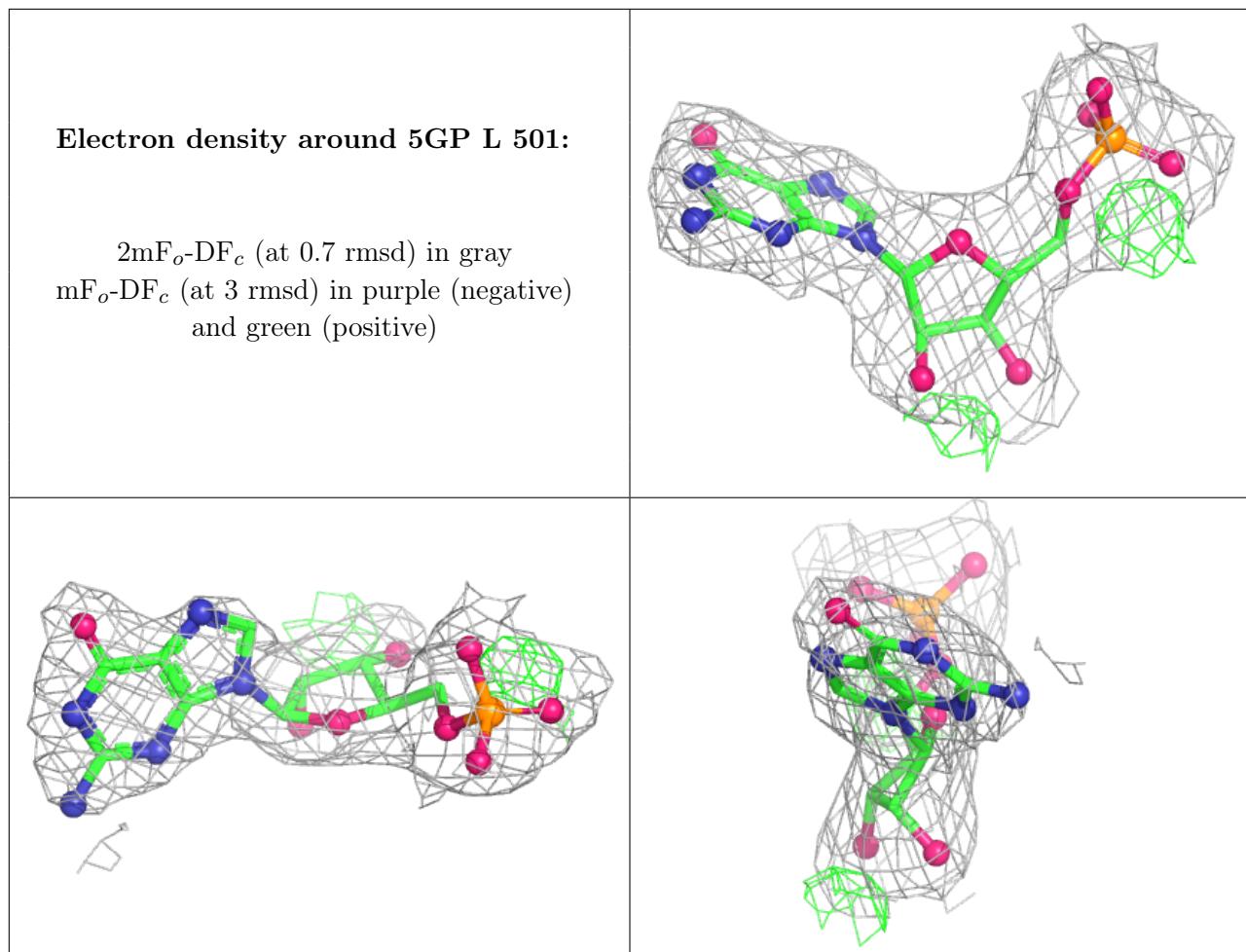
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

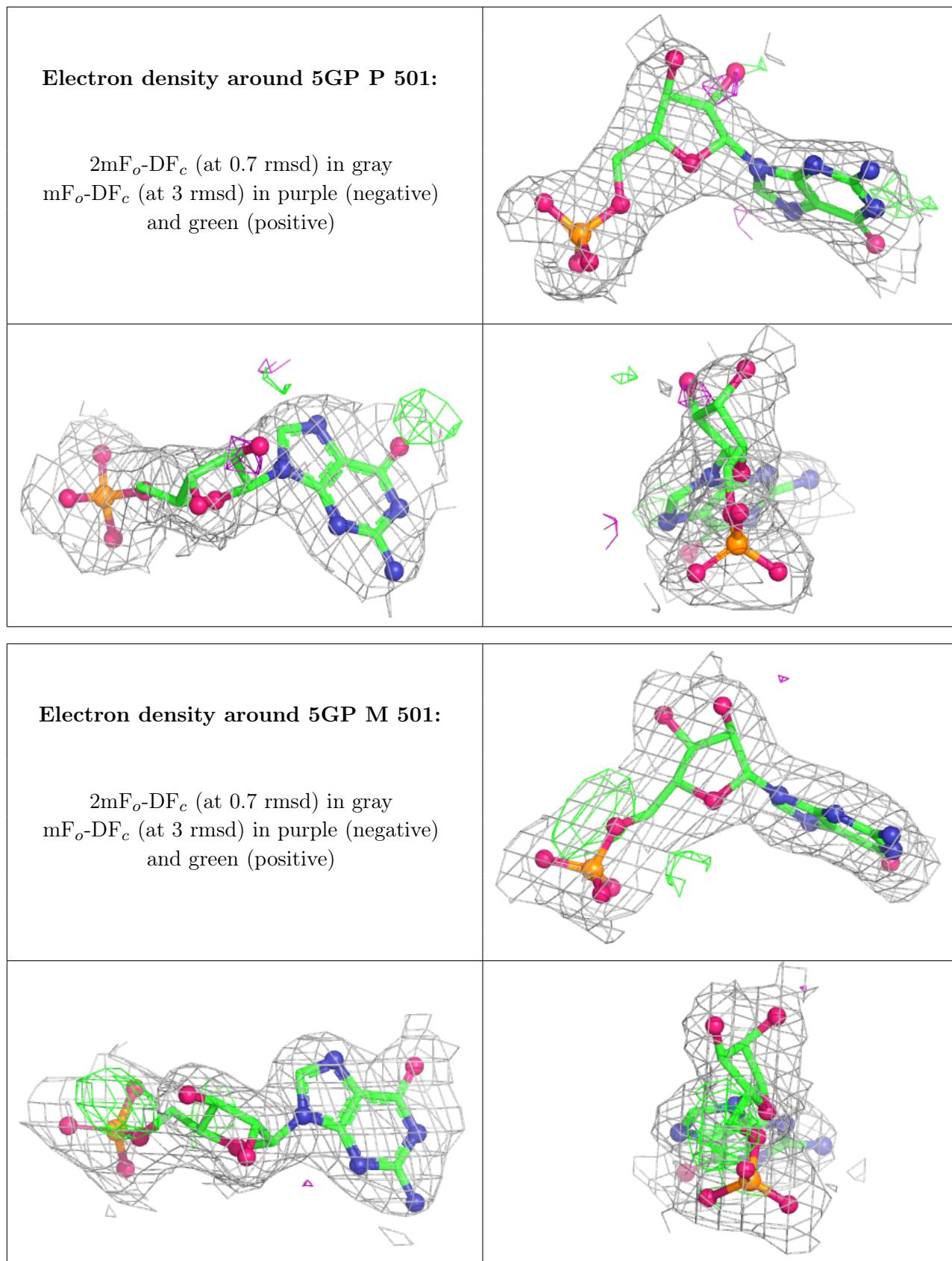


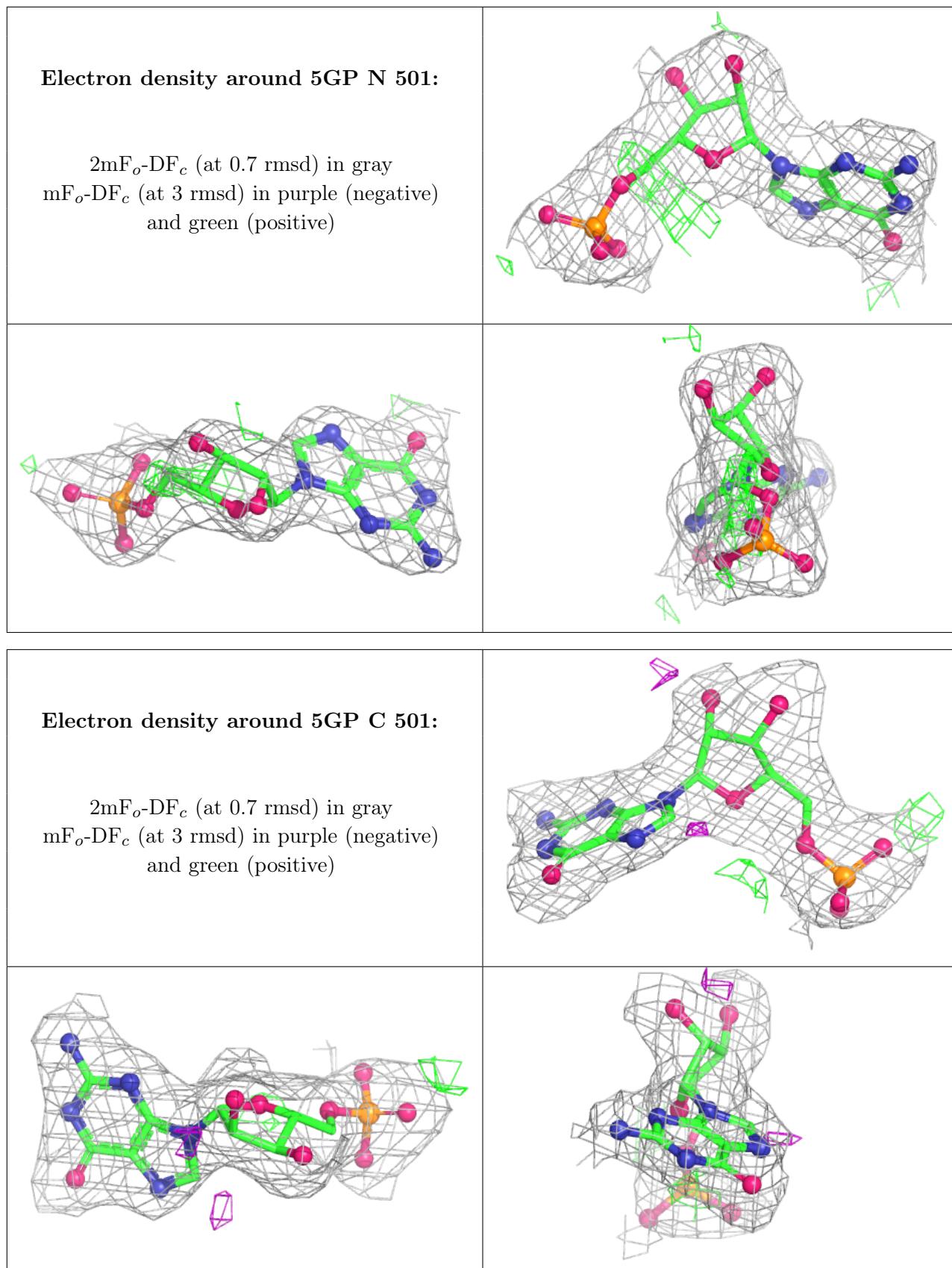


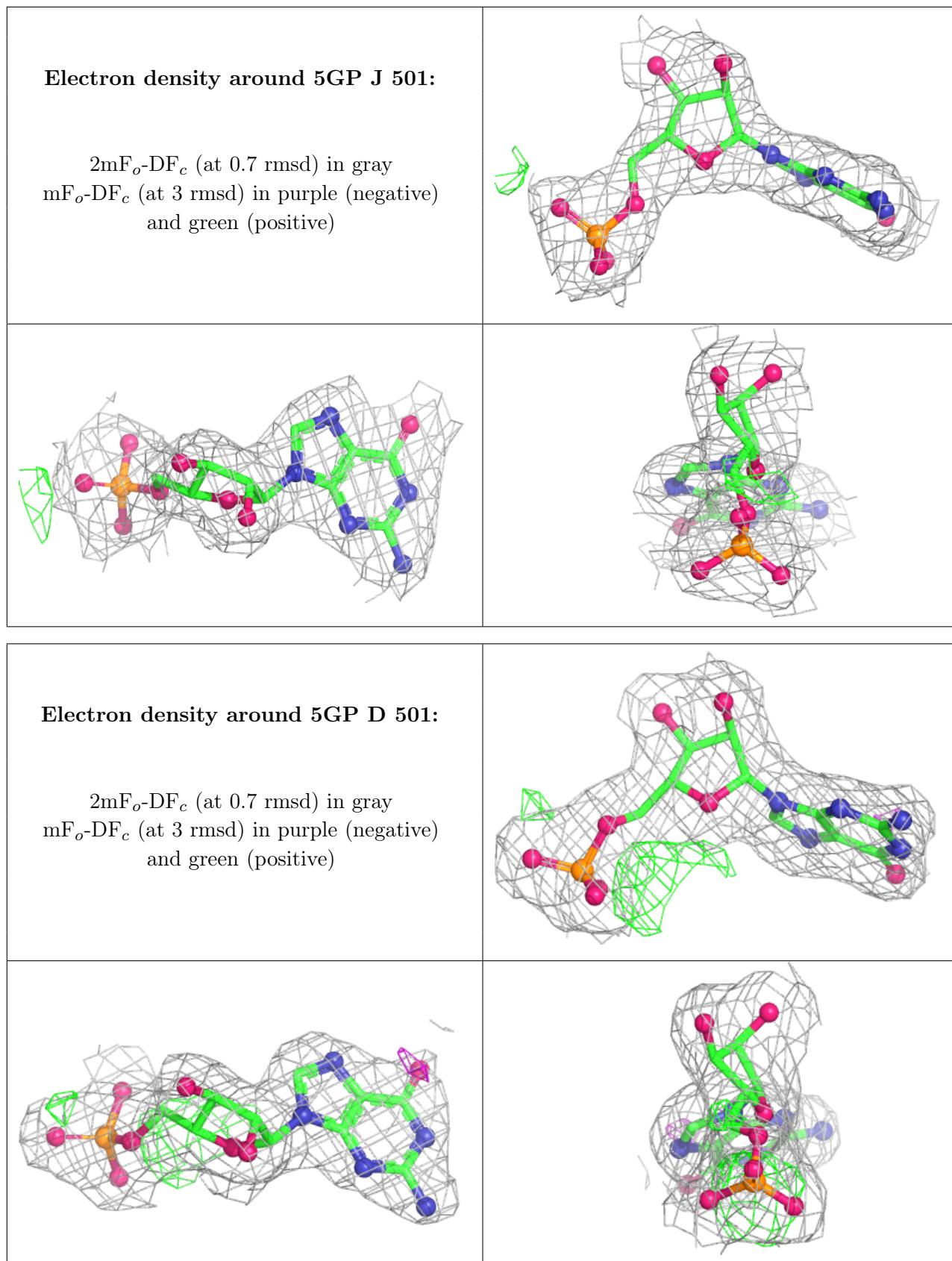


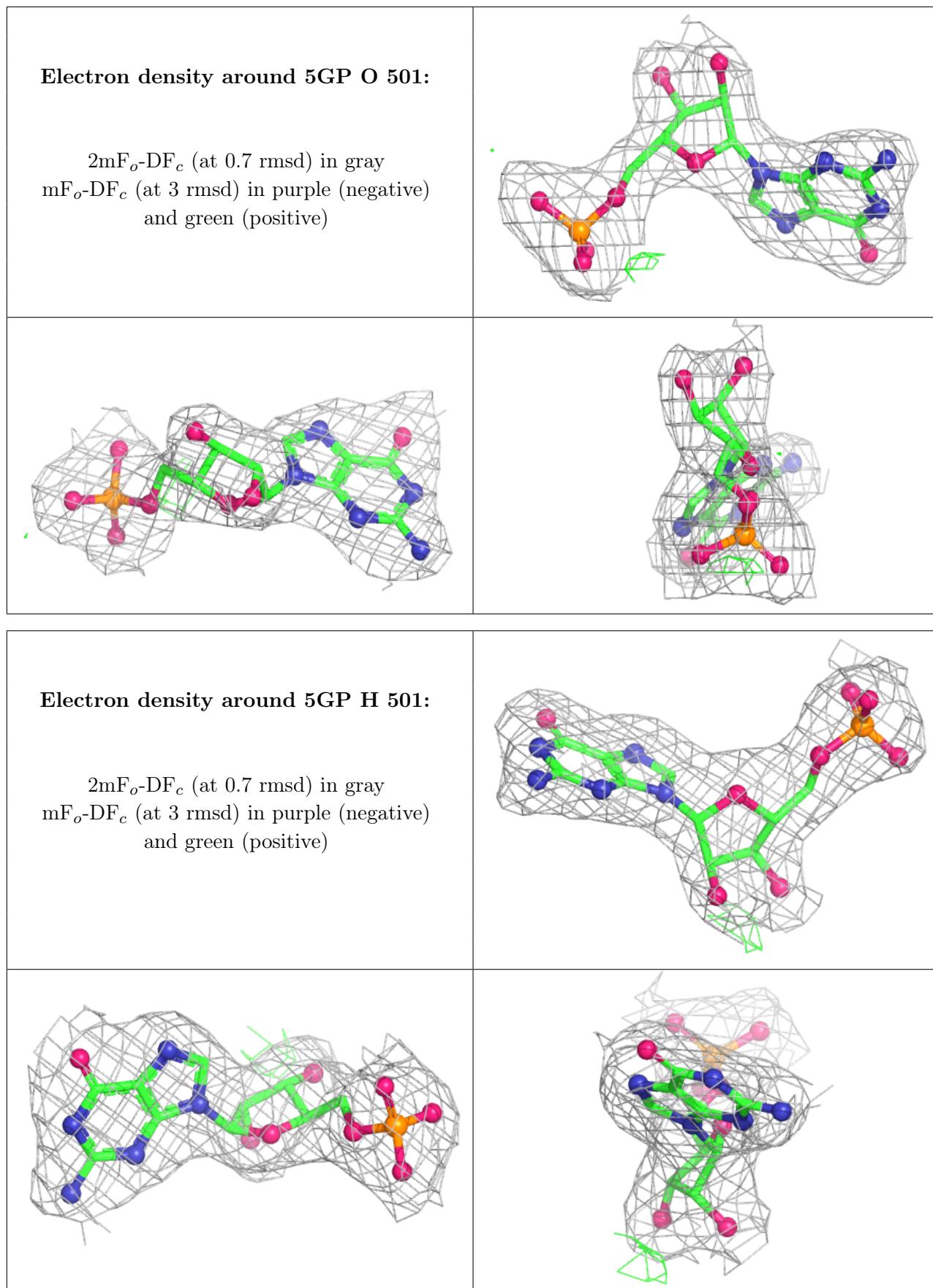


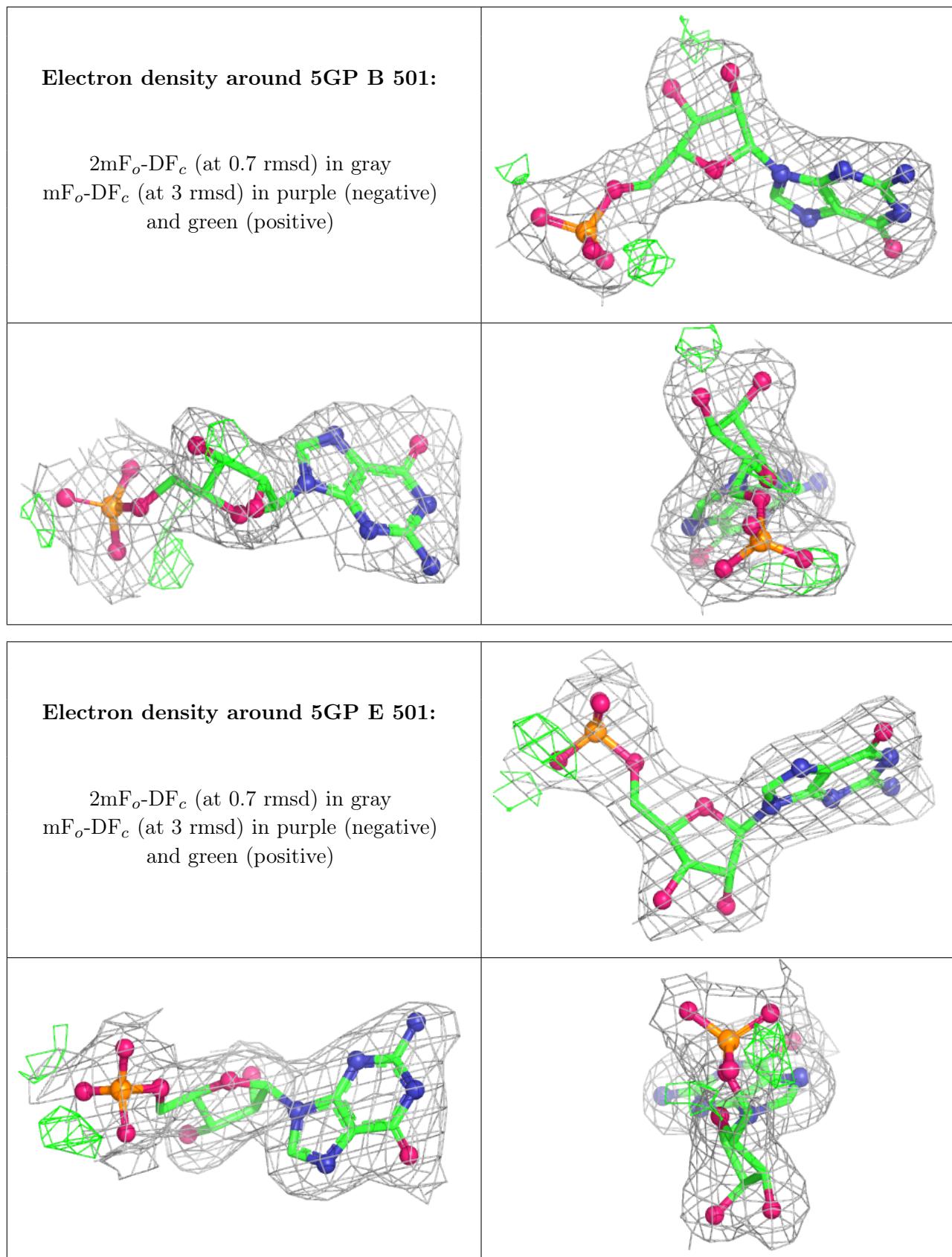












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.