Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 02:48 PM EST

PDB ID	:	3CMV
Title	:	Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors	:	Pavletich, N.P.
Deposited on	:	2008-03-24
Resolution	:	4.30 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

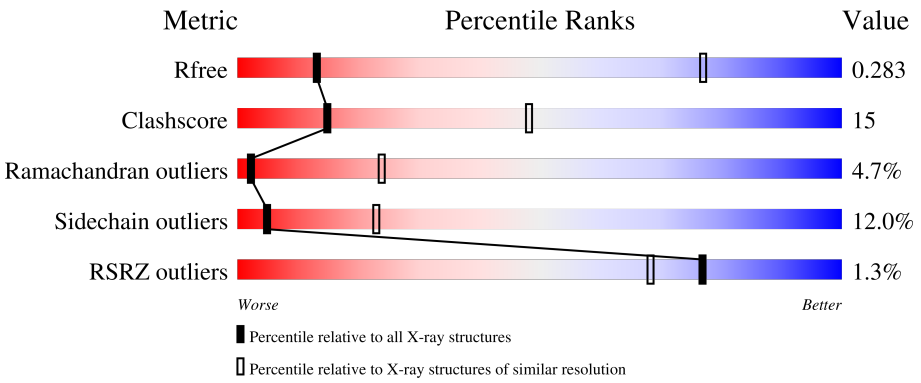
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.30 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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 <=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	1357	.% 55% 27% 6% • 12%
1	B	1357	.% 54% 27% 5% 14%
1	C	1357	.% 54% 27% 5% 13%
1	D	1357	2% 55% 27% 5% 13%
1	E	1357	.% 53% 27% 5% 14%

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Mol	Chain	Length	Quality of chain
1	F	1357	54% 27% 5% 13%
1	G	1357	54% 27% 5% 14%
1	H	1357	53% 28% 5% 14%

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	MG	B	1701	-	-	-	X
2	MG	C	701	-	-	-	X
2	MG	D	1701	-	-	-	X
2	MG	D	701	-	-	-	X
2	MG	E	701	-	-	-	X
2	MG	G	701	-	-	-	X
3	ANP	A	1400	X	-	-	-
3	ANP	A	2400	X	-	-	-
3	ANP	A	3400	X	-	-	-
3	ANP	A	400	X	-	-	-
3	ANP	B	1400	X	-	-	-
3	ANP	B	2400	X	-	-	-
3	ANP	B	3400	X	-	-	-
3	ANP	B	400	X	-	-	-
3	ANP	C	1400	X	-	-	-
3	ANP	C	2400	X	-	-	-
3	ANP	C	3400	X	-	-	-
3	ANP	C	400	X	-	-	-
3	ANP	D	1400	X	-	-	-
3	ANP	D	2400	X	-	-	-
3	ANP	D	3400	X	-	-	-
3	ANP	D	400	X	-	-	-
3	ANP	E	1400	X	-	-	-
3	ANP	E	2400	X	-	-	-
3	ANP	E	3400	X	-	-	-
3	ANP	E	400	X	-	-	-
3	ANP	F	1400	X	-	-	-
3	ANP	F	2400	X	-	-	X
3	ANP	F	3400	X	-	-	-
3	ANP	F	400	X	-	-	-
3	ANP	G	1400	X	-	-	-
3	ANP	G	2400	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ANP	G	3400	X	-	-	-
3	ANP	G	400	X	-	-	-
3	ANP	H	1400	X	-	-	-
3	ANP	H	2400	X	-	-	-
3	ANP	H	3400	X	-	-	-
3	ANP	H	400	X	-	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 71761 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 Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1190	8970	5660	1553	1719	38	0	0	0
1	B	1163	8769	5538	1519	1677	35	0	0	0
1	C	1175	8856	5587	1533	1700	36	0	0	0
1	D	1175	8856	5587	1533	1700	36	0	0	0
1	E	1165	8787	5548	1521	1683	35	0	0	0
1	F	1175	8856	5587	1533	1700	36	0	0	0
1	G	1167	8799	5554	1523	1687	35	0	0	0
1	H	1173	8844	5581	1531	1696	36	0	0	0

There are 400 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	linker	UNP P0A7G6
A	27	ALA	-	linker	UNP P0A7G6
A	28	MET	-	linker	UNP P0A7G6
A	29	HIS	-	linker	UNP P0A7G6
A	986	THR	-	linker	UNP P0A7G6
A	987	GLY	-	linker	UNP P0A7G6
A	988	SER	-	linker	UNP P0A7G6
A	989	THR	-	linker	UNP P0A7G6
A	990	GLY	-	linker	UNP P0A7G6
A	991	SER	-	linker	UNP P0A7G6
A	992	GLY	-	linker	UNP P0A7G6
A	993	THR	-	linker	UNP P0A7G6
A	994	THR	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	995	GLY	-	linker	UNP P0A7G6
A	996	SER	-	linker	UNP P0A7G6
A	997	THR	-	linker	UNP P0A7G6
A	998	GLY	-	linker	UNP P0A7G6
A	999	SER	-	linker	UNP P0A7G6
A	1000	MET	-	linker	UNP P0A7G6
A	1986	THR	-	linker	UNP P0A7G6
A	1987	GLY	-	linker	UNP P0A7G6
A	1988	SER	-	linker	UNP P0A7G6
A	1989	THR	-	linker	UNP P0A7G6
A	1990	GLY	-	linker	UNP P0A7G6
A	1991	SER	-	linker	UNP P0A7G6
A	1992	MET	-	linker	UNP P0A7G6
A	1993	GLY	-	linker	UNP P0A7G6
A	1994	HIS	-	linker	UNP P0A7G6
A	1995	THR	-	linker	UNP P0A7G6
A	1996	THR	-	linker	UNP P0A7G6
A	1997	GLY	-	linker	UNP P0A7G6
A	1998	SER	-	linker	UNP P0A7G6
A	1999	MET	-	linker	UNP P0A7G6
A	2000	SER	-	linker	UNP P0A7G6
A	2985	THR	-	linker	UNP P0A7G6
A	2986	GLY	-	linker	UNP P0A7G6
A	2987	SER	-	linker	UNP P0A7G6
A	2988	THR	-	linker	UNP P0A7G6
A	2989	GLY	-	linker	UNP P0A7G6
A	2990	SER	-	linker	UNP P0A7G6
A	2991	ALA	-	linker	UNP P0A7G6
A	2992	SER	-	linker	UNP P0A7G6
A	2993	GLY	-	linker	UNP P0A7G6
A	2994	SER	-	linker	UNP P0A7G6
A	2995	SER	-	linker	UNP P0A7G6
A	2996	THR	-	linker	UNP P0A7G6
A	2997	GLY	-	linker	UNP P0A7G6
A	2998	SER	-	linker	UNP P0A7G6
A	2999	MET	-	linker	UNP P0A7G6
A	3000	SER	-	linker	UNP P0A7G6
B	26	GLY	-	linker	UNP P0A7G6
B	27	ALA	-	linker	UNP P0A7G6
B	28	MET	-	linker	UNP P0A7G6
B	29	HIS	-	linker	UNP P0A7G6
B	986	THR	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	987	GLY	-	linker	UNP P0A7G6
B	988	SER	-	linker	UNP P0A7G6
B	989	THR	-	linker	UNP P0A7G6
B	990	GLY	-	linker	UNP P0A7G6
B	991	SER	-	linker	UNP P0A7G6
B	992	GLY	-	linker	UNP P0A7G6
B	993	THR	-	linker	UNP P0A7G6
B	994	THR	-	linker	UNP P0A7G6
B	995	GLY	-	linker	UNP P0A7G6
B	996	SER	-	linker	UNP P0A7G6
B	997	THR	-	linker	UNP P0A7G6
B	998	GLY	-	linker	UNP P0A7G6
B	999	SER	-	linker	UNP P0A7G6
B	1000	MET	-	linker	UNP P0A7G6
B	1986	THR	-	linker	UNP P0A7G6
B	1987	GLY	-	linker	UNP P0A7G6
B	1988	SER	-	linker	UNP P0A7G6
B	1989	THR	-	linker	UNP P0A7G6
B	1990	GLY	-	linker	UNP P0A7G6
B	1991	SER	-	linker	UNP P0A7G6
B	1992	MET	-	linker	UNP P0A7G6
B	1993	GLY	-	linker	UNP P0A7G6
B	1994	HIS	-	linker	UNP P0A7G6
B	1995	THR	-	linker	UNP P0A7G6
B	1996	THR	-	linker	UNP P0A7G6
B	1997	GLY	-	linker	UNP P0A7G6
B	1998	SER	-	linker	UNP P0A7G6
B	1999	MET	-	linker	UNP P0A7G6
B	2000	SER	-	linker	UNP P0A7G6
B	2985	THR	-	linker	UNP P0A7G6
B	2986	GLY	-	linker	UNP P0A7G6
B	2987	SER	-	linker	UNP P0A7G6
B	2988	THR	-	linker	UNP P0A7G6
B	2989	GLY	-	linker	UNP P0A7G6
B	2990	SER	-	linker	UNP P0A7G6
B	2991	ALA	-	linker	UNP P0A7G6
B	2992	SER	-	linker	UNP P0A7G6
B	2993	GLY	-	linker	UNP P0A7G6
B	2994	SER	-	linker	UNP P0A7G6
B	2995	SER	-	linker	UNP P0A7G6
B	2996	THR	-	linker	UNP P0A7G6
B	2997	GLY	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2998	SER	-	linker	UNP P0A7G6
B	2999	MET	-	linker	UNP P0A7G6
B	3000	SER	-	linker	UNP P0A7G6
C	26	GLY	-	linker	UNP P0A7G6
C	27	ALA	-	linker	UNP P0A7G6
C	28	MET	-	linker	UNP P0A7G6
C	29	HIS	-	linker	UNP P0A7G6
C	986	THR	-	linker	UNP P0A7G6
C	987	GLY	-	linker	UNP P0A7G6
C	988	SER	-	linker	UNP P0A7G6
C	989	THR	-	linker	UNP P0A7G6
C	990	GLY	-	linker	UNP P0A7G6
C	991	SER	-	linker	UNP P0A7G6
C	992	GLY	-	linker	UNP P0A7G6
C	993	THR	-	linker	UNP P0A7G6
C	994	THR	-	linker	UNP P0A7G6
C	995	GLY	-	linker	UNP P0A7G6
C	996	SER	-	linker	UNP P0A7G6
C	997	THR	-	linker	UNP P0A7G6
C	998	GLY	-	linker	UNP P0A7G6
C	999	SER	-	linker	UNP P0A7G6
C	1000	MET	-	linker	UNP P0A7G6
C	1986	THR	-	linker	UNP P0A7G6
C	1987	GLY	-	linker	UNP P0A7G6
C	1988	SER	-	linker	UNP P0A7G6
C	1989	THR	-	linker	UNP P0A7G6
C	1990	GLY	-	linker	UNP P0A7G6
C	1991	SER	-	linker	UNP P0A7G6
C	1992	MET	-	linker	UNP P0A7G6
C	1993	GLY	-	linker	UNP P0A7G6
C	1994	HIS	-	linker	UNP P0A7G6
C	1995	THR	-	linker	UNP P0A7G6
C	1996	THR	-	linker	UNP P0A7G6
C	1997	GLY	-	linker	UNP P0A7G6
C	1998	SER	-	linker	UNP P0A7G6
C	1999	MET	-	linker	UNP P0A7G6
C	2000	SER	-	linker	UNP P0A7G6
C	2985	THR	-	linker	UNP P0A7G6
C	2986	GLY	-	linker	UNP P0A7G6
C	2987	SER	-	linker	UNP P0A7G6
C	2988	THR	-	linker	UNP P0A7G6
C	2989	GLY	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2990	SER	-	linker	UNP P0A7G6
C	2991	ALA	-	linker	UNP P0A7G6
C	2992	SER	-	linker	UNP P0A7G6
C	2993	GLY	-	linker	UNP P0A7G6
C	2994	SER	-	linker	UNP P0A7G6
C	2995	SER	-	linker	UNP P0A7G6
C	2996	THR	-	linker	UNP P0A7G6
C	2997	GLY	-	linker	UNP P0A7G6
C	2998	SER	-	linker	UNP P0A7G6
C	2999	MET	-	linker	UNP P0A7G6
C	3000	SER	-	linker	UNP P0A7G6
D	26	GLY	-	linker	UNP P0A7G6
D	27	ALA	-	linker	UNP P0A7G6
D	28	MET	-	linker	UNP P0A7G6
D	29	HIS	-	linker	UNP P0A7G6
D	986	THR	-	linker	UNP P0A7G6
D	987	GLY	-	linker	UNP P0A7G6
D	988	SER	-	linker	UNP P0A7G6
D	989	THR	-	linker	UNP P0A7G6
D	990	GLY	-	linker	UNP P0A7G6
D	991	SER	-	linker	UNP P0A7G6
D	992	GLY	-	linker	UNP P0A7G6
D	993	THR	-	linker	UNP P0A7G6
D	994	THR	-	linker	UNP P0A7G6
D	995	GLY	-	linker	UNP P0A7G6
D	996	SER	-	linker	UNP P0A7G6
D	997	THR	-	linker	UNP P0A7G6
D	998	GLY	-	linker	UNP P0A7G6
D	999	SER	-	linker	UNP P0A7G6
D	1000	MET	-	linker	UNP P0A7G6
D	1986	THR	-	linker	UNP P0A7G6
D	1987	GLY	-	linker	UNP P0A7G6
D	1988	SER	-	linker	UNP P0A7G6
D	1989	THR	-	linker	UNP P0A7G6
D	1990	GLY	-	linker	UNP P0A7G6
D	1991	SER	-	linker	UNP P0A7G6
D	1992	MET	-	linker	UNP P0A7G6
D	1993	GLY	-	linker	UNP P0A7G6
D	1994	HIS	-	linker	UNP P0A7G6
D	1995	THR	-	linker	UNP P0A7G6
D	1996	THR	-	linker	UNP P0A7G6
D	1997	GLY	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1998	SER	-	linker	UNP P0A7G6
D	1999	MET	-	linker	UNP P0A7G6
D	2000	SER	-	linker	UNP P0A7G6
D	2985	THR	-	linker	UNP P0A7G6
D	2986	GLY	-	linker	UNP P0A7G6
D	2987	SER	-	linker	UNP P0A7G6
D	2988	THR	-	linker	UNP P0A7G6
D	2989	GLY	-	linker	UNP P0A7G6
D	2990	SER	-	linker	UNP P0A7G6
D	2991	ALA	-	linker	UNP P0A7G6
D	2992	SER	-	linker	UNP P0A7G6
D	2993	GLY	-	linker	UNP P0A7G6
D	2994	SER	-	linker	UNP P0A7G6
D	2995	SER	-	linker	UNP P0A7G6
D	2996	THR	-	linker	UNP P0A7G6
D	2997	GLY	-	linker	UNP P0A7G6
D	2998	SER	-	linker	UNP P0A7G6
D	2999	MET	-	linker	UNP P0A7G6
D	3000	SER	-	linker	UNP P0A7G6
E	26	GLY	-	linker	UNP P0A7G6
E	27	ALA	-	linker	UNP P0A7G6
E	28	MET	-	linker	UNP P0A7G6
E	29	HIS	-	linker	UNP P0A7G6
E	986	THR	-	linker	UNP P0A7G6
E	987	GLY	-	linker	UNP P0A7G6
E	988	SER	-	linker	UNP P0A7G6
E	989	THR	-	linker	UNP P0A7G6
E	990	GLY	-	linker	UNP P0A7G6
E	991	SER	-	linker	UNP P0A7G6
E	992	GLY	-	linker	UNP P0A7G6
E	993	THR	-	linker	UNP P0A7G6
E	994	THR	-	linker	UNP P0A7G6
E	995	GLY	-	linker	UNP P0A7G6
E	996	SER	-	linker	UNP P0A7G6
E	997	THR	-	linker	UNP P0A7G6
E	998	GLY	-	linker	UNP P0A7G6
E	999	SER	-	linker	UNP P0A7G6
E	1000	MET	-	linker	UNP P0A7G6
E	1986	THR	-	linker	UNP P0A7G6
E	1987	GLY	-	linker	UNP P0A7G6
E	1988	SER	-	linker	UNP P0A7G6
E	1989	THR	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1990	GLY	-	linker	UNP P0A7G6
E	1991	SER	-	linker	UNP P0A7G6
E	1992	MET	-	linker	UNP P0A7G6
E	1993	GLY	-	linker	UNP P0A7G6
E	1994	HIS	-	linker	UNP P0A7G6
E	1995	THR	-	linker	UNP P0A7G6
E	1996	THR	-	linker	UNP P0A7G6
E	1997	GLY	-	linker	UNP P0A7G6
E	1998	SER	-	linker	UNP P0A7G6
E	1999	MET	-	linker	UNP P0A7G6
E	2000	SER	-	linker	UNP P0A7G6
E	2985	THR	-	linker	UNP P0A7G6
E	2986	GLY	-	linker	UNP P0A7G6
E	2987	SER	-	linker	UNP P0A7G6
E	2988	THR	-	linker	UNP P0A7G6
E	2989	GLY	-	linker	UNP P0A7G6
E	2990	SER	-	linker	UNP P0A7G6
E	2991	ALA	-	linker	UNP P0A7G6
E	2992	SER	-	linker	UNP P0A7G6
E	2993	GLY	-	linker	UNP P0A7G6
E	2994	SER	-	linker	UNP P0A7G6
E	2995	SER	-	linker	UNP P0A7G6
E	2996	THR	-	linker	UNP P0A7G6
E	2997	GLY	-	linker	UNP P0A7G6
E	2998	SER	-	linker	UNP P0A7G6
E	2999	MET	-	linker	UNP P0A7G6
E	3000	SER	-	linker	UNP P0A7G6
F	26	GLY	-	linker	UNP P0A7G6
F	27	ALA	-	linker	UNP P0A7G6
F	28	MET	-	linker	UNP P0A7G6
F	29	HIS	-	linker	UNP P0A7G6
F	986	THR	-	linker	UNP P0A7G6
F	987	GLY	-	linker	UNP P0A7G6
F	988	SER	-	linker	UNP P0A7G6
F	989	THR	-	linker	UNP P0A7G6
F	990	GLY	-	linker	UNP P0A7G6
F	991	SER	-	linker	UNP P0A7G6
F	992	GLY	-	linker	UNP P0A7G6
F	993	THR	-	linker	UNP P0A7G6
F	994	THR	-	linker	UNP P0A7G6
F	995	GLY	-	linker	UNP P0A7G6
F	996	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	997	THR	-	linker	UNP P0A7G6
F	998	GLY	-	linker	UNP P0A7G6
F	999	SER	-	linker	UNP P0A7G6
F	1000	MET	-	linker	UNP P0A7G6
F	1986	THR	-	linker	UNP P0A7G6
F	1987	GLY	-	linker	UNP P0A7G6
F	1988	SER	-	linker	UNP P0A7G6
F	1989	THR	-	linker	UNP P0A7G6
F	1990	GLY	-	linker	UNP P0A7G6
F	1991	SER	-	linker	UNP P0A7G6
F	1992	MET	-	linker	UNP P0A7G6
F	1993	GLY	-	linker	UNP P0A7G6
F	1994	HIS	-	linker	UNP P0A7G6
F	1995	THR	-	linker	UNP P0A7G6
F	1996	THR	-	linker	UNP P0A7G6
F	1997	GLY	-	linker	UNP P0A7G6
F	1998	SER	-	linker	UNP P0A7G6
F	1999	MET	-	linker	UNP P0A7G6
F	2000	SER	-	linker	UNP P0A7G6
F	2985	THR	-	linker	UNP P0A7G6
F	2986	GLY	-	linker	UNP P0A7G6
F	2987	SER	-	linker	UNP P0A7G6
F	2988	THR	-	linker	UNP P0A7G6
F	2989	GLY	-	linker	UNP P0A7G6
F	2990	SER	-	linker	UNP P0A7G6
F	2991	ALA	-	linker	UNP P0A7G6
F	2992	SER	-	linker	UNP P0A7G6
F	2993	GLY	-	linker	UNP P0A7G6
F	2994	SER	-	linker	UNP P0A7G6
F	2995	SER	-	linker	UNP P0A7G6
F	2996	THR	-	linker	UNP P0A7G6
F	2997	GLY	-	linker	UNP P0A7G6
F	2998	SER	-	linker	UNP P0A7G6
F	2999	MET	-	linker	UNP P0A7G6
F	3000	SER	-	linker	UNP P0A7G6
G	26	GLY	-	linker	UNP P0A7G6
G	27	ALA	-	linker	UNP P0A7G6
G	28	MET	-	linker	UNP P0A7G6
G	29	HIS	-	linker	UNP P0A7G6
G	986	THR	-	linker	UNP P0A7G6
G	987	GLY	-	linker	UNP P0A7G6
G	988	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	989	THR	-	linker	UNP P0A7G6
G	990	GLY	-	linker	UNP P0A7G6
G	991	SER	-	linker	UNP P0A7G6
G	992	GLY	-	linker	UNP P0A7G6
G	993	THR	-	linker	UNP P0A7G6
G	994	THR	-	linker	UNP P0A7G6
G	995	GLY	-	linker	UNP P0A7G6
G	996	SER	-	linker	UNP P0A7G6
G	997	THR	-	linker	UNP P0A7G6
G	998	GLY	-	linker	UNP P0A7G6
G	999	SER	-	linker	UNP P0A7G6
G	1000	MET	-	linker	UNP P0A7G6
G	1986	THR	-	linker	UNP P0A7G6
G	1987	GLY	-	linker	UNP P0A7G6
G	1988	SER	-	linker	UNP P0A7G6
G	1989	THR	-	linker	UNP P0A7G6
G	1990	GLY	-	linker	UNP P0A7G6
G	1991	SER	-	linker	UNP P0A7G6
G	1992	MET	-	linker	UNP P0A7G6
G	1993	GLY	-	linker	UNP P0A7G6
G	1994	HIS	-	linker	UNP P0A7G6
G	1995	THR	-	linker	UNP P0A7G6
G	1996	THR	-	linker	UNP P0A7G6
G	1997	GLY	-	linker	UNP P0A7G6
G	1998	SER	-	linker	UNP P0A7G6
G	1999	MET	-	linker	UNP P0A7G6
G	2000	SER	-	linker	UNP P0A7G6
G	2985	THR	-	linker	UNP P0A7G6
G	2986	GLY	-	linker	UNP P0A7G6
G	2987	SER	-	linker	UNP P0A7G6
G	2988	THR	-	linker	UNP P0A7G6
G	2989	GLY	-	linker	UNP P0A7G6
G	2990	SER	-	linker	UNP P0A7G6
G	2991	ALA	-	linker	UNP P0A7G6
G	2992	SER	-	linker	UNP P0A7G6
G	2993	GLY	-	linker	UNP P0A7G6
G	2994	SER	-	linker	UNP P0A7G6
G	2995	SER	-	linker	UNP P0A7G6
G	2996	THR	-	linker	UNP P0A7G6
G	2997	GLY	-	linker	UNP P0A7G6
G	2998	SER	-	linker	UNP P0A7G6
G	2999	MET	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	3000	SER	-	linker	UNP P0A7G6
H	26	GLY	-	linker	UNP P0A7G6
H	27	ALA	-	linker	UNP P0A7G6
H	28	MET	-	linker	UNP P0A7G6
H	29	HIS	-	linker	UNP P0A7G6
H	986	THR	-	linker	UNP P0A7G6
H	987	GLY	-	linker	UNP P0A7G6
H	988	SER	-	linker	UNP P0A7G6
H	989	THR	-	linker	UNP P0A7G6
H	990	GLY	-	linker	UNP P0A7G6
H	991	SER	-	linker	UNP P0A7G6
H	992	GLY	-	linker	UNP P0A7G6
H	993	THR	-	linker	UNP P0A7G6
H	994	THR	-	linker	UNP P0A7G6
H	995	GLY	-	linker	UNP P0A7G6
H	996	SER	-	linker	UNP P0A7G6
H	997	THR	-	linker	UNP P0A7G6
H	998	GLY	-	linker	UNP P0A7G6
H	999	SER	-	linker	UNP P0A7G6
H	1000	MET	-	linker	UNP P0A7G6
H	1986	THR	-	linker	UNP P0A7G6
H	1987	GLY	-	linker	UNP P0A7G6
H	1988	SER	-	linker	UNP P0A7G6
H	1989	THR	-	linker	UNP P0A7G6
H	1990	GLY	-	linker	UNP P0A7G6
H	1991	SER	-	linker	UNP P0A7G6
H	1992	MET	-	linker	UNP P0A7G6
H	1993	GLY	-	linker	UNP P0A7G6
H	1994	HIS	-	linker	UNP P0A7G6
H	1995	THR	-	linker	UNP P0A7G6
H	1996	THR	-	linker	UNP P0A7G6
H	1997	GLY	-	linker	UNP P0A7G6
H	1998	SER	-	linker	UNP P0A7G6
H	1999	MET	-	linker	UNP P0A7G6
H	2000	SER	-	linker	UNP P0A7G6
H	2985	THR	-	linker	UNP P0A7G6
H	2986	GLY	-	linker	UNP P0A7G6
H	2987	SER	-	linker	UNP P0A7G6
H	2988	THR	-	linker	UNP P0A7G6
H	2989	GLY	-	linker	UNP P0A7G6
H	2990	SER	-	linker	UNP P0A7G6
H	2991	ALA	-	linker	UNP P0A7G6

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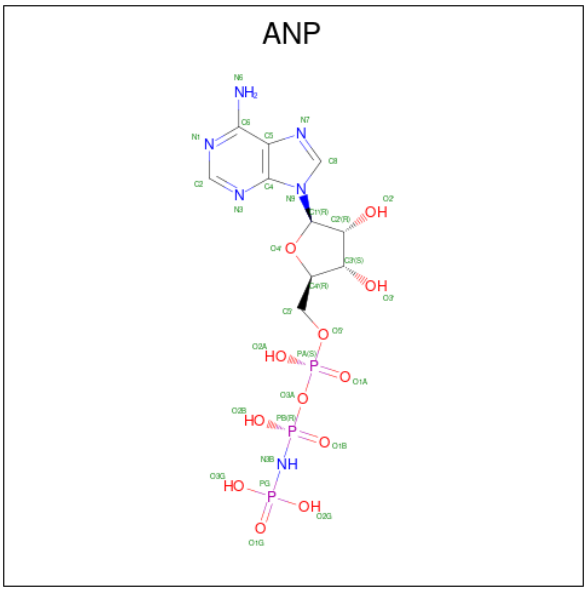
Chain	Residue	Modelled	Actual	Comment	Reference
H	2992	SER	-	linker	UNP P0A7G6
H	2993	GLY	-	linker	UNP P0A7G6
H	2994	SER	-	linker	UNP P0A7G6
H	2995	SER	-	linker	UNP P0A7G6
H	2996	THR	-	linker	UNP P0A7G6
H	2997	GLY	-	linker	UNP P0A7G6
H	2998	SER	-	linker	UNP P0A7G6
H	2999	MET	-	linker	UNP P0A7G6
H	3000	SER	-	linker	UNP P0A7G6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	4	4	4	0	0
2	B	4	4	4	0	0
2	C	4	4	4	0	0
2	D	4	4	4	0	0
2	E	4	4	4	0	0
2	F	4	4	4	0	0
2	G	4	4	4	0	0
2	H	4	4	4	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	A	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	A	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	A	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	B	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	B	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	B	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	B	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	C	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	C	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	C	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	C	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	D	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	D	1	31	10	6	12	3	0	0

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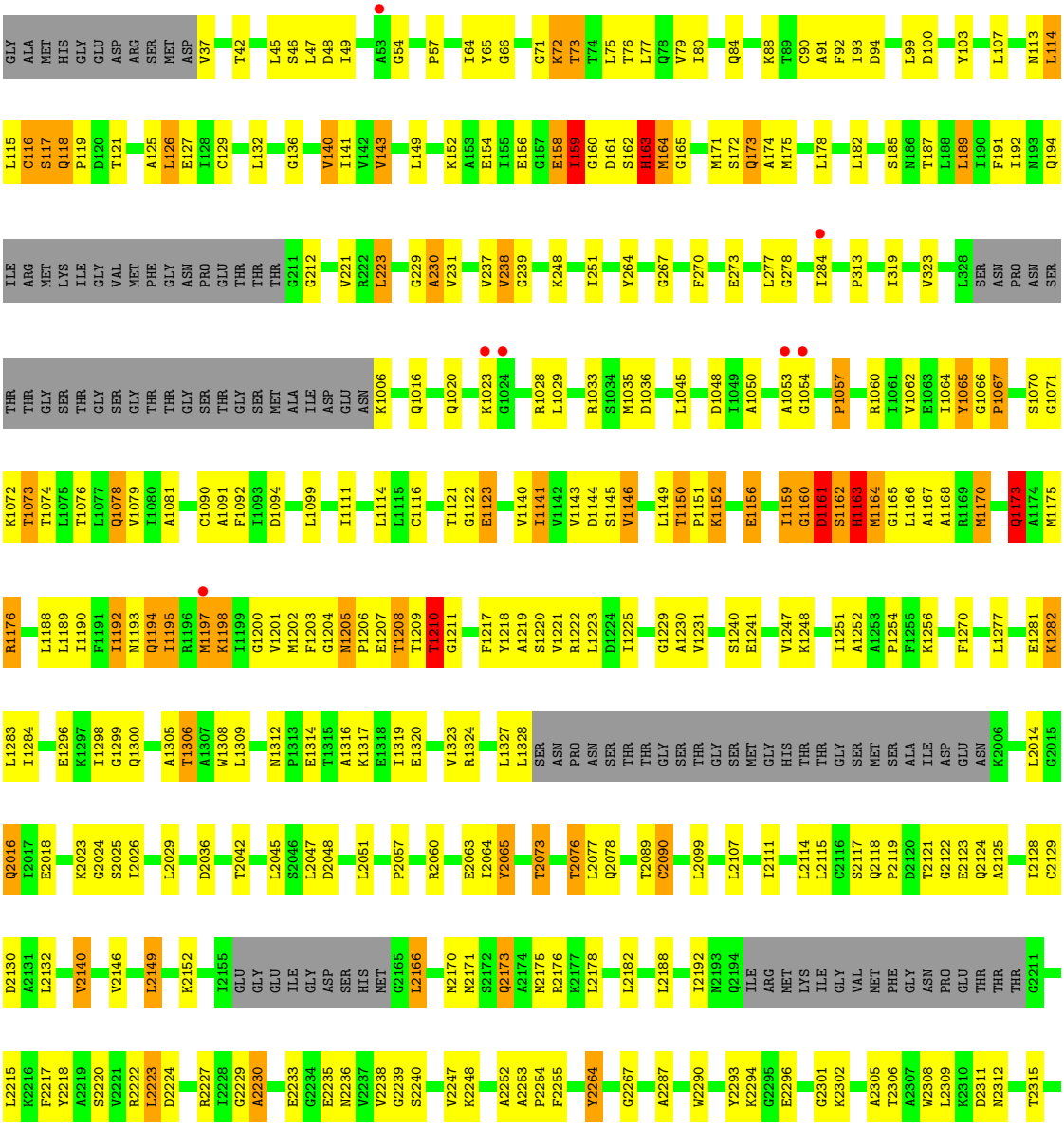
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	D	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	D	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	E	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	E	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	E	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	E	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	F	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	F	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	F	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	F	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	G	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	G	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	G	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	G	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	H	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	H	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	H	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
3	H	1	31	10	6	12	3	0	0

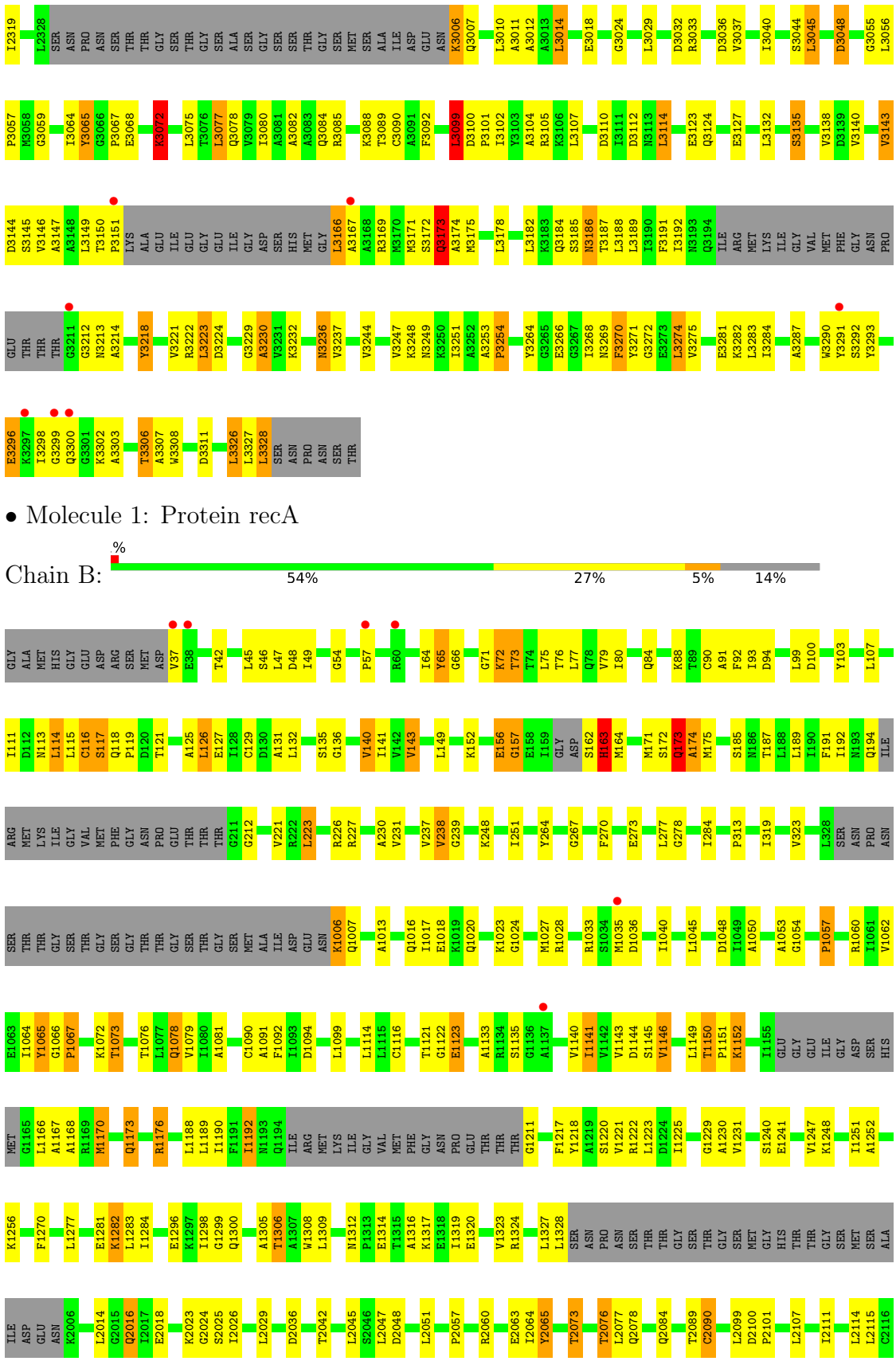
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Protein recA

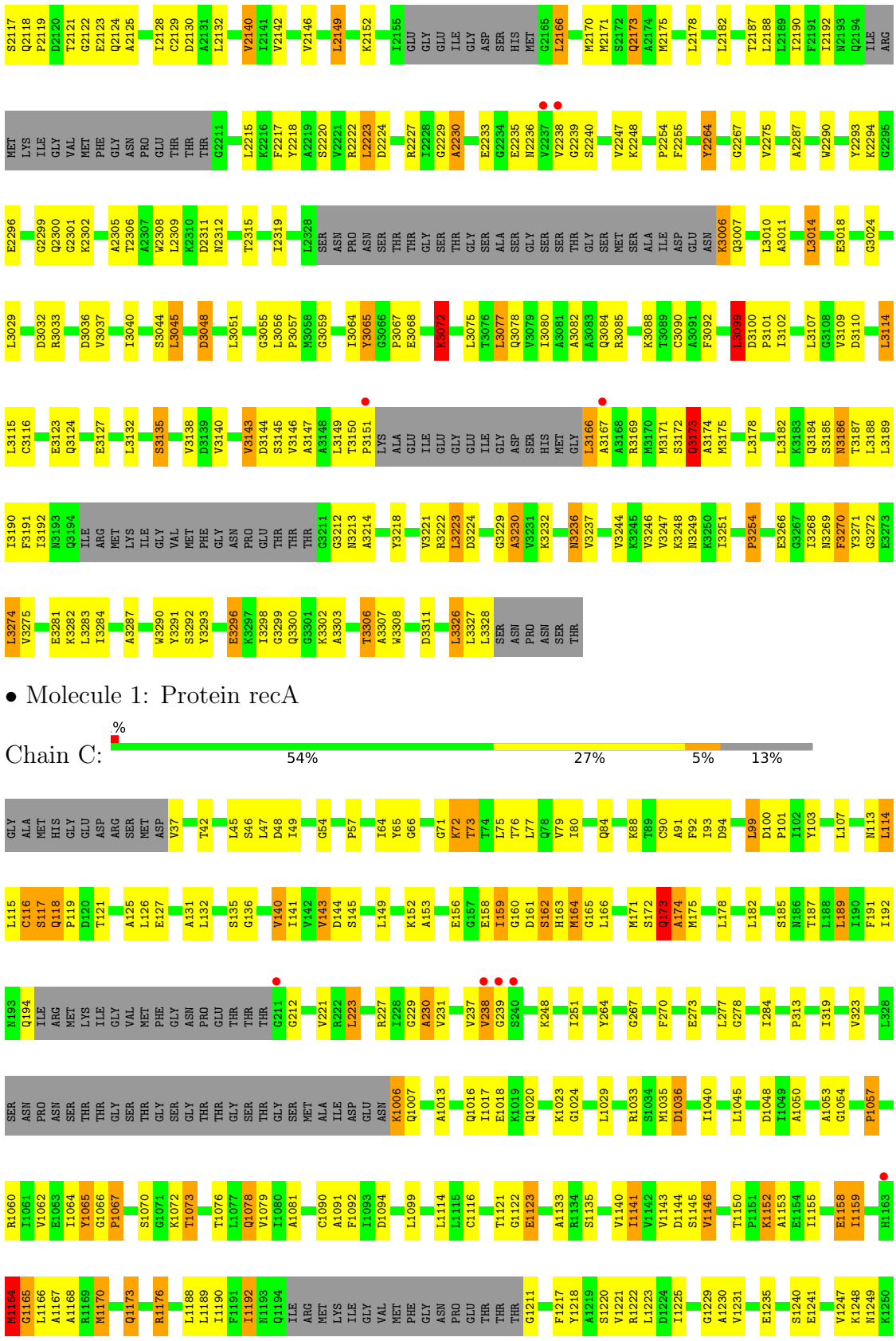
Chain A:





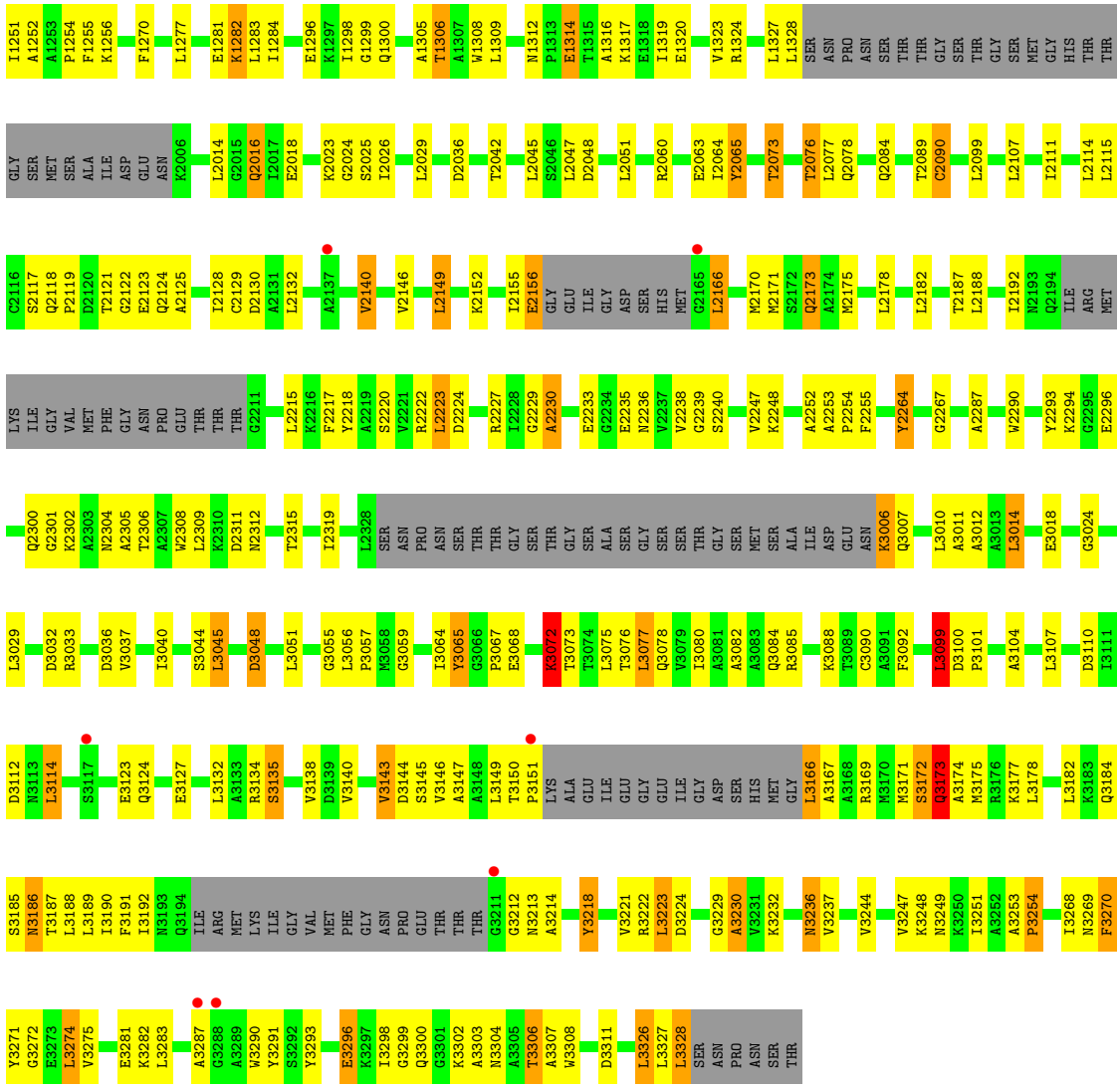
• Molecule 1: Protein recA

Chain B:



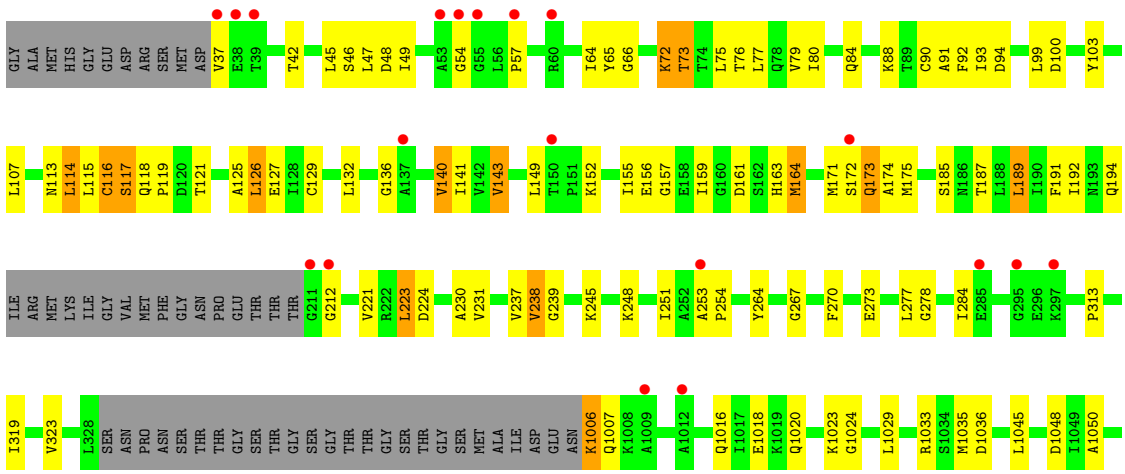
• Molecule 1: Protein recA

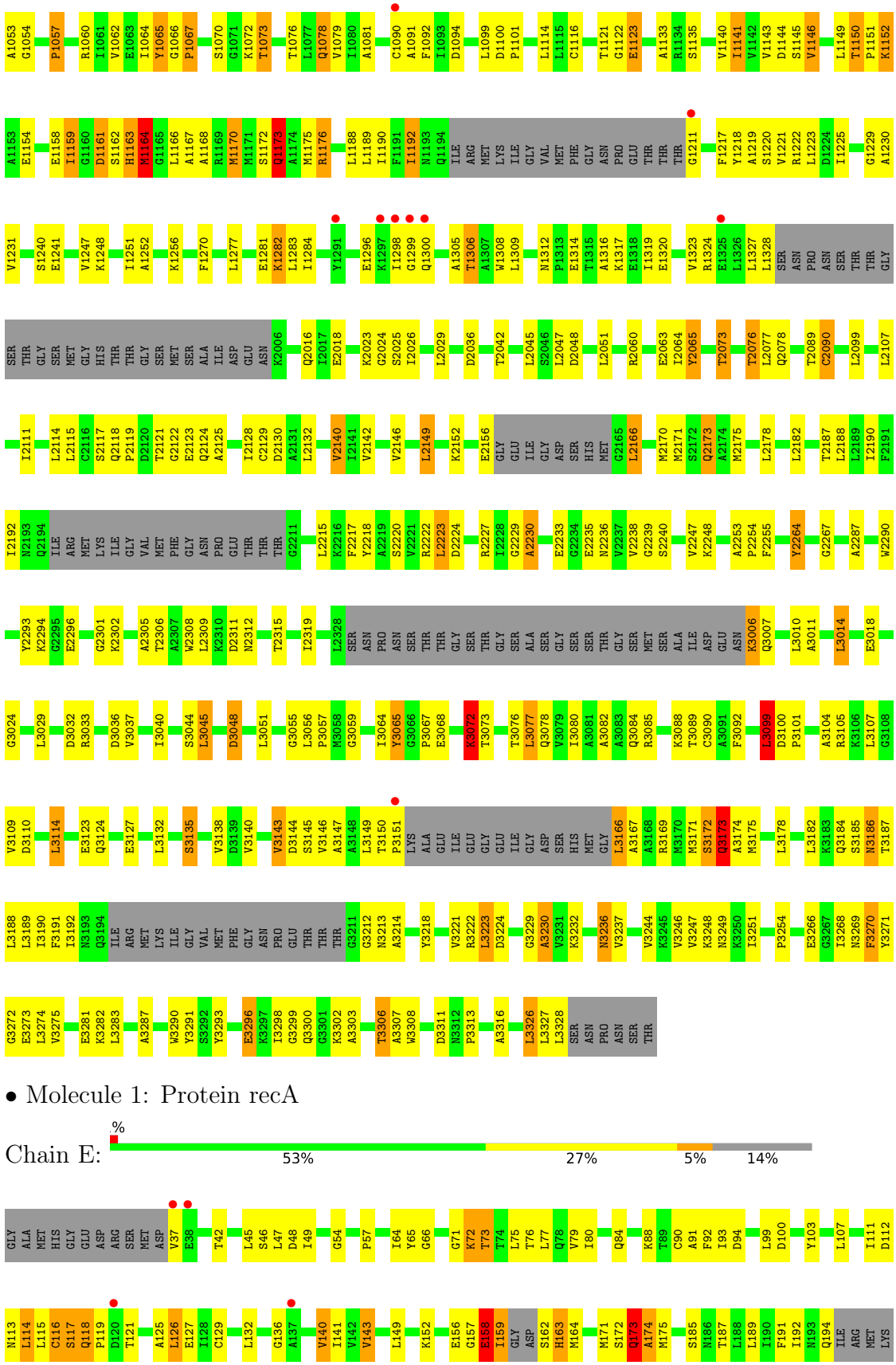
Chain C:



• Molecule 1: Protein recA

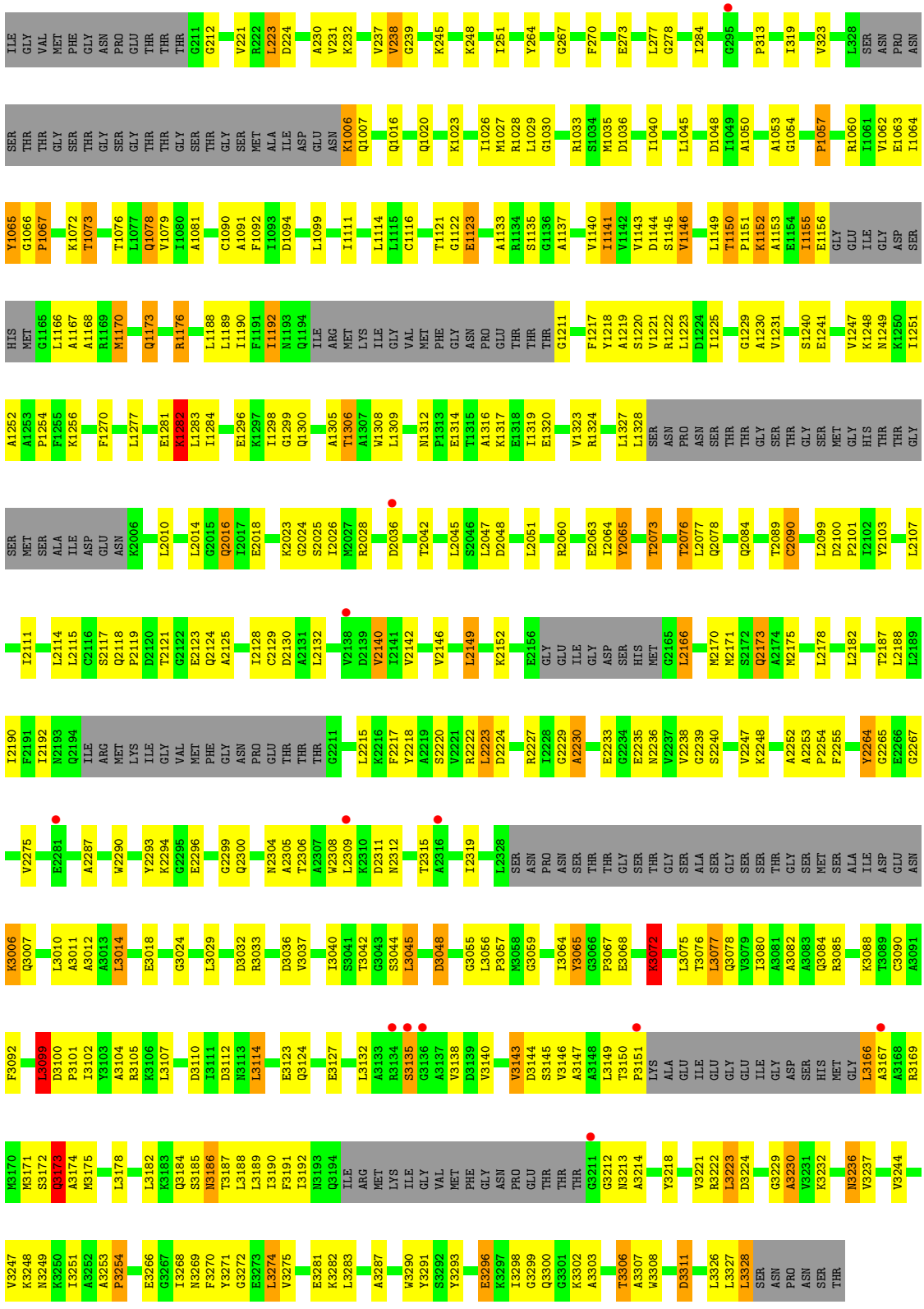
Chain D:





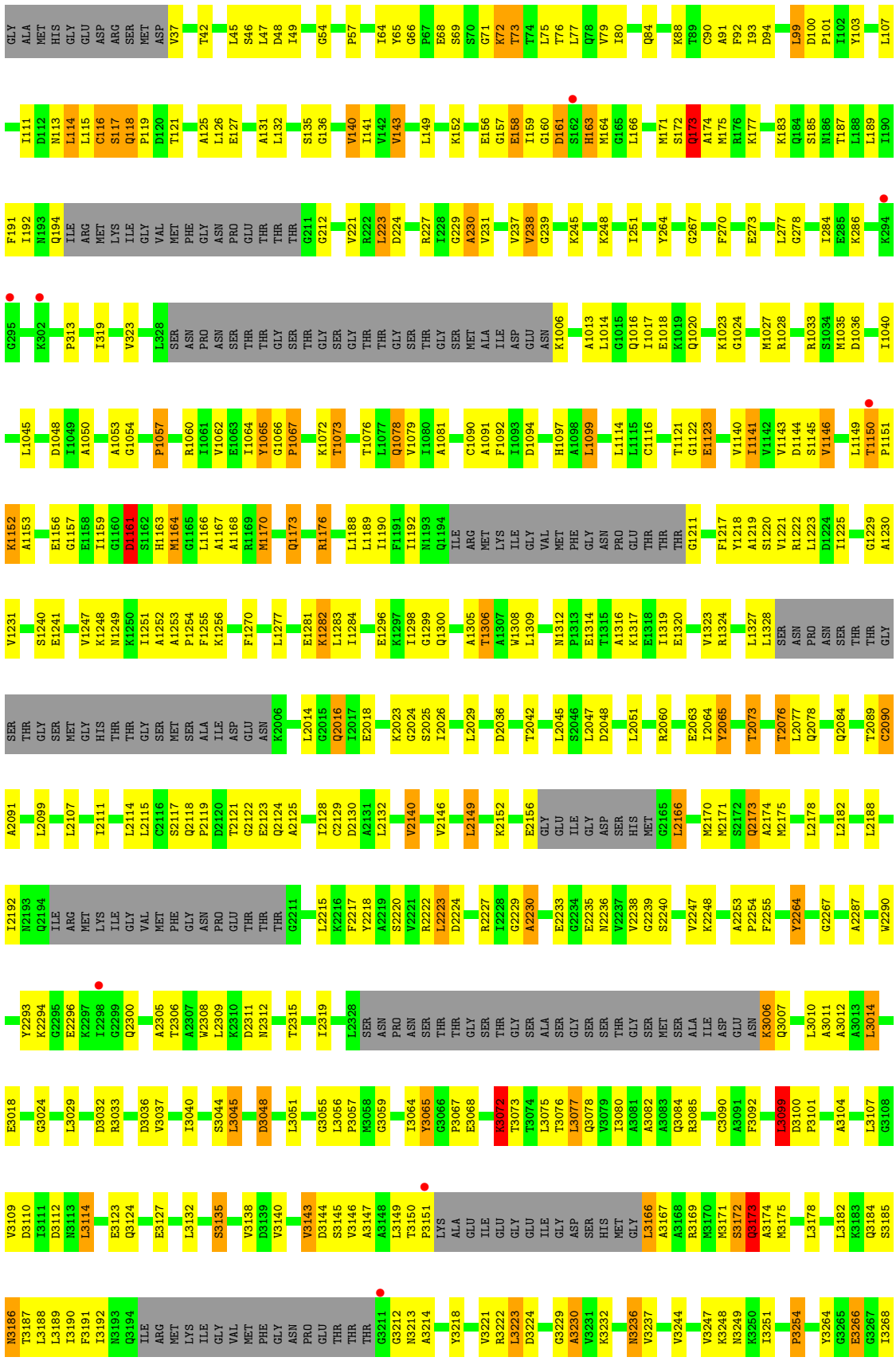
- Molecule 1: Protein recA

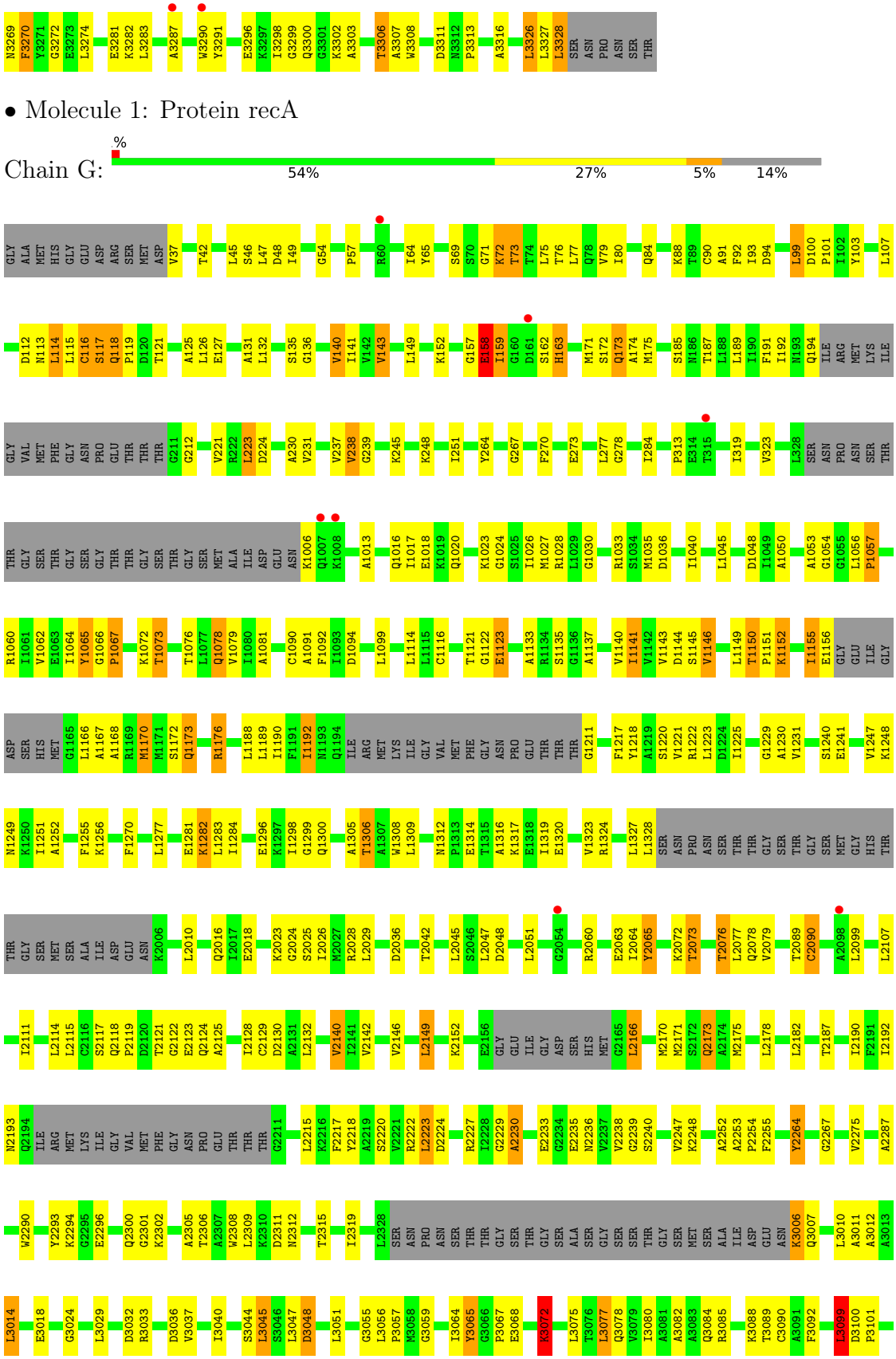
Chain E:



- Molecule 1: Protein recA

Chain F:


N3186 T3187 L3188 L3189 I3190 F3191 I3192 N3193 Q3194 ILE ARG MET LYS ILE GLY VAL MET PHE GLY ASN PRO GLU THR THR THR G3211 G3212 N3213 A3214 Y3218 Y3221 R3222 L3223 D3224 G3229 A3230 V3231 K3232 N3236 V3237 V3244 V3247 K3248 N3249 K3250 I3251 P3254 Y3264 G3265 E3266 G3267 I3268
V3109 D3110 I3111 D3112 N3113 L3114 E3123 Q3124 E3127 L3132 S3135 V3138 D3139 V3140 V3143 D3144 S3145 V3146 A3147 A3148 L3149 T3150 P3151 LYS ALA GLU ILE GLY ASP SER HIS MET GLY L3166 A3167 A3168 R3169 M3170 M3171 S3172 Q3173 A3174 M3175 L3178 L3182 K3183 Q3184 S3185
E3018 G3024 L3029 D3032 R3033 D3036 V3037 I3040 S3044 L3045 D3048 L3051 G3055 L3056 P3057 M3058 G3059 I3064 Y3065 G3066 P3067 E3068 K3072 T3073 T3074 L3075 T3076 L3077 Q3078 V3079 I3080 A3081 A3082 A3083 Q3084 R3085 C3090 A3091 F3092 L3099 D3100 P3101 A3104 L3107 G3108
Y2293 K2294 G2295 E2296 K2297 I2298 G2299 Q2300 A2305 T2306 A2307 W2308 L2309 K2310 D2311 N2312 T2315 I2319 L2328 SER ASN PRO ASN SER THR THR GLY SER THR GLY SER ALA SER GLY SER SER SER THR GLY SER MET SER ALA ILE ASP GLU ASN K3006 Q3007 L3010 A3011 A3012 A3013 L3014
I2192 N2193 Q2194 ILE ARG MET LYS ILE GLY VAL MET PHE GLY ASN PRO GLU THR THR THR G2211 L2215 K2216 F2217 Y2218 A2219 S2220 V2221 R2222 L2223 D2224 R2227 I2228 G2229 A2230 E2233 G2234 E2235 N2236 V2237 V2238 G2239 S2240 V2247 K2248 A2253 P2254 F2255 Y2264 G2267 A2287 W2290
A2091 L2099 L2107 I2111 L2114 L2115 C2116 S2117 Q2118 P2119 D2120 T2121 G2122 E2123 Q2124 A2125 I2128 C2129 D2130 A2131 L2132 V2140 V2146 L2149 K2152 E2156 GLY GLU ILE GLY ASP SER HIS MET G2165 L2166 M2170 M2171 S2172 Q2173 A2174 M2175 L2178 L2182 L2188
SER THR GLY SER MET GLY HIS THR THR GLY SER MET SER ALA ILE ASP GLU ASN K2006 L2014 G2015 Q2016 I2017 E2018 K2023 G2024 S2025 I2026 L2029 D2036 T2042 L2045 S2046 L2047 D2048 L2051 R2060 E2063 I2064 Y2065 T2073 T2076 L2077 Q2078 Q2084 T2089 C2090
V1231 S1240 E1241 V1247 K1248 N1249 K1250 I1251 A1252 A1253 P1254 F1255 K1256 F1270 L1277 E1281 K1282 L1283 I1284 E1296 K1297 I1298 G1299 Q1300 A1305 T1306 A1307 W1308 L1309 N1312 P1313 E1314 T1315 A1316 K1317 E1318 I1319 E1320 V1323 R1324 L1327 L1328 SER ASN PRO ASN SER THR THR GLY
K1152 A1153 E1156 G1157 E1158 I1159 G1160 D1161 S1162 H1163 M1164 G1165 L1166 A1167 A1168 R1169 M1170 Q1173 R1176 L1188 L1189 I1190 F1191 I1192 N1193 Q1194 ILE ARG MET LYS ILE GLY VAL MET PHE GLY ASN PRO GLU THR THR THR G1211 F1217 Y1218 A1219 S1220 V1221 R1222 L1223 D1224 I1225 G1229 A1230
L1045 D1048 I1049 A1050 A1053 G1054 P1057 R1060 I1061 V1062 E1063 I1064 Y1065 G1066 P1067 K1072 T1073 T1076 L1077 Q1078 V1079 I1080 A1081 C1090 A1091 F1092 I1093 D1094 H1097 A1098 L1099 L1114 L1115 C1116 T1121 G1122 E1123 V1140 I1141 V1142 V1143 D1144 S1145 V1146 L1149 T1150 P1151
G295 K302 P313 I319 V323 L328 SER ASN PRO ASN SER THR THR THR GLY SER THR THR THR GLY SER SER GLY THR THR THR GLY SER MET ALA ILE ILE ASP GLU ASN K1006 A1013 L1014 G1015 Q1016 I1017 E1018 K1019 Q1020 K1023 G1024 M1027 R1028 R1033 S1034 M1035 D1036 I1040
F191 I192 N193 Q194 ILE ARG MET LYS ILE GLY VAL MET PHE GLY ASN PRO GLU THR THR THR G211 G212 V221 R222 L223 D224 R227 I228 G229 A230 V231 V237 V238 G239 K245 K248 I251 Y264 G267 F270 E273 L277 G278 I284 E285 K286 K294
I111 D112 N113 L114 L115 C116 S117 Q118 P119 D120 T121 A125 L126 E127 A131 L132 S135 G136 V140 I141 V142 V143 L149 K152 E156 G157 E158 I159 G160 D161 S162 H163 M164 G165 L166 M171 S172 Q173 A174 M175 R176 K177 K183 Q184 S185 N186 T187 L188 L189 I190
GLY ALA MET HIS GLY GLU ASP ARG SER MET ASP V37 T42 L45 S46 L47 D48 I49 G54 P57 I64 Y65 G66 P67 E68 S69 S70 G71 K72 T73 T74 L75 T76 L77 Q78 V79 I80 Q84 K88 T89 C90 A91 F92 I93 D94 L99 D100 P101 I102 Y103 L107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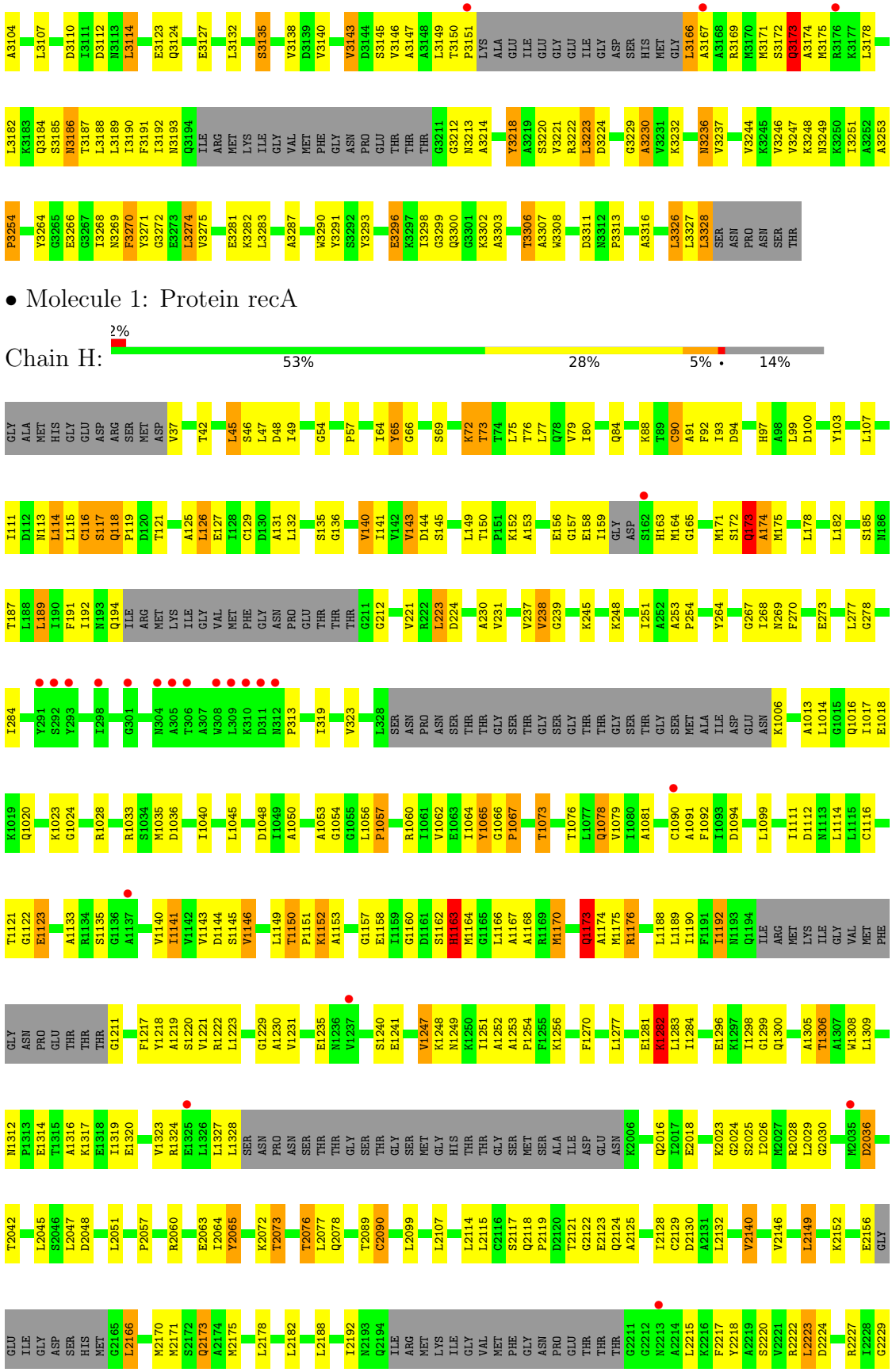
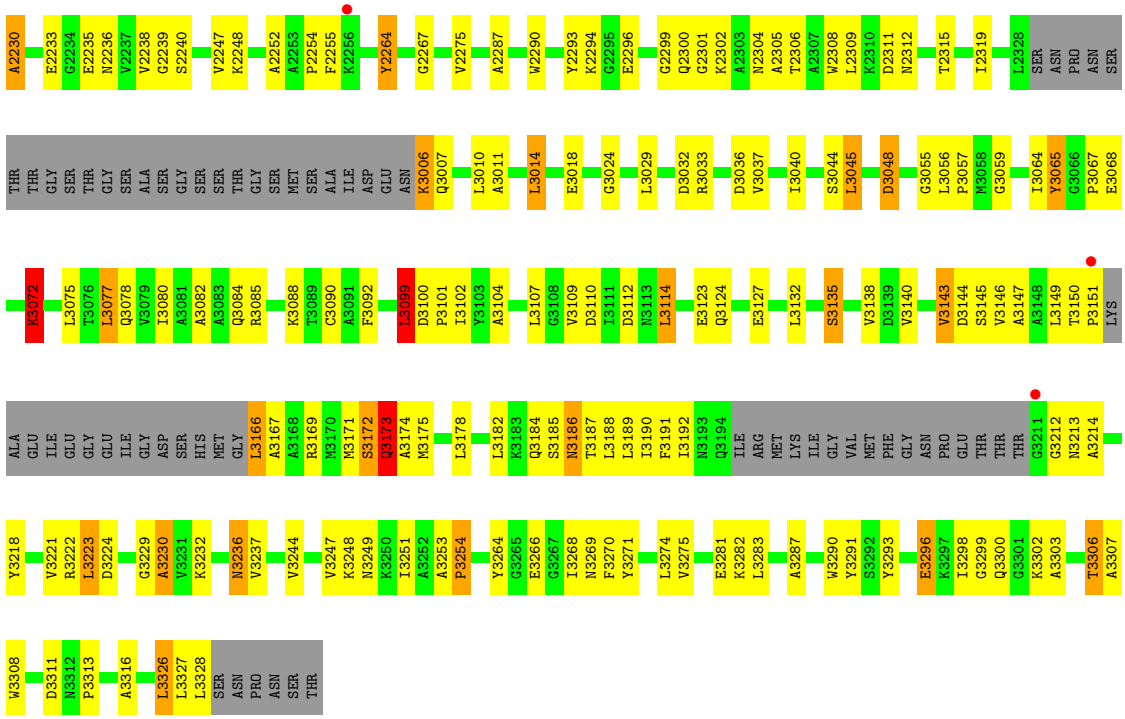
• Molecule 1: Protein recA
Chain G:
%
54%
27%
5%
14%
GLY ALA MET HIS GLY GLU ASP ARG SER MET ASP V37 T42 L45 S46 L47 D48 I49 G54 P57 R60 I64 Y65 S69 S70 G71 K72 T73 T74 L75 T76 L77 Q78 V79 I80 Q84 K88 T89 C90 A91 F92 I93 D94 L99 D100 P101 I102 Y103 L107
D112 N113 L114 L115 C116 S117 Q118 P119 D120 T121 A125 L126 E127 A131 L132 S135 G136 V140 I141 V142 V143 L149 K152 G157 E158 I159 G160 D161 S162 H163 M171 S172 Q173 A174 M175 S185 N186 T187 L188 L189 I190 F191 I192 N193 Q194 ILE ARG MET LYS ILE
GLY VAL MET PHE GLY ASN PRO GLU THR THR THR G211 G212 V221 R222 L223 D224 A230 V231 V237 V238 G239 K245 K248 I251 Y264 G267 F270 E273 L277 G278 I284 P313 E314 T315 I319 V323 L328 SER ASN PRO ASN SER THR
THR GLY SER THR GLY SER GLY THR THR GLY SER THR GLY SER MET ALA ILE ASP GLU ASN K1006 Q1007 K1008 A1013 Q1016 I1017 E1018 K1019 Q1020 K1023 G1024 S1025 I1026 M1027 R1028 L1029 G1030 R1033 S1034 M1035 D1036 I1040 L1045 D1048 I1049 A1050 A1053 G1054 G1055 L1056 P1057
R1060 I1061 V1062 E1063 I1064 Y1065 G1066 P1067 K1072 T1073 T1076 L1077 Q1078 V1079 I1080 A1081 C1090 A1091 F1092 I1093 D1094 L1099 L1114 L1115 C1116 T1121 G1122 E1123 A1133 R1134 S1135 G1136 A1137 V1140 I1141 V1142 V1143 D1144 S1145 V1146 L1149 T1150 P1151 K1152 I1155 E1156 GLY GLU ILE GLY
ASP SER HIS MET G1165 L1166 A1167 A1168 R1169 M1170 M1171 S1172 Q1173 R1176 L1188 L1189 I1190 F1191 I1192 N1193 Q1194 ILE ARG MET LYS ILE GLY VAL MET PHE GLY ASN PRO GLU THR THR THR G1211 F1217 Y1218 A1219 S1220 V1221 R1222 L1223 D1224 I1225 G1229 A1230 V1231 S1240 E1241 V1247 K1248
N1249 K1250 I1251 A1252 F1255 K1256 F1270 L1277 E1281 K1282 L1283 I1284 E1296 K1297 I1298 G1299 Q1300 A1305 T1306 A1307 W1308 L1309 N1312 P1313 E1314 T1315 A1316 K1317 E1318 I1319 E1320 V1323 R1324 L1327 L1328 SER ASN PRO ASN SER THR THR THR GLY SER THR GLY SER MET GLY HIS THR
THR GLY SER MET SER ALA ILE ASP GLU ASN K2006 L2010 Q2016 I2017 E2018 K2023 G2024 S2025 I2026 M2027 R2028 L2029 D2036 T2042 L2045 S2046 L2047 D2048 L2051 G2054 R2060 E2063 I2064 Y2065 K2072 T2073 T2076 L2077 Q2078 V2079 T2089 C2090 A2098 L2099 L2107
I2111 L2114 L2115 C2116 S2117 Q2118 P2119 D2120 T2121 G2122 E2123 Q2124 A2125 I2128 C2129 D2130 A2131 L2132 V2140 I2141 V2142 V2146 L2149 K2152 E2156 GLY GLU ILE GLY ASP SER HIS MET G2165 L2166 M2170 M2171 S2172 Q2173 A2174 M2175 L2178 L2182 T2187 I2190 F2191 I2192
N2193 Q2194 ILE ARG MET LYS ILE GLY VAL MET PHE GLY ASN PRO GLU THR THR THR G2211 L2215 K2216 F2217 Y2218 A2219 S2220 V2221 R2222 L2223 D2224 R2227 I2228 G2229 A2230 E2233 G2234 E2235 N2236 V2237 V2238 G2239 S2240 V2247 K2248 A2252 A2253 P2254 F2255 Y2264 G2267 V2275 A2287
W2290 Y2293 K2294 G2295 E2296 Q2300 G2301 K2302 A2305 T2306 A2307 W2308 L2309 K2310 D2311 N2312 T2315 I2319 L2328 SER ASN PRO ASN SER THR THR THR GLY SER THR GLY SER ALA SER GLY SER SER THR GLY SER MET SER ALA ILE ASP GLU ASN K3006 Q3007 L3010 A3011 A3012 A3013
L3014 E3018 G3024 L3029 D3032 R3033 D3036 V3037 I3040 S3044 L3045 S3046 L3047 D3048 L3051 G3055 L3056 P3057 M3058 G3059 I3064 Y3065 G3066 P3067 E3068 K3072 L3075 T3076 L3077 Q3078 V3079 I3080 A3081 A3082 A3083 Q3084 R3085 K3088 T3089 C3090 A3091 F3092 L3099 D3100 P3101



• Molecule 1: Protein recA

Chain H: 2% 53% 28% 5% • 14%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SER ASN PRO ASN SER
THR THR GLY SER THR GLY SER ALA SER GLY SER SER THR GLY SER MET SER ALA ILE ASP GLU ASN K3006 Q3007 L3010 A3011 L3014 E3018 G3024 L3029 D3032 R3033 D3036 V3037 I3040 S3044 L3045 D3048 G3055 L3056 P3057 M3058 G3059 I3064 Y3065 G3066 P3067 E3068
K3072 L3075 T3076 L3077 Q3078 V3079 I3080 A3081 A3082 A3083 Q3084 R3085 K3088 T3089 C3090 A3091 F3092 L3099 D3100 P3101 I3102 Y3103 A3104 L3107 G3108 V3109 D3110 T3111 D3112 N3113 L3114 E3123 Q3124 E3127 L3132 S3135 V3138 D3139 V3140 V3143 D3144 S3145 V3146 A3147 A3148 L3149 T3150 P3151
LYS
ALA GLU ILE GLU GLY GLU ILE GLY ASP SER HIS MET GLY L3166 A3167 A3168 R3169 M3170 M3171 S3172 Q3173 A3174 M3175 L3178 L3182 K3183 Q3184 S3185 N3186 T3187 L3188 L3189 I3190 F3191 I3192 N3193 Q3194 ILE ARG MET LYS ILE GLY VAL MET PHE GLY ASN PRO GLU THR THR THR G3211 G3212 N3213 A3214
Y3218 V3221 R3222 L3223 D3224 G3229 A3230 V3231 K3232 N3236 V3237 V3244 V3247 K3248 N3249 K3250 I3251 A3252 A3253 P3254 Y3264 G3265 E3266 G3267 I3268 N3269 F3270 Y3271 L3274 V3275 E3281 K3282 L3283 A3287 W3290 Y3291 S3292 Y3293 E3296 K3297 I3298 G3299 Q3300 G3301 K3302 A3303 T3306 A3307
W3308 D3311 N3312 P3313 A3316 L3326 L3327 L3328
SER ASN PRO ASN SER THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	176.60Å 189.80Å 424.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.30 39.93 – 4.30	Depositor EDS
% Data completeness (in resolution range)	92.7 (20.00-4.30) 92.7 (39.93-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.261 0.274 , 0.283	Depositor DCC
R_{free} test set	1946 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	170.2	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 116.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	71761	wwPDB-VP
Average B, all atoms (Å^2)	220.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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: ANP, MG

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	0.81	6/9068 (0.1%)	0.80	10/12192 (0.1%)
1	B	0.76	4/8861 (0.0%)	0.76	1/11910 (0.0%)
1	C	0.77	0/8951	0.77	4/12033 (0.0%)
1	D	0.74	3/8951 (0.0%)	0.75	4/12033 (0.0%)
1	E	0.72	1/8879 (0.0%)	0.75	2/11934 (0.0%)
1	F	0.77	4/8951 (0.0%)	0.77	2/12033 (0.0%)
1	G	0.77	2/8892 (0.0%)	0.76	3/11953 (0.0%)
1	H	0.72	2/8938 (0.0%)	0.75	3/12014 (0.0%)
All	All	0.76	22/71491 (0.0%)	0.77	29/96102 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	3
1	C	0	4
1	D	0	7
1	E	0	6
1	F	0	6
1	G	0	5
1	H	0	4
All	All	0	46

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	HIS	N-CA	7.46	1.61	1.46
1	B	3266	GLU	CG-CD	6.68	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1164	MET	CB-CG	6.66	1.72	1.51
1	D	156	GLU	CG-CD	5.97	1.60	1.51
1	F	3270	PHE	CE1-CZ	5.74	1.48	1.37
1	D	3266	GLU	CG-CD	5.71	1.60	1.51
1	G	3270	PHE	CE1-CZ	5.63	1.48	1.37
1	F	3266	GLU	CG-CD	5.57	1.60	1.51
1	G	3266	GLU	CG-CD	5.55	1.60	1.51
1	B	3266	GLU	CB-CG	5.53	1.62	1.52
1	F	3270	PHE	CG-CD2	5.49	1.47	1.38
1	B	3270	PHE	CE1-CZ	5.49	1.47	1.37
1	A	3266	GLU	CG-CD	5.48	1.60	1.51
1	B	3270	PHE	CG-CD2	5.39	1.46	1.38
1	H	90	CYS	CB-SG	-5.38	1.73	1.81
1	E	3266	GLU	CG-CD	5.33	1.59	1.51
1	A	3270	PHE	CE1-CZ	5.29	1.47	1.37
1	F	1156	GLU	CG-CD	5.22	1.59	1.51
1	A	159	ILE	CA-C	5.19	1.66	1.52
1	D	3270	PHE	CE1-CZ	5.16	1.47	1.37
1	H	3266	GLU	CG-CD	5.15	1.59	1.51
1	A	1208	THR	CA-CB	5.04	1.66	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1164	MET	C-N-CA	-8.01	105.48	122.30
1	D	2166	LEU	CA-CB-CG	7.24	131.94	115.30
1	G	2166	LEU	CA-CB-CG	7.23	131.93	115.30
1	H	2166	LEU	CA-CB-CG	7.23	131.93	115.30
1	E	2166	LEU	CA-CB-CG	7.21	131.89	115.30
1	C	2166	LEU	CA-CB-CG	7.20	131.85	115.30
1	A	2166	LEU	CA-CB-CG	7.17	131.78	115.30
1	B	2166	LEU	CA-CB-CG	7.17	131.78	115.30
1	F	2166	LEU	CA-CB-CG	7.16	131.76	115.30
1	A	1164	MET	CB-CG-SD	6.70	132.50	112.40
1	G	158	GLU	N-CA-C	6.58	128.76	111.00
1	A	163	HIS	N-CA-C	6.40	128.28	111.00
1	H	2036	ASP	C-N-CA	5.59	135.68	121.70
1	D	1163	HIS	N-CA-C	5.55	126.00	111.00
1	C	1164	MET	N-CA-C	5.38	125.52	111.00
1	A	3072	LYS	CD-CE-NZ	5.36	124.04	111.70
1	D	3328	LEU	CA-CB-CG	5.34	127.57	115.30
1	G	3328	LEU	CA-CB-CG	5.32	127.52	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1210	THR	C-N-CA	5.22	133.26	122.30
1	H	3328	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	1194	GLN	O-C-N	-5.18	114.41	122.70
1	A	1210	THR	CA-C-N	-5.14	105.91	116.20
1	F	3328	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	3328	LEU	CA-CB-CG	5.08	126.98	115.30
1	D	1164	MET	CB-CG-SD	5.07	127.61	112.40
1	C	1036	ASP	O-C-N	5.06	130.79	122.70
1	A	1210	THR	CA-C-O	5.04	130.68	120.10
1	C	3328	LEU	CA-CB-CG	5.02	126.84	115.30
1	E	3328	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1161	ASP	Peptide
1	A	1163	HIS	Peptide
1	A	1197	MET	Peptide
1	A	1198	LYS	Peptide
1	A	1210	THR	Peptide
1	A	158	GLU	Peptide
1	A	161	ASP	Peptide
1	A	163	HIS	Peptide
1	A	3138	VAL	Peptide
1	A	3149	LEU	Peptide
1	A	3150	THR	Peptide
1	B	3138	VAL	Peptide
1	B	3149	LEU	Peptide
1	B	3150	THR	Peptide
1	C	1164	MET	Peptide
1	C	3138	VAL	Peptide
1	C	3149	LEU	Peptide
1	C	3150	THR	Peptide
1	D	1161	ASP	Peptide
1	D	1162	SER	Peptide
1	D	1164	MET	Peptide
1	D	164	MET	Peptide
1	D	3138	VAL	Peptide
1	D	3149	LEU	Peptide
1	D	3150	THR	Peptide
1	E	1155	ILE	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
1	E	163	HIS	Peptide
1	E	3138	VAL	Peptide
1	E	3149	LEU	Peptide
1	E	3150	THR	Peptide
1	F	1164	MET	Peptide
1	F	161	ASP	Peptide
1	F	164	MET	Peptide
1	F	3138	VAL	Peptide
1	F	3149	LEU	Peptide
1	F	3150	THR	Peptide
1	G	1155	ILE	Mainchain
1	G	158	GLU	Peptide
1	G	3138	VAL	Peptide
1	G	3149	LEU	Peptide
1	G	3150	THR	Peptide
1	H	1163	HIS	Peptide
1	H	3138	VAL	Peptide
1	H	3149	LEU	Peptide
1	H	3150	THR	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	8970	0	9264	308	1
1	B	8769	0	9070	275	0
1	C	8856	0	9139	294	1
1	D	8856	0	9139	268	0
1	E	8787	0	9082	304	0
1	F	8856	0	9139	314	0
1	G	8799	0	9090	269	0
1	H	8844	0	9131	304	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	4	0	0	0	0
2	H	4	0	0	0	0
3	A	124	0	52	7	0
3	B	124	0	52	2	0
3	C	124	0	52	3	0
3	D	124	0	52	2	0
3	E	124	0	52	3	0
3	F	124	0	52	9	0
3	G	124	0	52	4	0
3	H	124	0	52	4	0
All	All	71761	0	73470	2200	1

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 15.

All (2200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:GLY:HA2	1:B:3115:LEU:CD2	1.50	1.42
1:A:1194:GLN:O	1:A:1195:ILE:CG2	1.73	1.37
1:A:162:SER:O	1:A:165:GLY:CA	1.71	1.35
1:A:1194:GLN:O	1:A:1195:ILE:CB	1.81	1.27
1:A:1194:GLN:O	1:A:1195:ILE:HG22	1.25	1.22
1:C:3151:PRO:HG2	1:D:3151:PRO:HG2	1.24	1.15
1:E:3151:PRO:HG2	1:F:3151:PRO:HG2	1.25	1.15
1:A:1204:GLY:CA	1:B:3115:LEU:HD22	1.77	1.13
1:C:3177:LYS:HE2	1:F:173:GLN:CG	1.80	1.11
1:C:3177:LYS:CE	1:F:173:GLN:HG3	1.80	1.11
1:G:3151:PRO:HG2	1:H:3151:PRO:HG2	1.32	1.11
1:C:3177:LYS:HE2	1:F:173:GLN:HG3	1.21	1.10
1:A:162:SER:O	1:A:165:GLY:HA3	0.91	1.09
1:D:1161:ASP:HB2	1:F:183:LYS:NZ	1.68	1.08
1:D:1161:ASP:HB3	1:F:183:LYS:HE2	1.28	1.08
1:F:156:GLU:OE2	1:F:1176:ARG:HG3	1.52	1.07
1:F:1161:ASP:HB3	1:F:1166:LEU:CD1	1.85	1.05
1:F:1161:ASP:HB3	1:F:1166:LEU:HD13	1.34	1.04
1:D:1161:ASP:HB2	1:F:183:LYS:HZ1	1.21	1.03
1:A:1204:GLY:HA2	1:B:3115:LEU:HD22	1.03	1.02
1:E:3105:ARG:HD3	1:F:227:ARG:NH2	1.74	1.01
1:E:3105:ARG:HD3	1:F:227:ARG:HH22	1.20	0.99
1:A:1194:GLN:O	1:A:1195:ILE:HB	1.61	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:GLY:CA	1:B:3115:LEU:CD2	2.38	0.97
1:E:3300:GLN:H	1:H:1300:GLN:NE2	1.64	0.96
1:F:3166:LEU:HB2	1:F:3169:ARG:HB2	1.47	0.96
1:A:3166:LEU:HB2	1:A:3169:ARG:HB2	1.47	0.96
1:C:3166:LEU:HB2	1:C:3169:ARG:HB2	1.47	0.95
1:B:3166:LEU:HB2	1:B:3169:ARG:HB2	1.47	0.95
1:E:3166:LEU:HB2	1:E:3169:ARG:HB2	1.47	0.95
1:D:3166:LEU:HB2	1:D:3169:ARG:HB2	1.48	0.95
1:H:3166:LEU:HB2	1:H:3169:ARG:HB2	1.48	0.95
1:E:1300:GLN:NE2	1:H:3300:GLN:H	1.65	0.93
1:E:1300:GLN:H	1:H:3300:GLN:NE2	1.66	0.93
1:G:3166:LEU:HB2	1:G:3169:ARG:HB2	1.47	0.93
1:F:1163:HIS:HB2	1:F:1166:LEU:HG	1.49	0.93
1:D:1161:ASP:HB3	1:F:183:LYS:CE	1.98	0.93
1:D:1161:ASP:CB	1:F:183:LYS:NZ	2.31	0.93
1:A:1164:MET:O	1:A:1166:LEU:N	2.01	0.91
1:A:1204:GLY:HA2	1:B:3115:LEU:HD23	1.51	0.91
1:A:158:GLU:HA	1:A:159:ILE:HD13	1.51	0.90
1:H:3064:ILE:HG12	1:H:3223:LEU:HB2	1.54	0.89
1:F:3064:ILE:HG12	1:F:3223:LEU:HB2	1.53	0.89
1:A:3064:ILE:HG12	1:A:3223:LEU:HB2	1.55	0.89
1:D:3064:ILE:HG12	1:D:3223:LEU:HB2	1.54	0.88
1:H:3072:LYS:HE3	3:H:3400:ANP:O1B	1.74	0.88
1:D:1159:ILE:HG21	1:D:1163:HIS:HD1	1.37	0.88
1:B:3064:ILE:HG12	1:B:3223:LEU:HB2	1.55	0.88
1:A:1193:ASN:ND2	1:A:1209:THR:HG23	1.88	0.87
1:A:162:SER:C	1:A:165:GLY:HA3	1.93	0.87
1:G:3064:ILE:HG12	1:G:3223:LEU:HB2	1.55	0.87
1:C:3064:ILE:HG12	1:C:3223:LEU:HB2	1.53	0.87
1:E:3064:ILE:HG12	1:E:3223:LEU:HB2	1.55	0.87
1:F:1153:ALA:O	1:F:1157:GLY:HA2	1.75	0.86
1:C:164:MET:O	1:C:166:LEU:N	2.09	0.85
1:F:3072:LYS:HE3	3:F:3400:ANP:O1B	1.74	0.85
1:C:2156:GLU:HA	1:C:3172:SER:OG	1.77	0.85
1:C:1164:MET:HG3	1:C:1165:GLY:HA3	1.60	0.84
1:F:3143:VAL:HG23	1:F:3191:PHE:HA	1.59	0.84
1:E:3072:LYS:HE3	3:E:3400:ANP:O1B	1.79	0.83
1:E:3300:GLN:H	1:H:1300:GLN:HE22	1.27	0.83
1:E:3300:GLN:NE2	1:H:1300:GLN:H	1.76	0.83
1:G:3143:VAL:HG23	1:G:3191:PHE:HA	1.61	0.82
1:D:3072:LYS:HE3	3:D:3400:ANP:O1B	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:SER:O	1:C:119:PRO:HD3	1.81	0.81
1:D:90:CYS:SG	1:D:140:VAL:HG13	2.21	0.81
1:D:1158:GLU:O	1:D:1159:ILE:HB	1.81	0.81
1:E:117:SER:O	1:E:119:PRO:HD3	1.81	0.81
1:G:3151:PRO:HG2	1:H:3151:PRO:CG	2.10	0.81
1:A:90:CYS:SG	1:A:140:VAL:HG13	2.21	0.81
1:B:90:CYS:SG	1:B:140:VAL:HG13	2.20	0.81
1:H:117:SER:O	1:H:119:PRO:HD3	1.81	0.81
1:A:163:HIS:C	1:A:165:GLY:H	1.80	0.81
1:B:117:SER:O	1:B:119:PRO:HD3	1.81	0.81
1:E:2300:GLN:HE22	1:H:2299:GLY:HA2	1.45	0.81
1:E:2300:GLN:H	1:H:2300:GLN:NE2	1.79	0.80
1:G:117:SER:O	1:G:119:PRO:HD3	1.81	0.80
1:D:117:SER:O	1:D:119:PRO:HD3	1.80	0.80
1:F:1123:GLU:HB2	1:F:1152:LYS:HE3	1.63	0.80
1:E:90:CYS:SG	1:E:140:VAL:HG13	2.21	0.80
1:F:117:SER:O	1:F:119:PRO:HD3	1.81	0.80
1:G:90:CYS:SG	1:G:140:VAL:HG13	2.21	0.80
1:D:1222:ARG:HB2	1:D:1248:LYS:HB3	1.64	0.80
1:D:3143:VAL:HG23	1:D:3191:PHE:HA	1.63	0.80
1:E:1123:GLU:HB2	1:E:1152:LYS:HE3	1.64	0.80
1:C:3143:VAL:HG23	1:C:3191:PHE:HA	1.64	0.80
1:A:162:SER:O	1:A:165:GLY:C	2.20	0.80
1:H:1123:GLU:HB2	1:H:1152:LYS:HE3	1.65	0.80
1:E:3175:MET:HG3	1:E:3218:TYR:HD1	1.47	0.79
1:G:3151:PRO:CG	1:H:3151:PRO:HG2	2.11	0.79
1:D:3077:LEU:HA	1:D:3080:ILE:HD12	1.64	0.79
1:A:1123:GLU:HB2	1:A:1152:LYS:HE3	1.64	0.79
1:A:117:SER:O	1:A:119:PRO:HD3	1.82	0.79
1:B:1222:ARG:HB2	1:B:1248:LYS:HB3	1.64	0.79
1:H:80:ILE:O	1:H:84:GLN:HB2	1.82	0.79
1:C:1123:GLU:HB2	1:C:1152:LYS:HE3	1.65	0.79
1:E:1222:ARG:HB2	1:E:1248:LYS:HB3	1.65	0.79
1:B:80:ILE:O	1:B:84:GLN:HB2	1.83	0.78
1:B:1123:GLU:HB2	1:B:1152:LYS:HE3	1.66	0.78
1:B:3175:MET:HG3	1:B:3218:TYR:HD1	1.47	0.78
1:C:90:CYS:SG	1:C:140:VAL:HG13	2.23	0.78
1:B:3143:VAL:HG23	1:B:3191:PHE:HA	1.64	0.78
1:D:80:ILE:O	1:D:84:GLN:HB2	1.82	0.78
1:H:3143:VAL:HG23	1:H:3191:PHE:HA	1.62	0.78
1:F:80:ILE:O	1:F:84:GLN:HB2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:ILE:O	1:G:84:GLN:HB2	1.83	0.78
1:E:3143:VAL:HG23	1:E:3191:PHE:HA	1.64	0.78
1:F:3175:MET:HG3	1:F:3218:TYR:HD1	1.48	0.78
1:F:90:CYS:SG	1:F:140:VAL:HG13	2.23	0.78
1:A:1300:GLN:NE2	1:D:3300:GLN:H	1.81	0.78
1:C:80:ILE:O	1:C:84:GLN:HB2	1.84	0.78
1:A:3072:LYS:HE3	3:A:3400:ANP:O1B	1.84	0.78
1:A:3175:MET:HG3	1:A:3218:TYR:HD1	1.48	0.78
1:A:80:ILE:O	1:A:84:GLN:HB2	1.83	0.78
1:A:3143:VAL:HG23	1:A:3191:PHE:HA	1.64	0.78
1:G:3175:MET:HG3	1:G:3218:TYR:HD1	1.49	0.78
1:H:90:CYS:SG	1:H:140:VAL:HG13	2.24	0.78
1:C:1222:ARG:HB2	1:C:1248:LYS:HB3	1.65	0.77
1:H:1222:ARG:HB2	1:H:1248:LYS:HB3	1.65	0.77
1:D:1123:GLU:HB2	1:D:1152:LYS:HE3	1.65	0.77
1:D:3175:MET:HG3	1:D:3218:TYR:HD1	1.48	0.77
1:E:1300:GLN:HE22	1:H:3299:GLY:HA2	1.49	0.77
1:G:1123:GLU:HB2	1:G:1152:LYS:HE3	1.65	0.77
1:H:3077:LEU:HA	1:H:3080:ILE:HD12	1.67	0.77
1:H:3175:MET:HG3	1:H:3218:TYR:HD1	1.48	0.77
1:A:1197:MET:H	1:A:1198:LYS:HG3	1.47	0.77
1:E:80:ILE:O	1:E:84:GLN:HB2	1.84	0.77
1:F:1222:ARG:HB2	1:F:1248:LYS:HB3	1.65	0.77
1:G:1222:ARG:HB2	1:G:1248:LYS:HB3	1.66	0.76
1:F:71:GLY:HA2	3:F:400:ANP:H5'1	1.68	0.76
1:A:1156:GLU:OE2	1:A:2176:ARG:HB2	1.85	0.75
1:E:93:ILE:HA	1:E:117:SER:OG	1.86	0.75
1:A:1222:ARG:HB2	1:A:1248:LYS:HB3	1.66	0.75
1:C:3175:MET:HG3	1:C:3218:TYR:HD1	1.49	0.75
1:C:3177:LYS:HE2	1:F:173:GLN:CD	2.06	0.75
1:A:1195:ILE:HD11	1:A:1206:PRO:HB3	1.69	0.75
1:B:2300:GLN:NE2	1:C:2300:GLN:H	1.86	0.74
1:D:1161:ASP:CB	1:F:183:LYS:CE	2.66	0.74
1:B:3077:LEU:HA	1:B:3080:ILE:HD12	1.69	0.74
1:F:143:VAL:HG23	1:F:191:PHE:HA	1.70	0.74
1:D:2156:GLU:HA	1:D:3172:SER:OG	1.88	0.74
1:B:143:VAL:HG23	1:B:191:PHE:HA	1.70	0.74
1:A:156:GLU:OE1	1:A:1176:ARG:HG3	1.89	0.73
1:G:2121:THR:HG23	1:G:2124:GLN:H	1.54	0.73
1:A:143:VAL:HG23	1:A:191:PHE:HA	1.68	0.73
1:C:3077:LEU:HA	1:C:3080:ILE:HD12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3077:LEU:HA	1:G:3080:ILE:HD12	1.68	0.73
1:A:2121:THR:HG23	1:A:2124:GLN:H	1.53	0.73
1:D:1159:ILE:HG21	1:D:1163:HIS:ND1	2.04	0.73
1:H:2121:THR:HG23	1:H:2124:GLN:H	1.53	0.73
1:A:3151:PRO:HG2	1:B:3151:PRO:HG2	1.71	0.73
1:C:3072:LYS:HE3	3:C:3400:ANP:O1B	1.88	0.73
1:H:93:ILE:HA	1:H:117:SER:OG	1.89	0.73
1:C:143:VAL:HG23	1:C:191:PHE:HA	1.70	0.72
1:E:143:VAL:HG23	1:E:191:PHE:HA	1.70	0.72
1:E:2121:THR:HG23	1:E:2124:GLN:H	1.54	0.72
1:A:93:ILE:HA	1:A:117:SER:OG	1.89	0.72
1:B:91:ALA:HB3	1:B:141:ILE:HG12	1.72	0.72
1:B:2121:THR:HG23	1:B:2124:GLN:H	1.54	0.72
1:A:91:ALA:HB3	1:A:141:ILE:HG12	1.72	0.72
1:B:2300:GLN:H	1:C:2300:GLN:NE2	1.88	0.72
1:E:3151:PRO:HG2	1:F:3151:PRO:CG	2.13	0.72
1:G:143:VAL:HG23	1:G:191:PHE:HA	1.71	0.72
1:H:143:VAL:HG23	1:H:191:PHE:HA	1.70	0.72
1:C:3151:PRO:HG2	1:D:3151:PRO:CG	2.12	0.72
1:G:3044:SER:OG	1:G:3045:LEU:N	2.23	0.72
1:D:157:GLY:CA	1:D:1172:SER:HB3	2.20	0.72
1:A:1071:GLY:HA2	3:A:1400:ANP:H5'1	1.72	0.72
1:D:143:VAL:HG23	1:D:191:PHE:HA	1.71	0.72
1:F:3044:SER:OG	1:F:3045:LEU:N	2.20	0.72
1:F:3077:LEU:HA	1:F:3080:ILE:HD12	1.70	0.72
1:A:1163:HIS:HB2	1:A:1166:LEU:HD12	1.71	0.71
1:C:2121:THR:HG23	1:C:2124:GLN:H	1.54	0.71
1:F:2121:THR:HG23	1:F:2124:GLN:H	1.55	0.71
1:A:1300:GLN:HE22	1:D:3300:GLN:H	1.36	0.71
1:E:3077:LEU:HA	1:E:3080:ILE:HD12	1.70	0.71
1:B:2118:GLN:HE22	1:B:3249:ASN:H	1.39	0.71
1:E:115:LEU:HA	1:E:1027:MET:O	1.91	0.71
1:D:2118:GLN:HE22	1:D:3249:ASN:H	1.39	0.71
1:E:2300:GLN:NE2	1:H:2300:GLN:H	1.87	0.71
1:A:156:GLU:OE2	1:A:1176:ARG:CG	2.38	0.71
1:D:1161:ASP:CB	1:F:183:LYS:HE2	2.16	0.71
1:D:2121:THR:HG23	1:D:2124:GLN:H	1.55	0.71
1:E:114:LEU:O	1:E:1028:ARG:HA	1.90	0.71
1:F:91:ALA:HB3	1:F:141:ILE:HG12	1.73	0.71
1:A:3077:LEU:HA	1:A:3080:ILE:HD12	1.72	0.71
1:D:93:ILE:HA	1:D:117:SER:OG	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1146:VAL:HG11	1:A:1211:GLY:HA3	1.73	0.71
1:E:3044:SER:OG	1:E:3045:LEU:N	2.24	0.71
1:F:1163:HIS:CG	1:F:1166:LEU:HD21	2.26	0.70
1:A:156:GLU:CD	1:A:1176:ARG:HG3	2.11	0.70
1:B:3072:LYS:HE3	3:B:3400:ANP:O1B	1.91	0.70
1:E:91:ALA:HB3	1:E:141:ILE:HG12	1.73	0.70
1:D:91:ALA:HB3	1:D:141:ILE:HG12	1.73	0.70
1:D:157:GLY:HA2	1:D:1172:SER:HB3	1.73	0.70
1:H:91:ALA:HB3	1:H:141:ILE:HG12	1.73	0.70
1:E:2304:ASN:HB3	1:H:2300:GLN:OE1	1.91	0.70
1:F:1163:HIS:CD2	1:F:1166:LEU:HD21	2.27	0.70
1:B:93:ILE:HA	1:B:117:SER:OG	1.91	0.70
1:F:2118:GLN:HE22	1:F:3249:ASN:H	1.37	0.70
1:G:91:ALA:HB3	1:G:141:ILE:HG12	1.73	0.70
1:H:2118:GLN:HE22	1:H:3249:ASN:H	1.39	0.70
1:D:3044:SER:OG	1:D:3045:LEU:N	2.23	0.70
1:F:93:ILE:HA	1:F:117:SER:OG	1.91	0.70
1:E:1300:GLN:H	1:H:3300:GLN:HE22	1.37	0.69
1:A:1161:ASP:OD1	1:A:1161:ASP:N	2.25	0.69
1:C:2118:GLN:HE22	1:C:3249:ASN:H	1.40	0.69
1:E:2304:ASN:HB3	1:H:2300:GLN:CD	2.12	0.69
1:G:93:ILE:HA	1:G:117:SER:OG	1.91	0.69
1:C:93:ILE:HA	1:C:117:SER:OG	1.92	0.69
1:C:91:ALA:HB3	1:C:141:ILE:HG12	1.74	0.68
1:E:1146:VAL:HG11	1:E:1211:GLY:HA3	1.76	0.68
1:H:131:ALA:HB1	1:H:1017:ILE:HD12	1.76	0.68
1:F:1217:PHE:HA	1:F:1248:LYS:HE3	1.76	0.68
1:A:163:HIS:C	1:A:165:GLY:N	2.47	0.68
1:B:2300:GLN:N	1:C:2300:GLN:NE2	2.42	0.68
1:G:157:GLY:HA2	1:G:1172:SER:CB	2.23	0.68
1:H:1146:VAL:HG11	1:H:1211:GLY:HA3	1.76	0.68
1:A:2117:SER:O	1:A:2119:PRO:HD3	1.94	0.68
1:A:2118:GLN:HE22	1:A:3249:ASN:H	1.41	0.68
1:A:1300:GLN:H	1:D:3300:GLN:NE2	1.92	0.67
1:E:2118:GLN:HE22	1:E:3249:ASN:H	1.43	0.67
1:G:2118:GLN:HE22	1:G:3249:ASN:H	1.42	0.67
1:H:1217:PHE:HA	1:H:1248:LYS:HE3	1.77	0.67
1:A:156:GLU:OE2	1:A:1176:ARG:HG2	1.95	0.67
1:C:2063:GLU:OE1	1:C:2222:ARG:HD2	1.95	0.67
1:H:3044:SER:OG	1:H:3045:LEU:N	2.26	0.67
1:B:2300:GLN:HE22	1:C:2300:GLN:H	1.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1146:VAL:HG11	1:C:1211:GLY:HA3	1.76	0.67
1:C:1217:PHE:HA	1:C:1248:LYS:HE3	1.77	0.67
1:D:1146:VAL:HG11	1:D:1211:GLY:HA3	1.77	0.67
1:G:1146:VAL:HG11	1:G:1211:GLY:HA3	1.76	0.67
1:A:3044:SER:OG	1:A:3045:LEU:N	2.27	0.67
1:B:3044:SER:OG	1:B:3045:LEU:N	2.25	0.67
1:C:3044:SER:OG	1:C:3045:LEU:N	2.27	0.67
1:E:3300:GLN:HE22	1:H:1300:GLN:H	1.43	0.67
1:C:2117:SER:O	1:C:2119:PRO:HD3	1.95	0.66
1:D:2117:SER:O	1:D:2119:PRO:HD3	1.95	0.66
1:B:1217:PHE:HA	1:B:1248:LYS:HE3	1.77	0.66
1:F:1123:GLU:HB2	1:F:1152:LYS:CE	2.25	0.66
1:F:1146:VAL:HG11	1:F:1211:GLY:HA3	1.77	0.66
1:G:1217:PHE:HA	1:G:1248:LYS:HE3	1.77	0.66
1:A:1160:GLY:C	1:A:1161:ASP:OD1	2.34	0.66
1:E:2117:SER:O	1:E:2119:PRO:HD3	1.95	0.66
1:H:156:GLU:CG	1:H:1176:ARG:HG3	2.26	0.66
1:H:2117:SER:O	1:H:2119:PRO:HD3	1.95	0.66
1:D:1217:PHE:HA	1:D:1248:LYS:HE3	1.77	0.66
1:D:3018:GLU:HG2	1:D:3024:GLY:H	1.61	0.65
1:G:114:LEU:O	1:G:1028:ARG:HA	1.96	0.65
1:C:3151:PRO:CG	1:D:3151:PRO:HG2	2.15	0.65
1:G:2117:SER:O	1:G:2119:PRO:HD3	1.95	0.65
1:E:1217:PHE:HA	1:E:1248:LYS:HE3	1.77	0.65
1:E:114:LEU:HB3	1:E:1029:LEU:HD12	1.78	0.65
1:A:1123:GLU:HB2	1:A:1152:LYS:CE	2.26	0.65
1:A:1217:PHE:HA	1:A:1248:LYS:HE3	1.79	0.65
1:D:1123:GLU:HB2	1:D:1152:LYS:CE	2.27	0.65
1:E:1123:GLU:HB2	1:E:1152:LYS:CE	2.26	0.65
1:H:1123:GLU:HB2	1:H:1152:LYS:CE	2.27	0.65
1:C:1123:GLU:HB2	1:C:1152:LYS:CE	2.27	0.65
1:C:1123:GLU:HB2	1:C:1152:LYS:HZ1	1.61	0.65
1:D:2063:GLU:OE1	1:D:2222:ARG:HD2	1.96	0.65
1:B:1146:VAL:HG11	1:B:1211:GLY:HA3	1.78	0.64
1:E:3300:GLN:N	1:H:1300:GLN:NE2	2.43	0.64
1:G:1123:GLU:HB2	1:G:1152:LYS:HZ1	1.62	0.64
1:G:1123:GLU:HB2	1:G:1152:LYS:CE	2.27	0.64
1:E:1308:TRP:HE3	1:E:1309:LEU:HD23	1.62	0.64
1:B:2117:SER:O	1:B:2119:PRO:HD3	1.97	0.64
1:H:2063:GLU:OE1	1:H:2222:ARG:HD2	1.97	0.64
1:A:1209:THR:HG22	1:A:1209:THR:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2063:GLU:OE1	1:A:2222:ARG:HD2	1.97	0.64
1:B:1123:GLU:HB2	1:B:1152:LYS:HZ1	1.63	0.64
1:A:1300:GLN:H	1:D:3300:GLN:HE22	1.46	0.64
1:C:3177:LYS:CE	1:F:173:GLN:CG	2.58	0.64
1:E:1300:GLN:NE2	1:H:3300:GLN:N	2.41	0.64
1:B:2063:GLU:OE1	1:B:2222:ARG:HD2	1.98	0.64
1:G:1156:GLU:N	1:G:1156:GLU:OE2	2.31	0.64
1:E:3018:GLU:HG2	1:E:3024:GLY:H	1.63	0.64
1:F:143:VAL:O	1:F:192:ILE:HG12	1.97	0.64
1:F:160:GLY:HA2	1:F:166:LEU:HD11	1.79	0.64
1:G:157:GLY:HA2	1:G:1172:SER:HB3	1.79	0.64
1:G:2076:THR:HG22	1:G:2077:LEU:HD12	1.80	0.64
1:H:3029:LEU:HD23	1:H:3254:PRO:HD2	1.80	0.64
1:G:2063:GLU:OE1	1:G:2222:ARG:HD2	1.98	0.64
1:H:156:GLU:HG2	1:H:1176:ARG:HG3	1.80	0.64
1:B:1123:GLU:HB2	1:B:1152:LYS:CE	2.28	0.63
1:B:1300:GLN:H	1:C:3300:GLN:NE2	1.97	0.63
1:C:1308:TRP:HE3	1:C:1309:LEU:HD23	1.63	0.63
1:F:1308:TRP:HE3	1:F:1309:LEU:HD23	1.61	0.63
1:D:1308:TRP:HE3	1:D:1309:LEU:HD23	1.62	0.63
1:F:68:GLU:HB2	3:F:400:ANP:O2G	1.98	0.63
1:D:143:VAL:O	1:D:192:ILE:HG12	1.98	0.63
1:F:3029:LEU:HD23	1:F:3254:PRO:HD2	1.80	0.63
1:A:1308:TRP:HE3	1:A:1309:LEU:HD23	1.62	0.63
1:B:2076:THR:HG22	1:B:2077:LEU:HD12	1.81	0.63
1:C:143:VAL:O	1:C:192:ILE:HG12	1.98	0.63
1:C:1164:MET:HG3	1:C:1165:GLY:CA	2.28	0.63
1:D:1123:GLU:HB2	1:D:1152:LYS:HZ1	1.63	0.63
1:E:2063:GLU:OE1	1:E:2222:ARG:HD2	1.98	0.63
1:H:143:VAL:O	1:H:192:ILE:HG12	1.97	0.63
1:C:3029:LEU:HD23	1:C:3254:PRO:HD2	1.80	0.63
1:G:3018:GLU:HG2	1:G:3024:GLY:H	1.64	0.63
1:H:118:GLN:HE21	1:H:1254:PRO:HB3	1.64	0.63
1:H:1308:TRP:HE3	1:H:1309:LEU:HD23	1.62	0.63
1:A:1123:GLU:HB2	1:A:1152:LYS:HZ1	1.63	0.63
1:E:1300:GLN:HE22	1:H:3300:GLN:H	1.45	0.63
1:H:1140:VAL:HG12	1:H:1188:LEU:HB3	1.81	0.63
1:B:2300:GLN:NE2	1:C:2300:GLN:N	2.46	0.62
1:G:1305:ALA:O	1:G:1306:THR:C	2.38	0.62
1:G:1308:TRP:HE3	1:G:1309:LEU:HD23	1.64	0.62
1:B:237:VAL:O	1:B:239:GLY:N	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1140:VAL:HG12	1:D:1188:LEU:HB3	1.81	0.62
1:F:1300:GLN:H	1:G:3300:GLN:NE2	1.97	0.62
1:G:3029:LEU:HD23	1:G:3254:PRO:HD2	1.81	0.62
1:B:3029:LEU:HD23	1:B:3254:PRO:HD2	1.81	0.62
1:D:3029:LEU:HD23	1:D:3254:PRO:HD2	1.80	0.62
1:F:2063:GLU:OE1	1:F:2222:ARG:HD2	1.98	0.62
1:F:2117:SER:O	1:F:2119:PRO:HD3	1.98	0.62
1:F:3018:GLU:HG2	1:F:3024:GLY:H	1.63	0.62
1:F:3185:SER:C	1:F:3187:THR:H	2.03	0.62
1:B:1308:TRP:HE3	1:B:1309:LEU:HD23	1.63	0.62
1:F:1140:VAL:HG12	1:F:1188:LEU:HB3	1.81	0.62
1:A:1156:GLU:OE2	1:A:2176:ARG:CB	2.47	0.62
1:B:3018:GLU:HG2	1:B:3024:GLY:H	1.64	0.62
1:B:3185:SER:C	1:B:3187:THR:H	2.02	0.62
1:E:1123:GLU:HB2	1:E:1152:LYS:HZ1	1.64	0.62
1:F:1123:GLU:HB2	1:F:1152:LYS:HZ1	1.64	0.62
1:E:3029:LEU:HD23	1:E:3254:PRO:HD2	1.80	0.62
1:C:3018:GLU:HG2	1:C:3024:GLY:H	1.64	0.62
1:F:1153:ALA:O	1:F:1157:GLY:CA	2.47	0.62
1:C:1305:ALA:O	1:C:1306:THR:C	2.37	0.61
1:C:3177:LYS:NZ	1:F:173:GLN:HG3	2.15	0.61
1:F:1305:ALA:O	1:F:1306:THR:C	2.39	0.61
1:A:3018:GLU:HG2	1:A:3024:GLY:H	1.64	0.61
1:E:2076:THR:HG22	1:E:2077:LEU:HD12	1.82	0.61
1:G:3229:GLY:O	1:G:3230:ALA:CB	2.48	0.61
1:A:1159:ILE:HG22	1:A:1160:GLY:H	1.64	0.61
1:C:2076:THR:HG22	1:C:2077:LEU:HD12	1.82	0.61
1:D:1053:ALA:HB2	1:D:1251:ILE:HG21	1.83	0.61
1:A:3029:LEU:HD23	1:A:3254:PRO:HD2	1.81	0.61
1:B:1300:GLN:NE2	1:C:3300:GLN:H	1.98	0.61
1:D:3185:SER:C	1:D:3187:THR:H	2.04	0.61
1:H:3018:GLU:HG2	1:H:3024:GLY:H	1.64	0.61
1:A:2076:THR:HG22	1:A:2077:LEU:HD12	1.83	0.61
1:E:143:VAL:O	1:E:192:ILE:HG12	2.01	0.61
1:G:237:VAL:O	1:G:239:GLY:N	2.30	0.61
1:G:3185:SER:C	1:G:3187:THR:H	2.04	0.61
1:B:2300:GLN:HE21	1:C:2300:GLN:HB3	1.66	0.61
1:B:3229:GLY:O	1:B:3230:ALA:CB	2.49	0.61
1:C:1140:VAL:HG12	1:C:1188:LEU:HB3	1.83	0.61
1:G:143:VAL:O	1:G:192:ILE:HG12	2.00	0.61
1:H:143:VAL:HG21	1:H:191:PHE:CD1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG21	1:A:191:PHE:CD1	2.36	0.60
1:G:1281:GLU:O	1:G:1283:LEU:N	2.33	0.60
1:D:3229:GLY:O	1:D:3230:ALA:CB	2.49	0.60
1:E:1140:VAL:HG12	1:E:1188:LEU:HB3	1.83	0.60
1:E:3105:ARG:CD	1:F:227:ARG:HH22	2.04	0.60
1:E:3229:GLY:O	1:E:3230:ALA:CB	2.49	0.60
1:F:143:VAL:HG21	1:F:191:PHE:CD1	2.36	0.60
1:A:1121:THR:OG1	1:A:1122:GLY:N	2.33	0.60
1:D:2076:THR:HG22	1:D:2077:LEU:HD12	1.82	0.60
1:E:3185:SER:C	1:E:3187:THR:H	2.05	0.60
1:A:1071:GLY:HA2	3:A:1400:ANP:C5'	2.31	0.60
1:A:1193:ASN:HD22	1:A:1209:THR:HG23	1.61	0.60
1:B:42:THR:HG21	1:B:47:LEU:HD22	1.84	0.60
1:D:1230:ALA:H	1:D:1241:GLU:H	1.50	0.60
1:A:3185:SER:C	1:A:3187:THR:H	2.05	0.60
1:B:143:VAL:HG21	1:B:191:PHE:CD1	2.37	0.60
1:C:1121:THR:OG1	1:C:1122:GLY:N	2.35	0.60
1:C:2090:CYS:HB3	1:C:2140:VAL:HG13	1.84	0.60
1:C:3185:SER:C	1:C:3187:THR:H	2.05	0.60
1:D:1161:ASP:CB	1:F:183:LYS:HZ3	2.14	0.60
1:E:2090:CYS:HB3	1:E:2140:VAL:HG13	1.84	0.60
1:A:1193:ASN:HD21	1:A:1211:GLY:H	1.47	0.60
1:A:1305:ALA:O	1:A:1306:THR:C	2.40	0.60
1:G:143:VAL:HG21	1:G:191:PHE:CD1	2.36	0.60
1:G:2090:CYS:HB3	1:G:2140:VAL:HG13	1.83	0.60
1:B:1140:VAL:HG12	1:B:1188:LEU:HB3	1.83	0.60
1:C:2155:ILE:O	1:C:2156:GLU:HG3	2.02	0.60
1:C:2229:GLY:O	1:C:2230:ALA:HB2	2.01	0.60
1:D:1305:ALA:O	1:D:1306:THR:C	2.40	0.60
1:E:2300:GLN:NE2	1:H:2300:GLN:N	2.49	0.60
1:G:1121:THR:OG1	1:G:1122:GLY:N	2.34	0.60
1:A:1053:ALA:HB2	1:A:1251:ILE:HG21	1.83	0.60
1:B:2229:GLY:O	1:B:2230:ALA:HB2	2.02	0.60
1:D:1161:ASP:HB2	1:F:183:LYS:HZ3	1.61	0.60
1:G:3082:ALA:HA	1:G:3085:ARG:HB2	1.83	0.60
1:A:114:LEU:HB3	1:A:1029:LEU:HD12	1.84	0.60
1:C:71:GLY:HA2	3:C:400:ANP:H5'1	1.84	0.60
1:F:2229:GLY:O	1:F:2230:ALA:HB2	2.02	0.60
1:H:2229:GLY:O	1:H:2230:ALA:HB2	2.02	0.60
1:C:3229:GLY:O	1:C:3230:ALA:CB	2.49	0.60
1:E:1053:ALA:HB2	1:E:1251:ILE:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:THR:HG21	1:F:47:LEU:HD22	1.84	0.59
1:F:2090:CYS:HB3	1:F:2140:VAL:HG13	1.84	0.59
1:A:1161:ASP:HB3	1:A:1166:LEU:HD13	1.83	0.59
1:A:2090:CYS:HB3	1:A:2140:VAL:HG13	1.84	0.59
1:A:2229:GLY:O	1:A:2230:ALA:HB2	2.02	0.59
1:A:3229:GLY:O	1:A:3230:ALA:CB	2.50	0.59
1:B:2090:CYS:HB3	1:B:2140:VAL:HG13	1.82	0.59
1:F:1053:ALA:HB2	1:F:1251:ILE:HG21	1.84	0.59
1:H:2076:THR:HG22	1:H:2077:LEU:HD12	1.82	0.59
1:C:2018:GLU:HG2	1:C:2024:GLY:H	1.67	0.59
1:E:143:VAL:HG21	1:E:191:PHE:CD1	2.37	0.59
1:C:1281:GLU:O	1:C:1283:LEU:N	2.35	0.59
1:E:2229:GLY:O	1:E:2230:ALA:HB2	2.03	0.59
1:G:3057:PRO:O	1:G:3188:LEU:HD13	2.02	0.59
1:E:237:VAL:O	1:E:239:GLY:N	2.30	0.59
1:B:143:VAL:O	1:B:192:ILE:HG12	2.01	0.59
1:D:270:PHE:HA	1:D:273:GLU:HG2	1.84	0.59
1:D:2229:GLY:O	1:D:2230:ALA:HB2	2.02	0.59
1:B:156:GLU:CD	1:B:1176:ARG:HG3	2.23	0.59
1:C:237:VAL:O	1:C:239:GLY:N	2.31	0.59
1:C:3057:PRO:O	1:C:3188:LEU:HD13	2.02	0.59
1:D:2090:CYS:HB3	1:D:2140:VAL:HG13	1.84	0.59
1:G:1053:ALA:HB2	1:G:1251:ILE:HG21	1.84	0.59
1:H:1281:GLU:O	1:H:1283:LEU:N	2.36	0.59
1:H:3229:GLY:O	1:H:3230:ALA:CB	2.50	0.59
1:E:3082:ALA:HA	1:E:3085:ARG:HB2	1.84	0.59
1:H:1123:GLU:HB2	1:H:1152:LYS:HZ1	1.66	0.59
1:A:42:THR:HG21	1:A:47:LEU:HD22	1.84	0.59
1:B:1053:ALA:HB2	1:B:1251:ILE:HG21	1.84	0.59
1:D:42:THR:HG21	1:D:47:LEU:HD22	1.85	0.59
1:D:3082:ALA:HA	1:D:3085:ARG:HB2	1.84	0.59
1:H:3185:SER:C	1:H:3187:THR:H	2.05	0.59
1:A:1163:HIS:O	1:A:1164:MET:C	2.41	0.59
1:B:2300:GLN:H	1:C:2300:GLN:HE22	1.49	0.59
1:E:1092:PHE:CE2	1:E:1094:ASP:HB2	2.38	0.59
1:F:3064:ILE:HG12	1:F:3223:LEU:CB	2.31	0.59
1:F:3229:GLY:O	1:F:3230:ALA:CB	2.50	0.59
1:G:270:PHE:HA	1:G:273:GLU:HG2	1.84	0.59
1:C:1053:ALA:HB2	1:C:1251:ILE:HG21	1.84	0.58
1:D:237:VAL:O	1:D:239:GLY:N	2.30	0.58
1:D:3175:MET:HG3	1:D:3218:TYR:CD1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1230:ALA:H	1:E:1241:GLU:H	1.51	0.58
1:E:3300:GLN:NE2	1:H:1300:GLN:N	2.49	0.58
1:F:3057:PRO:O	1:F:3188:LEU:HD13	2.03	0.58
1:H:3057:PRO:O	1:H:3188:LEU:HD13	2.03	0.58
1:A:143:VAL:O	1:A:192:ILE:HG12	2.03	0.58
1:A:2018:GLU:HG2	1:A:2024:GLY:H	1.67	0.58
1:A:3082:ALA:HA	1:A:3085:ARG:HB2	1.84	0.58
1:C:143:VAL:HG21	1:C:191:PHE:CD1	2.38	0.58
1:D:143:VAL:HG21	1:D:191:PHE:CD1	2.38	0.58
1:D:3057:PRO:O	1:D:3188:LEU:HD13	2.03	0.58
1:F:2076:THR:HG22	1:F:2077:LEU:HD12	1.82	0.58
1:F:3006:LYS:HG3	1:F:3007:GLN:H	1.68	0.58
1:H:1230:ALA:H	1:H:1241:GLU:H	1.51	0.58
1:B:2018:GLU:HG2	1:B:2024:GLY:H	1.69	0.58
1:H:237:VAL:O	1:H:239:GLY:N	2.31	0.58
1:B:1121:THR:OG1	1:B:1122:GLY:N	2.36	0.58
1:D:1141:ILE:HG21	1:D:1189:LEU:HD12	1.85	0.58
1:D:1281:GLU:O	1:D:1283:LEU:N	2.37	0.58
1:E:1145:SER:HB2	1:E:1192:ILE:O	2.02	0.58
1:F:1121:THR:OG1	1:F:1122:GLY:N	2.36	0.58
1:G:1140:VAL:HG12	1:G:1188:LEU:HB3	1.85	0.58
1:G:3006:LYS:HG3	1:G:3007:GLN:H	1.69	0.58
1:H:1053:ALA:HB2	1:H:1251:ILE:HG21	1.84	0.58
1:A:1230:ALA:H	1:A:1241:GLU:H	1.52	0.58
1:B:1092:PHE:CE2	1:B:1094:ASP:HB2	2.39	0.58
1:B:3057:PRO:O	1:B:3188:LEU:HD13	2.03	0.58
1:A:1141:ILE:HG21	1:A:1189:LEU:HD12	1.85	0.58
1:C:1092:PHE:CE2	1:C:1094:ASP:HB2	2.39	0.58
1:D:1092:PHE:CE2	1:D:1094:ASP:HB2	2.38	0.58
1:F:1114:LEU:HB3	1:F:2029:LEU:HD12	1.86	0.58
1:B:2217:PHE:O	1:B:2248:LYS:NZ	2.37	0.58
1:E:270:PHE:HA	1:E:273:GLU:HG2	1.85	0.58
1:E:3057:PRO:O	1:E:3188:LEU:HD13	2.04	0.58
1:B:1299:GLY:HA2	1:C:3300:GLN:HE22	1.68	0.58
1:E:42:THR:HG21	1:E:47:LEU:HD22	1.85	0.58
1:F:3082:ALA:HA	1:F:3085:ARG:HB2	1.86	0.58
1:A:1145:SER:HB2	1:A:1192:ILE:O	2.03	0.58
1:D:2018:GLU:HG2	1:D:2024:GLY:H	1.69	0.58
1:F:1161:ASP:CB	1:F:1166:LEU:HD13	2.23	0.58
1:G:42:THR:HG21	1:G:47:LEU:HD22	1.86	0.58
1:G:3072:LYS:HE3	3:G:3400:ANP:O1B	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:VAL:HG12	1:A:1188:LEU:HB3	1.85	0.58
1:C:1230:ALA:HA	1:C:1240:SER:HA	1.86	0.58
1:C:3006:LYS:HG3	1:C:3007:GLN:H	1.68	0.58
1:F:3300:GLN:NE2	1:G:1300:GLN:H	2.02	0.58
1:G:2229:GLY:O	1:G:2230:ALA:HB2	2.03	0.58
1:A:1161:ASP:CB	1:A:1166:LEU:HD13	2.34	0.57
1:A:1281:GLU:O	1:A:1283:LEU:N	2.37	0.57
1:D:1145:SER:HB2	1:D:1192:ILE:O	2.04	0.57
1:E:1230:ALA:HA	1:E:1240:SER:HA	1.86	0.57
1:E:1300:GLN:N	1:H:3300:GLN:NE2	2.46	0.57
1:E:2018:GLU:HG2	1:E:2024:GLY:H	1.69	0.57
1:E:2300:GLN:N	1:H:2300:GLN:NE2	2.50	0.57
1:F:3300:GLN:H	1:G:1300:GLN:NE2	2.02	0.57
1:G:1141:ILE:HG21	1:G:1189:LEU:HD12	1.86	0.57
1:C:1230:ALA:H	1:C:1241:GLU:H	1.52	0.57
1:C:2217:PHE:O	1:C:2248:LYS:NZ	2.36	0.57
1:E:1141:ILE:HG21	1:E:1189:LEU:HD12	1.86	0.57
1:H:2090:CYS:HB3	1:H:2140:VAL:HG13	1.85	0.57
1:B:1230:ALA:H	1:B:1241:GLU:H	1.52	0.57
1:F:2018:GLU:HG2	1:F:2024:GLY:H	1.68	0.57
1:F:3175:MET:HG3	1:F:3218:TYR:CD1	2.37	0.57
1:H:3082:ALA:HA	1:H:3085:ARG:HB2	1.87	0.57
1:A:1230:ALA:HA	1:A:1240:SER:HA	1.87	0.57
1:C:42:THR:HG21	1:C:47:LEU:HD22	1.86	0.57
1:D:92:PHE:N	1:D:115:LEU:O	2.37	0.57
1:F:92:PHE:N	1:F:115:LEU:O	2.37	0.57
1:H:153:ALA:O	1:H:157:GLY:N	2.37	0.57
1:H:270:PHE:HA	1:H:273:GLU:HG2	1.85	0.57
1:H:2018:GLU:HG2	1:H:2024:GLY:H	1.69	0.57
1:A:237:VAL:O	1:A:239:GLY:N	2.31	0.57
1:C:3082:ALA:HA	1:C:3085:ARG:HB2	1.85	0.57
1:H:1092:PHE:CE2	1:H:1094:ASP:HB2	2.39	0.57
1:H:1305:ALA:O	1:H:1306:THR:C	2.43	0.57
1:H:3006:LYS:HG3	1:H:3007:GLN:H	1.70	0.57
1:A:2217:PHE:O	1:A:2248:LYS:NZ	2.37	0.57
1:B:1305:ALA:O	1:B:1306:THR:C	2.41	0.57
1:C:270:PHE:HA	1:C:273:GLU:HG2	1.84	0.57
1:E:3006:LYS:HG3	1:E:3007:GLN:H	1.70	0.57
1:F:1230:ALA:HA	1:F:1240:SER:HA	1.86	0.57
1:A:3306:THR:O	1:A:3308:TRP:N	2.38	0.57
1:C:1091:ALA:HB3	1:C:1141:ILE:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2217:PHE:O	1:D:2248:LYS:NZ	2.37	0.57
1:G:2018:GLU:HG2	1:G:2024:GLY:H	1.69	0.57
1:B:3006:LYS:HG3	1:B:3007:GLN:H	1.70	0.57
1:E:1121:THR:OG1	1:E:1122:GLY:N	2.37	0.57
1:E:1300:GLN:HE21	1:H:3300:GLN:H	1.53	0.57
1:F:2217:PHE:O	1:F:2248:LYS:NZ	2.37	0.57
1:G:1230:ALA:H	1:G:1241:GLU:H	1.52	0.57
1:B:2300:GLN:N	1:C:2300:GLN:HE22	2.02	0.57
1:D:3006:LYS:HG3	1:D:3007:GLN:H	1.69	0.57
1:G:42:THR:HA	1:G:79:VAL:HG12	1.87	0.57
1:E:2217:PHE:O	1:E:2248:LYS:NZ	2.38	0.57
1:F:1092:PHE:CE2	1:F:1094:ASP:HB2	2.39	0.56
1:F:1145:SER:HB2	1:F:1192:ILE:O	2.04	0.56
1:H:1230:ALA:HA	1:H:1240:SER:HA	1.86	0.56
1:A:270:PHE:HA	1:A:273:GLU:HG2	1.85	0.56
1:D:3064:ILE:HG12	1:D:3223:LEU:CB	2.31	0.56
1:B:3082:ALA:HA	1:B:3085:ARG:HB2	1.86	0.56
1:C:92:PHE:N	1:C:115:LEU:O	2.36	0.56
1:C:1060:ARG:HB3	1:C:1220:SER:OG	2.06	0.56
1:D:1230:ALA:HA	1:D:1240:SER:HA	1.86	0.56
1:F:131:ALA:HB1	1:F:1017:ILE:HD12	1.87	0.56
1:G:1155:ILE:C	1:G:1156:GLU:OE2	2.44	0.56
1:G:2217:PHE:O	1:G:2248:LYS:NZ	2.38	0.56
1:H:92:PHE:N	1:H:115:LEU:O	2.37	0.56
1:A:1092:PHE:CE2	1:A:1094:ASP:HB2	2.40	0.56
1:A:3006:LYS:HG3	1:A:3007:GLN:H	1.70	0.56
1:C:3306:THR:O	1:C:3308:TRP:N	2.39	0.56
1:E:1091:ALA:HB3	1:E:1141:ILE:HG12	1.88	0.56
1:F:270:PHE:HA	1:F:273:GLU:HG2	1.86	0.56
1:G:1092:PHE:CE2	1:G:1094:ASP:HB2	2.40	0.56
1:G:1230:ALA:HA	1:G:1240:SER:HA	1.87	0.56
1:E:92:PHE:N	1:E:115:LEU:O	2.39	0.56
1:F:1163:HIS:HB2	1:F:1166:LEU:CG	2.29	0.56
1:F:1230:ALA:H	1:F:1241:GLU:H	1.53	0.56
1:H:1091:ALA:HB3	1:H:1141:ILE:HG12	1.88	0.56
1:H:2217:PHE:O	1:H:2248:LYS:NZ	2.39	0.56
1:B:1281:GLU:O	1:B:1283:LEU:N	2.38	0.56
1:F:1281:GLU:O	1:F:1283:LEU:N	2.39	0.56
1:H:1145:SER:HB2	1:H:1192:ILE:O	2.05	0.56
1:B:1145:SER:HB2	1:B:1192:ILE:O	2.05	0.56
1:C:1145:SER:HB2	1:C:1192:ILE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1145:SER:HB2	1:G:1192:ILE:O	2.05	0.56
1:B:1091:ALA:HB3	1:B:1141:ILE:HG12	1.88	0.56
1:E:3311:ASP:HB3	1:F:286:LYS:NZ	2.20	0.56
1:H:42:THR:HG21	1:H:47:LEU:HD22	1.87	0.56
1:A:1060:ARG:HB3	1:A:1220:SER:OG	2.06	0.56
1:B:1141:ILE:HG21	1:B:1189:LEU:HD12	1.87	0.56
1:E:1305:ALA:O	1:E:1306:THR:C	2.43	0.56
1:F:237:VAL:O	1:F:239:GLY:N	2.33	0.56
1:C:1298:ILE:HG13	1:C:1299:GLY:N	2.20	0.56
1:D:1091:ALA:HB3	1:D:1141:ILE:HG12	1.88	0.56
1:E:3151:PRO:CG	1:F:3151:PRO:HG2	2.18	0.56
1:H:1141:ILE:HG21	1:H:1189:LEU:HD12	1.87	0.56
1:A:154:GLU:O	1:A:156:GLU:O	2.23	0.55
1:E:3175:MET:HG3	1:E:3218:TYR:CD1	2.35	0.55
1:F:3065:TYR:C	1:F:3065:TYR:CD2	2.80	0.55
1:H:3064:ILE:HG12	1:H:3223:LEU:CB	2.32	0.55
1:A:3064:ILE:HG12	1:A:3223:LEU:CB	2.32	0.55
1:F:1141:ILE:HG21	1:F:1189:LEU:HD12	1.87	0.55
1:F:3300:GLN:HE22	1:G:1300:GLN:H	1.54	0.55
1:G:1060:ARG:HB3	1:G:1220:SER:OG	2.06	0.55
1:G:3175:MET:HG3	1:G:3218:TYR:CD1	2.37	0.55
1:B:1230:ALA:HA	1:B:1240:SER:HA	1.88	0.55
1:F:3072:LYS:CE	3:F:3400:ANP:O1B	2.50	0.55
1:B:270:PHE:HA	1:B:273:GLU:HG2	1.87	0.55
1:B:3175:MET:HG3	1:B:3218:TYR:CD1	2.35	0.55
1:B:3306:THR:O	1:B:3308:TRP:N	2.39	0.55
1:C:1078:GLN:O	1:C:1081:ALA:HB3	2.06	0.55
1:C:1153:ALA:O	1:C:1158:GLU:HA	2.06	0.55
1:E:3065:TYR:HD2	1:E:3065:TYR:C	2.10	0.55
1:F:3306:THR:O	1:F:3308:TRP:N	2.39	0.55
1:A:42:THR:HA	1:A:79:VAL:HG12	1.88	0.55
1:B:42:THR:HA	1:B:79:VAL:HG12	1.89	0.55
1:B:92:PHE:N	1:B:115:LEU:O	2.38	0.55
1:C:42:THR:HA	1:C:79:VAL:HG12	1.89	0.55
1:D:3065:TYR:HD2	1:D:3065:TYR:C	2.10	0.55
1:H:1121:THR:OG1	1:H:1122:GLY:N	2.37	0.55
1:E:1281:GLU:O	1:E:1283:LEU:N	2.38	0.55
1:C:1141:ILE:HG21	1:C:1189:LEU:HD12	1.88	0.55
1:F:42:THR:HA	1:F:79:VAL:HG12	1.88	0.55
1:F:1123:GLU:HB2	1:F:1152:LYS:NZ	2.21	0.55
1:E:42:THR:HA	1:E:79:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:GLN:NE2	1:F:1249:ASN:H	2.04	0.55
1:H:3065:TYR:HD2	1:H:3065:TYR:C	2.10	0.55
1:A:1204:GLY:HA3	1:B:3115:LEU:HD22	1.84	0.55
1:D:42:THR:HA	1:D:79:VAL:HG12	1.88	0.55
1:E:3065:TYR:C	1:E:3065:TYR:CD2	2.80	0.55
1:G:3306:THR:O	1:G:3308:TRP:N	2.40	0.55
1:A:3057:PRO:O	1:A:3188:LEU:HD13	2.07	0.54
1:D:1121:THR:OG1	1:D:1122:GLY:N	2.37	0.54
1:E:3306:THR:O	1:E:3308:TRP:N	2.40	0.54
1:F:3065:TYR:C	1:F:3065:TYR:HD2	2.10	0.54
1:F:1057:PRO:HB2	1:F:1060:ARG:HG3	1.89	0.54
1:B:1060:ARG:HB3	1:B:1220:SER:OG	2.08	0.54
1:D:1060:ARG:HB3	1:D:1220:SER:OG	2.08	0.54
1:D:3065:TYR:C	1:D:3065:TYR:CD2	2.81	0.54
1:H:3065:TYR:C	1:H:3065:TYR:CD2	2.81	0.54
1:H:3072:LYS:CE	3:H:3400:ANP:O1B	2.53	0.54
1:E:1123:GLU:HB2	1:E:1152:LYS:NZ	2.22	0.54
1:F:3268:ILE:HG22	1:F:3269:ASN:N	2.23	0.54
1:B:1057:PRO:HB2	1:B:1060:ARG:HG3	1.90	0.54
1:B:2300:GLN:HE22	1:C:2300:GLN:N	2.03	0.54
1:E:1060:ARG:HB3	1:E:1220:SER:OG	2.08	0.54
1:A:1057:PRO:HB2	1:A:1060:ARG:HG3	1.90	0.54
1:C:1123:GLU:HB2	1:C:1152:LYS:NZ	2.22	0.54
1:C:1229:GLY:O	1:C:1230:ALA:HB3	2.08	0.54
1:A:156:GLU:OE2	1:A:1176:ARG:HG3	2.07	0.54
1:C:156:GLU:HG2	1:C:1176:ARG:HG2	1.89	0.54
1:C:3064:ILE:HG12	1:C:3223:LEU:CB	2.30	0.54
1:G:131:ALA:HB1	1:G:1017:ILE:HD12	1.88	0.54
1:G:1078:GLN:O	1:G:1081:ALA:HB3	2.08	0.54
1:G:3065:TYR:HD2	1:G:3065:TYR:C	2.12	0.54
1:H:1114:LEU:HB3	1:H:2029:LEU:HD12	1.89	0.54
1:D:1123:GLU:HB2	1:D:1152:LYS:NZ	2.22	0.54
1:F:1060:ARG:HB3	1:F:1220:SER:OG	2.08	0.54
1:H:1057:PRO:HB2	1:H:1060:ARG:HG3	1.90	0.54
1:A:1229:GLY:O	1:A:1230:ALA:HB3	2.07	0.54
1:D:155:ILE:C	1:D:157:GLY:N	2.60	0.54
1:C:1057:PRO:HB2	1:C:1060:ARG:HG3	1.90	0.54
1:D:1143:VAL:O	1:D:1192:ILE:HG13	2.08	0.54
1:G:1057:PRO:HB2	1:G:1060:ARG:HG3	1.89	0.54
1:A:1123:GLU:HB2	1:A:1152:LYS:NZ	2.22	0.53
1:B:1143:VAL:O	1:B:1192:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ARG:NH2	1:D:3105:ARG:HD3	2.24	0.53
1:G:1091:ALA:HB3	1:G:1141:ILE:HG12	1.89	0.53
1:G:2029:LEU:HD23	1:G:2254:PRO:HD2	1.89	0.53
1:G:3065:TYR:C	1:G:3065:TYR:CD2	2.82	0.53
1:A:1161:ASP:CG	1:A:1166:LEU:HD13	2.29	0.53
1:A:3065:TYR:HD2	1:A:3065:TYR:C	2.12	0.53
1:B:1092:PHE:HB2	1:B:1114:LEU:HD11	1.90	0.53
1:C:3084:GLN:HG2	1:C:3110:ASP:H	1.74	0.53
1:D:157:GLY:HA3	1:D:1172:SER:HB3	1.90	0.53
1:F:1091:ALA:HB3	1:F:1141:ILE:HG12	1.90	0.53
1:F:2156:GLU:HA	1:F:3172:SER:OG	2.08	0.53
1:C:3065:TYR:HD2	1:C:3065:TYR:C	2.12	0.53
1:G:92:PHE:N	1:G:115:LEU:O	2.39	0.53
1:G:3143:VAL:HG21	1:G:3191:PHE:CD1	2.44	0.53
1:B:1078:GLN:O	1:B:1081:ALA:HB3	2.09	0.53
1:E:3064:ILE:HG12	1:E:3223:LEU:CB	2.33	0.53
1:F:3100:ASP:O	1:F:3101:PRO:C	2.46	0.53
1:G:1123:GLU:HB2	1:G:1152:LYS:NZ	2.23	0.53
1:H:1123:GLU:HB2	1:H:1152:LYS:NZ	2.23	0.53
1:A:1298:ILE:HG13	1:A:1299:GLY:N	2.23	0.53
1:B:131:ALA:HB1	1:B:1017:ILE:HD12	1.90	0.53
1:E:1229:GLY:O	1:E:1230:ALA:HB3	2.08	0.53
1:G:1298:ILE:HG13	1:G:1299:GLY:N	2.23	0.53
1:H:1060:ARG:HB3	1:H:1220:SER:OG	2.09	0.53
1:H:3084:GLN:HG2	1:H:3110:ASP:H	1.74	0.53
1:H:3306:THR:O	1:H:3308:TRP:N	2.41	0.53
1:G:3059:GLY:HA2	1:G:3187:THR:O	2.08	0.53
1:A:3105:ARG:HD3	1:B:227:ARG:NH2	2.24	0.53
1:B:1123:GLU:HB2	1:B:1152:LYS:NZ	2.23	0.53
1:C:3175:MET:HG3	1:C:3218:TYR:CD1	2.37	0.53
1:E:3300:GLN:HE22	1:H:1299:GLY:HA2	1.73	0.53
1:G:1229:GLY:O	1:G:1230:ALA:HB3	2.09	0.53
1:A:1091:ALA:HB3	1:A:1141:ILE:HG12	1.89	0.53
1:C:1073:THR:HA	1:C:1076:THR:HB	1.91	0.53
1:C:3065:TYR:C	1:C:3065:TYR:CD2	2.82	0.53
1:D:3100:ASP:O	1:D:3101:PRO:C	2.46	0.53
1:E:2300:GLN:H	1:H:2300:GLN:HE22	1.55	0.53
1:A:46:SER:HA	1:A:49:ILE:HD12	1.91	0.53
1:A:1176:ARG:HA	1:A:1218:TYR:HE1	1.74	0.53
1:C:1065:TYR:C	1:C:1065:TYR:CD1	2.82	0.53
1:D:1057:PRO:HB2	1:D:1060:ARG:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1222:ARG:HB2	1:D:1248:LYS:CB	2.37	0.53
1:E:1057:PRO:HB2	1:E:1060:ARG:HG3	1.90	0.53
1:F:3143:VAL:HG21	1:F:3191:PHE:CD1	2.44	0.53
1:G:1143:VAL:O	1:G:1192:ILE:HG13	2.09	0.53
1:H:42:THR:HA	1:H:79:VAL:HG12	1.90	0.53
1:F:1308:TRP:CE3	1:F:1309:LEU:HD23	2.44	0.52
1:C:153:ALA:O	1:C:158:GLU:HB2	2.09	0.52
1:D:1229:GLY:O	1:D:1230:ALA:HB3	2.09	0.52
1:G:1176:ARG:HA	1:G:1218:TYR:HE1	1.74	0.52
1:H:1112:ASP:HA	1:H:2030:GLY:HA3	1.91	0.52
1:A:1092:PHE:HB2	1:A:1114:LEU:HD11	1.91	0.52
1:A:3084:GLN:HG2	1:A:3110:ASP:H	1.73	0.52
1:B:1176:ARG:HA	1:B:1218:TYR:HE1	1.73	0.52
1:B:1229:GLY:O	1:B:1230:ALA:HB3	2.08	0.52
1:D:3306:THR:O	1:D:3308:TRP:N	2.42	0.52
1:G:3064:ILE:HG12	1:G:3223:LEU:CB	2.33	0.52
1:B:156:GLU:O	1:B:157:GLY:O	2.28	0.52
1:D:2178:LEU:O	1:D:2182:LEU:HG	2.09	0.52
1:E:1222:ARG:HB2	1:E:1248:LYS:CB	2.37	0.52
1:H:1065:TYR:CD1	1:H:1065:TYR:C	2.83	0.52
1:A:1078:GLN:O	1:A:1081:ALA:HB3	2.09	0.52
1:A:1208:THR:HG21	1:A:1222:ARG:HH22	1.75	0.52
1:B:121:THR:HG21	1:B:152:LYS:HG3	1.92	0.52
1:C:1114:LEU:HB3	1:C:2029:LEU:HD12	1.90	0.52
1:C:1143:VAL:O	1:C:1192:ILE:HG13	2.10	0.52
1:C:2178:LEU:O	1:C:2182:LEU:HG	2.10	0.52
1:D:1176:ARG:HA	1:D:1218:TYR:HE1	1.75	0.52
1:F:1176:ARG:HA	1:F:1218:TYR:HE1	1.74	0.52
1:A:1143:VAL:O	1:A:1192:ILE:HG13	2.09	0.52
1:A:3221:VAL:HA	1:A:3248:LYS:O	2.10	0.52
1:H:1092:PHE:HB2	1:H:1114:LEU:HD11	1.91	0.52
1:H:3059:GLY:HA2	1:H:3187:THR:O	2.10	0.52
1:C:1222:ARG:HB2	1:C:1248:LYS:CB	2.37	0.52
1:C:1316:ALA:O	1:C:1319:ILE:N	2.43	0.52
1:D:1159:ILE:HG22	1:D:1161:ASP:H	1.74	0.52
1:E:3300:GLN:N	1:H:1300:GLN:HE22	2.02	0.52
1:G:2178:LEU:O	1:G:2182:LEU:HG	2.10	0.52
1:H:118:GLN:NE2	1:H:1254:PRO:HB3	2.25	0.52
1:A:114:LEU:O	1:A:1028:ARG:HA	2.10	0.52
1:C:3177:LYS:CE	1:F:173:GLN:CD	2.76	0.52
1:E:1065:TYR:CD1	1:E:1065:TYR:C	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2178:LEU:O	1:B:2182:LEU:HG	2.10	0.52
1:C:1176:ARG:HA	1:C:1218:TYR:HE1	1.74	0.52
1:D:157:GLY:HA2	1:D:1172:SER:CB	2.39	0.52
1:D:1065:TYR:CD1	1:D:1065:TYR:C	2.83	0.52
1:D:1298:ILE:HG13	1:D:1299:GLY:N	2.24	0.52
1:B:1065:TYR:CD1	1:B:1065:TYR:C	2.84	0.52
1:C:2155:ILE:C	1:C:2156:GLU:HG3	2.30	0.52
1:C:3072:LYS:CE	3:C:3400:ANP:O1B	2.57	0.52
1:D:1078:GLN:O	1:D:1081:ALA:HB3	2.10	0.52
1:D:3268:ILE:HG22	1:D:3269:ASN:N	2.25	0.52
1:E:3105:ARG:HH11	1:F:227:ARG:NH2	2.09	0.52
1:F:71:GLY:CA	3:F:400:ANP:H5'1	2.38	0.52
1:F:1222:ARG:HB2	1:F:1248:LYS:CB	2.37	0.52
1:F:1229:GLY:O	1:F:1230:ALA:HB3	2.10	0.52
1:G:1065:TYR:CD1	1:G:1065:TYR:C	2.84	0.52
1:A:92:PHE:N	1:A:115:LEU:O	2.38	0.51
1:B:1298:ILE:HG13	1:B:1299:GLY:N	2.23	0.51
1:E:1092:PHE:HB2	1:E:1114:LEU:HD11	1.91	0.51
1:F:2146:VAL:HA	1:F:2149:LEU:HD23	1.92	0.51
1:F:2178:LEU:O	1:F:2182:LEU:HG	2.10	0.51
1:H:3175:MET:HG3	1:H:3218:TYR:CD1	2.36	0.51
1:A:1222:ARG:HB2	1:A:1248:LYS:CB	2.38	0.51
1:F:46:SER:HA	1:F:49:ILE:HD12	1.92	0.51
1:F:107:LEU:CD2	1:F:267:GLY:HA3	2.40	0.51
1:H:1229:GLY:O	1:H:1230:ALA:HB3	2.09	0.51
1:H:3143:VAL:HG21	1:H:3191:PHE:CD1	2.45	0.51
1:A:1091:ALA:HB3	1:A:1141:ILE:HA	1.93	0.51
1:B:3065:TYR:C	1:B:3065:TYR:CD2	2.84	0.51
1:B:3249:ASN:OD1	1:B:3251:ILE:HG22	2.10	0.51
1:E:1143:VAL:O	1:E:1192:ILE:HG13	2.10	0.51
1:F:2118:GLN:NE2	1:F:3249:ASN:H	2.08	0.51
1:G:121:THR:HG21	1:G:152:LYS:HG3	1.92	0.51
1:G:3100:ASP:O	1:G:3101:PRO:C	2.49	0.51
1:A:132:LEU:HB2	1:A:141:ILE:HD11	1.92	0.51
1:A:3065:TYR:C	1:A:3065:TYR:CD2	2.82	0.51
1:C:121:THR:HG21	1:C:152:LYS:HG3	1.93	0.51
1:C:2123:GLU:HG3	1:C:2170:MET:HG3	1.92	0.51
1:D:1092:PHE:HB2	1:D:1114:LEU:HD11	1.92	0.51
1:F:3298:ILE:HG13	1:F:3299:GLY:N	2.26	0.51
1:A:2178:LEU:O	1:A:2182:LEU:HG	2.10	0.51
1:D:3084:GLN:HG2	1:D:3110:ASP:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1078:GLN:O	1:E:1081:ALA:HB3	2.09	0.51
1:F:99:LEU:HD23	1:F:1255:PHE:CZ	2.46	0.51
1:F:118:GLN:HE21	1:F:1249:ASN:H	1.57	0.51
1:A:1065:TYR:CD1	1:A:1065:TYR:C	2.84	0.51
1:A:2042:THR:HG21	1:A:2047:LEU:HD22	1.93	0.51
1:C:131:ALA:HB1	1:C:1017:ILE:HD12	1.93	0.51
1:D:46:SER:HA	1:D:49:ILE:HD12	1.93	0.51
1:D:2308:TRP:HE3	1:D:2309:LEU:HD23	1.75	0.51
1:D:3059:GLY:HA2	1:D:3187:THR:O	2.10	0.51
1:F:3221:VAL:HA	1:F:3248:LYS:O	2.11	0.51
1:H:2178:LEU:O	1:H:2182:LEU:HG	2.10	0.51
1:A:3175:MET:HG3	1:A:3218:TYR:CD1	2.37	0.51
1:A:3249:ASN:OD1	1:A:3251:ILE:HG22	2.10	0.51
1:B:2299:GLY:HA2	1:C:2300:GLN:HE22	1.76	0.51
1:E:1176:ARG:HA	1:E:1218:TYR:HE1	1.75	0.51
1:F:1065:TYR:C	1:F:1065:TYR:CD1	2.83	0.51
1:H:114:LEU:O	1:H:1028:ARG:HA	2.10	0.51
1:H:1222:ARG:HB2	1:H:1248:LYS:CB	2.38	0.51
1:B:3100:ASP:O	1:B:3101:PRO:C	2.47	0.51
1:E:1053:ALA:HB2	1:E:1251:ILE:CG2	2.41	0.51
1:E:2300:GLN:NE2	1:H:2299:GLY:HA2	2.21	0.51
1:E:3084:GLN:HG2	1:E:3110:ASP:H	1.75	0.51
1:F:121:THR:HG21	1:F:152:LYS:HG3	1.93	0.51
1:F:1092:PHE:HB2	1:F:1114:LEU:HD11	1.91	0.51
1:F:3300:GLN:H	1:G:1300:GLN:HE22	1.59	0.51
1:H:115:LEU:CD2	1:H:1028:ARG:HG2	2.41	0.51
1:H:1176:ARG:HA	1:H:1218:TYR:HE1	1.75	0.51
1:B:3221:VAL:HA	1:B:3248:LYS:O	2.11	0.51
1:C:164:MET:C	1:C:166:LEU:H	2.14	0.51
1:C:3059:GLY:HA2	1:C:3187:THR:O	2.10	0.51
1:G:132:LEU:HB2	1:G:141:ILE:HD11	1.92	0.51
1:H:135:SER:OG	1:H:1013:ALA:HB1	2.11	0.51
1:H:3221:VAL:HA	1:H:3248:LYS:O	2.11	0.51
1:A:107:LEU:CD2	1:A:267:GLY:HA3	2.41	0.51
1:A:2123:GLU:HG3	1:A:2170:MET:HG3	1.93	0.51
1:A:3143:VAL:HG21	1:A:3191:PHE:CD1	2.46	0.51
1:B:107:LEU:CD2	1:B:267:GLY:HA3	2.41	0.51
1:B:3059:GLY:HA2	1:B:3187:THR:O	2.11	0.51
1:D:107:LEU:CD2	1:D:267:GLY:HA3	2.42	0.51
1:F:1143:VAL:O	1:F:1192:ILE:HG13	2.11	0.51
1:G:3221:VAL:HA	1:G:3248:LYS:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3078:GLN:HG3	1:H:3268:ILE:HG13	1.93	0.51
1:C:185:SER:HB2	1:C:187:THR:OG1	2.10	0.50
1:D:132:LEU:HB2	1:D:141:ILE:HD11	1.93	0.50
1:D:2107:LEU:CD2	1:D:2267:GLY:HA3	2.41	0.50
1:D:3249:ASN:OD1	1:D:3251:ILE:HG22	2.11	0.50
1:E:232:LYS:NZ	1:F:3266:GLU:HG3	2.26	0.50
1:G:185:SER:HB2	1:G:187:THR:OG1	2.11	0.50
1:H:1078:GLN:O	1:H:1081:ALA:HB3	2.11	0.50
1:A:1145:SER:O	1:A:1146:VAL:C	2.50	0.50
1:A:2107:LEU:CD2	1:A:2267:GLY:HA3	2.42	0.50
1:B:1073:THR:HA	1:B:1076:THR:HB	1.93	0.50
1:C:3143:VAL:HG21	1:C:3191:PHE:CD1	2.47	0.50
1:C:3221:VAL:HA	1:C:3248:LYS:O	2.10	0.50
1:D:1091:ALA:HB3	1:D:1141:ILE:HA	1.94	0.50
1:D:3221:VAL:HA	1:D:3248:LYS:O	2.11	0.50
1:D:3298:ILE:HG13	1:D:3299:GLY:N	2.27	0.50
1:F:1078:GLN:O	1:F:1081:ALA:HB3	2.11	0.50
1:F:2308:TRP:HE3	1:F:2309:LEU:HD23	1.76	0.50
1:G:107:LEU:CD2	1:G:267:GLY:HA3	2.42	0.50
1:G:1092:PHE:HB2	1:G:1114:LEU:HD11	1.93	0.50
1:H:2042:THR:HG21	1:H:2047:LEU:HD22	1.94	0.50
1:A:1197:MET:O	1:A:1202:MET:HB2	2.11	0.50
1:B:1308:TRP:CE3	1:B:1309:LEU:HD23	2.46	0.50
1:B:3065:TYR:C	1:B:3065:TYR:HD2	2.15	0.50
1:B:3065:TYR:HE2	1:B:3224:ASP:CG	2.15	0.50
1:C:1092:PHE:HB2	1:C:1114:LEU:HD11	1.92	0.50
1:D:185:SER:HB2	1:D:187:THR:OG1	2.12	0.50
1:E:121:THR:HG21	1:E:152:LYS:HG3	1.92	0.50
1:E:1091:ALA:HB3	1:E:1141:ILE:HA	1.93	0.50
1:F:1300:GLN:NE2	1:G:3300:GLN:H	2.10	0.50
1:H:46:SER:HA	1:H:49:ILE:HD12	1.92	0.50
1:A:3064:ILE:O	1:A:3192:ILE:HA	2.11	0.50
1:B:162:SER:O	1:B:163:HIS:HB2	2.12	0.50
1:B:1222:ARG:HB2	1:B:1248:LYS:CB	2.37	0.50
1:E:185:SER:HB2	1:E:187:THR:OG1	2.12	0.50
1:E:1298:ILE:HG13	1:E:1299:GLY:N	2.25	0.50
1:F:1298:ILE:HG13	1:F:1299:GLY:N	2.26	0.50
1:F:2073:THR:HG23	1:F:2077:LEU:HD13	1.93	0.50
1:F:2300:GLN:HB3	1:G:2300:GLN:HE21	1.76	0.50
1:F:3078:GLN:HG3	1:F:3268:ILE:HG13	1.93	0.50
1:G:1222:ARG:HB2	1:G:1248:LYS:CB	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1308:TRP:CE3	1:G:1309:LEU:HD23	2.46	0.50
1:H:152:LYS:O	1:H:156:GLU:OE2	2.29	0.50
1:C:2073:THR:HG23	1:C:2077:LEU:HD13	1.94	0.50
1:C:3222:ARG:HG3	1:C:3248:LYS:HB3	1.93	0.50
1:E:1153:ALA:O	1:E:1156:GLU:C	2.50	0.50
1:E:1308:TRP:CE3	1:E:1309:LEU:HD23	2.45	0.50
1:F:3084:GLN:HG2	1:F:3110:ASP:H	1.76	0.50
1:G:1316:ALA:O	1:G:1319:ILE:N	2.44	0.50
1:H:1143:VAL:O	1:H:1192:ILE:HG13	2.11	0.50
1:H:2107:LEU:CD2	1:H:2267:GLY:HA3	2.41	0.50
1:C:107:LEU:CD2	1:C:267:GLY:HA3	2.41	0.50
1:C:1091:ALA:HB3	1:C:1141:ILE:HA	1.92	0.50
1:D:2173:GLN:C	1:D:2175:MET:H	2.15	0.50
1:D:3222:ARG:HG3	1:D:3248:LYS:HB3	1.93	0.50
1:E:2107:LEU:CD2	1:E:2267:GLY:HA3	2.42	0.50
1:E:3059:GLY:HA2	1:E:3187:THR:O	2.11	0.50
1:E:3143:VAL:HG21	1:E:3191:PHE:CD1	2.46	0.50
1:E:3145:SER:O	1:E:3147:ALA:N	2.44	0.50
1:E:3222:ARG:HG3	1:E:3248:LYS:HB3	1.93	0.50
1:F:132:LEU:HB2	1:F:141:ILE:HD11	1.93	0.50
1:F:3059:GLY:HA2	1:F:3187:THR:O	2.11	0.50
1:G:2042:THR:HG21	1:G:2047:LEU:HD22	1.92	0.50
1:G:2073:THR:HG23	1:G:2077:LEU:HD13	1.94	0.50
1:H:121:THR:HG21	1:H:152:LYS:HG3	1.92	0.50
1:H:1308:TRP:CE3	1:H:1309:LEU:HD23	2.44	0.50
1:A:185:SER:HB2	1:A:187:THR:OG1	2.11	0.50
1:B:2073:THR:HG23	1:B:2077:LEU:HD13	1.94	0.50
1:C:132:LEU:HB2	1:C:141:ILE:HD11	1.94	0.50
1:D:2073:THR:HG23	1:D:2077:LEU:HD13	1.94	0.50
1:D:3143:VAL:HG21	1:D:3191:PHE:CD1	2.47	0.50
1:G:2308:TRP:HE3	1:G:2309:LEU:HD23	1.77	0.50
1:G:3249:ASN:OD1	1:G:3251:ILE:HG22	2.12	0.50
1:H:132:LEU:HB2	1:H:141:ILE:HD11	1.93	0.50
1:H:278:GLY:HA3	1:H:284:ILE:HD12	1.94	0.50
1:H:3249:ASN:OD1	1:H:3251:ILE:HG22	2.11	0.50
1:A:1193:ASN:ND2	1:A:1209:THR:CG2	2.68	0.50
1:A:1300:GLN:NE2	1:D:3300:GLN:N	2.57	0.50
1:A:1319:ILE:O	1:A:1323:VAL:HG23	2.12	0.50
1:B:132:LEU:HB2	1:B:141:ILE:HD11	1.93	0.50
1:C:319:ILE:O	1:C:323:VAL:HG23	2.11	0.50
1:C:1308:TRP:CE3	1:C:1309:LEU:HD23	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1016:GLN:O	1:E:1020:GLN:HB2	2.12	0.50
1:E:1299:GLY:HA2	1:H:3300:GLN:HE22	1.76	0.50
1:E:2300:GLN:HB3	1:H:2300:GLN:HB3	1.93	0.50
1:A:3222:ARG:HG3	1:A:3248:LYS:HB3	1.93	0.50
1:B:2123:GLU:HG3	1:B:2170:MET:HG3	1.94	0.50
1:B:2300:GLN:HB3	1:C:2300:GLN:HB3	1.94	0.50
1:D:157:GLY:CA	1:D:1172:SER:CB	2.88	0.50
1:D:1319:ILE:O	1:D:1323:VAL:HG23	2.12	0.50
1:E:46:SER:HA	1:E:49:ILE:HD12	1.93	0.50
1:F:1073:THR:HA	1:F:1076:THR:HB	1.93	0.50
1:G:2123:GLU:HG3	1:G:2170:MET:HG3	1.93	0.50
1:H:45:LEU:HD23	1:H:270:PHE:CD1	2.47	0.50
1:B:2308:TRP:HE3	1:B:2309:LEU:HD23	1.77	0.49
1:C:2264:TYR:H	1:C:2264:TYR:HD2	1.60	0.49
1:D:121:THR:HG21	1:D:152:LYS:HG3	1.93	0.49
1:D:1053:ALA:HB2	1:D:1251:ILE:CG2	2.42	0.49
1:E:112:ASP:HA	1:E:1030:GLY:H	1.77	0.49
1:E:2178:LEU:O	1:E:2182:LEU:HG	2.10	0.49
1:E:3221:VAL:HA	1:E:3248:LYS:O	2.12	0.49
1:E:3249:ASN:OD1	1:E:3251:ILE:HG22	2.12	0.49
1:F:2042:THR:HG21	1:F:2047:LEU:HD22	1.94	0.49
1:F:2173:GLN:C	1:F:2175:MET:H	2.15	0.49
1:F:3171:MET:O	1:F:3173:GLN:N	2.45	0.49
1:G:3084:GLN:HG2	1:G:3110:ASP:H	1.77	0.49
1:B:2264:TYR:HD2	1:B:2264:TYR:H	1.60	0.49
1:C:46:SER:HA	1:C:49:ILE:HD12	1.93	0.49
1:C:2107:LEU:CD2	1:C:2267:GLY:HA3	2.41	0.49
1:D:2264:TYR:H	1:D:2264:TYR:HD2	1.60	0.49
1:G:3145:SER:O	1:G:3147:ALA:N	2.45	0.49
1:H:2173:GLN:C	1:H:2175:MET:H	2.15	0.49
1:E:132:LEU:HB2	1:E:141:ILE:HD11	1.93	0.49
1:E:2073:THR:HG23	1:E:2077:LEU:HD13	1.94	0.49
1:E:2123:GLU:HG3	1:E:2170:MET:HG3	1.94	0.49
1:F:185:SER:HB2	1:F:187:THR:OG1	2.12	0.49
1:F:3222:ARG:HG3	1:F:3248:LYS:HB3	1.94	0.49
1:H:1091:ALA:HB3	1:H:1141:ILE:HA	1.92	0.49
1:A:2173:GLN:C	1:A:2175:MET:H	2.16	0.49
1:A:3059:GLY:HA2	1:A:3187:THR:O	2.11	0.49
1:B:71:GLY:HA2	3:B:400:ANP:H5'1	1.94	0.49
1:B:1176:ARG:HA	1:B:1218:TYR:CE1	2.47	0.49
1:B:2042:THR:HG21	1:B:2047:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1065:TYR:C	1:C:1065:TYR:HD1	2.16	0.49
1:D:2123:GLU:HG3	1:D:2170:MET:HG3	1.93	0.49
1:E:2173:GLN:C	1:E:2175:MET:H	2.15	0.49
1:G:319:ILE:O	1:G:323:VAL:HG23	2.12	0.49
1:G:1073:THR:HA	1:G:1076:THR:HB	1.94	0.49
1:G:3222:ARG:HG3	1:G:3248:LYS:HB3	1.94	0.49
1:H:156:GLU:HG3	1:H:1176:ARG:HG3	1.93	0.49
1:H:1316:ALA:O	1:H:1319:ILE:N	2.46	0.49
1:B:2107:LEU:CD2	1:B:2267:GLY:HA3	2.43	0.49
1:B:2118:GLN:NE2	1:B:3249:ASN:H	2.10	0.49
1:B:3222:ARG:HG3	1:B:3248:LYS:HB3	1.94	0.49
1:C:3100:ASP:O	1:C:3101:PRO:C	2.50	0.49
1:E:107:LEU:CD2	1:E:267:GLY:HA3	2.43	0.49
1:E:1073:THR:HA	1:E:1076:THR:HB	1.94	0.49
1:E:2042:THR:HG21	1:E:2047:LEU:HD22	1.93	0.49
1:A:1053:ALA:HB2	1:A:1251:ILE:CG2	2.42	0.49
1:B:319:ILE:O	1:B:323:VAL:HG23	2.13	0.49
1:B:3178:LEU:O	1:B:3182:LEU:HG	2.13	0.49
1:C:48:ASP:HB3	1:C:54:GLY:HA2	1.95	0.49
1:C:1166:LEU:O	1:C:1168:ALA:N	2.46	0.49
1:C:3078:GLN:HG3	1:C:3268:ILE:HG13	1.95	0.49
1:F:1176:ARG:HA	1:F:1218:TYR:CE1	2.48	0.49
1:F:2107:LEU:CD2	1:F:2267:GLY:HA3	2.43	0.49
1:G:2107:LEU:CD2	1:G:2267:GLY:HA3	2.43	0.49
1:G:2175:MET:HG3	1:G:2218:TYR:HD1	1.78	0.49
1:H:1298:ILE:HG13	1:H:1299:GLY:N	2.26	0.49
1:H:2107:LEU:HD21	1:H:2267:GLY:HA3	1.95	0.49
1:H:2123:GLU:HG3	1:H:2170:MET:HG3	1.94	0.49
1:H:2308:TRP:HE3	1:H:2309:LEU:HD23	1.77	0.49
1:A:2146:VAL:HA	1:A:2149:LEU:HD23	1.95	0.49
1:A:2308:TRP:HE3	1:A:2309:LEU:HD23	1.78	0.49
1:B:1319:ILE:O	1:B:1323:VAL:HG23	2.13	0.49
1:B:2107:LEU:HD21	1:B:2267:GLY:HA3	1.95	0.49
1:B:2300:GLN:HB3	1:C:2300:GLN:HE21	1.78	0.49
1:B:3298:ILE:HG13	1:B:3299:GLY:N	2.27	0.49
1:C:1176:ARG:HA	1:C:1218:TYR:CE1	2.48	0.49
1:D:2107:LEU:HD21	1:D:2267:GLY:HA3	1.94	0.49
1:F:319:ILE:O	1:F:323:VAL:HG23	2.12	0.49
1:F:3249:ASN:OD1	1:F:3251:ILE:HG22	2.13	0.49
1:G:1091:ALA:HB3	1:G:1141:ILE:HA	1.93	0.49
1:H:1065:TYR:C	1:H:1065:TYR:HD1	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2042:THR:HG21	1:C:2047:LEU:HD22	1.93	0.49
1:C:3145:SER:O	1:C:3147:ALA:N	2.46	0.49
1:D:2146:VAL:HA	1:D:2149:LEU:HD23	1.94	0.49
1:D:3078:GLN:HG3	1:D:3268:ILE:HG13	1.95	0.49
1:E:48:ASP:HB3	1:E:54:GLY:HA2	1.95	0.49
1:E:2264:TYR:H	1:E:2264:TYR:HD2	1.61	0.49
1:E:2308:TRP:HE3	1:E:2309:LEU:HD23	1.78	0.49
1:F:2175:MET:HG3	1:F:2218:TYR:HD1	1.78	0.49
1:H:3100:ASP:O	1:H:3101:PRO:C	2.51	0.49
1:H:3222:ARG:HG3	1:H:3248:LYS:HB3	1.93	0.49
1:A:2107:LEU:HD21	1:A:2267:GLY:HA3	1.94	0.49
1:B:1091:ALA:HB3	1:B:1141:ILE:HA	1.93	0.49
1:B:2173:GLN:C	1:B:2175:MET:H	2.16	0.49
1:E:1319:ILE:O	1:E:1323:VAL:HG23	2.12	0.49
1:E:2175:MET:HG3	1:E:2218:TYR:HD1	1.78	0.49
1:F:156:GLU:OE2	1:F:1176:ARG:CG	2.42	0.49
1:F:2264:TYR:H	1:F:2264:TYR:HD2	1.60	0.49
1:G:46:SER:HA	1:G:49:ILE:HD12	1.94	0.49
1:G:1319:ILE:O	1:G:1323:VAL:HG23	2.13	0.49
1:G:3298:ILE:HG13	1:G:3299:GLY:N	2.28	0.49
1:H:1053:ALA:HB2	1:H:1251:ILE:CG2	2.43	0.49
1:H:3145:SER:O	1:H:3147:ALA:N	2.46	0.49
1:A:118:GLN:HE21	1:A:1254:PRO:HB3	1.78	0.49
1:A:2264:TYR:H	1:A:2264:TYR:HD2	1.61	0.49
1:B:46:SER:HA	1:B:49:ILE:HD12	1.93	0.49
1:C:2308:TRP:HE3	1:C:2309:LEU:HD23	1.78	0.49
1:D:1073:THR:HA	1:D:1076:THR:HB	1.93	0.49
1:E:2146:VAL:HA	1:E:2149:LEU:HD23	1.95	0.49
1:A:121:THR:HG21	1:A:152:LYS:HG3	1.93	0.48
1:A:1073:THR:HA	1:A:1076:THR:HB	1.94	0.48
1:A:1166:LEU:O	1:A:1168:ALA:N	2.46	0.48
1:A:1166:LEU:C	1:A:1168:ALA:H	2.16	0.48
1:A:1308:TRP:CE3	1:A:1309:LEU:HD23	2.45	0.48
1:A:3298:ILE:HG13	1:A:3299:GLY:N	2.27	0.48
1:B:1053:ALA:HB2	1:B:1251:ILE:CG2	2.43	0.48
1:C:2173:GLN:C	1:C:2175:MET:H	2.16	0.48
1:C:2175:MET:HG3	1:C:2218:TYR:HD1	1.78	0.48
1:D:319:ILE:O	1:D:323:VAL:HG23	2.13	0.48
1:D:2042:THR:HG21	1:D:2047:LEU:HD22	1.94	0.48
1:D:3048:ASP:OD1	1:D:3048:ASP:N	2.46	0.48
1:E:2107:LEU:HD21	1:E:2267:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2299:GLY:HA2	1:H:2300:GLN:HE22	1.77	0.48
1:F:1091:ALA:HB3	1:F:1141:ILE:HA	1.94	0.48
1:F:2114:LEU:HD22	1:F:2115:LEU:H	1.78	0.48
1:F:2123:GLU:HG3	1:F:2170:MET:HG3	1.94	0.48
1:H:107:LEU:CD2	1:H:267:GLY:HA3	2.43	0.48
1:H:3171:MET:C	1:H:3173:GLN:N	2.67	0.48
1:B:3064:ILE:HG12	1:B:3223:LEU:CB	2.33	0.48
1:B:3269:ASN:O	1:B:3272:GLY:N	2.46	0.48
1:C:1166:LEU:C	1:C:1168:ALA:H	2.16	0.48
1:D:1308:TRP:CE3	1:D:1309:LEU:HD23	2.45	0.48
1:E:3064:ILE:O	1:E:3192:ILE:HA	2.13	0.48
1:F:2178:LEU:HD23	1:F:2182:LEU:HD11	1.95	0.48
1:F:3064:ILE:O	1:F:3192:ILE:HA	2.13	0.48
1:G:1053:ALA:HB2	1:G:1251:ILE:CG2	2.43	0.48
1:G:1166:LEU:C	1:G:1168:ALA:H	2.17	0.48
1:H:1073:THR:HA	1:H:1076:THR:HB	1.94	0.48
1:A:48:ASP:HB3	1:A:54:GLY:HA2	1.95	0.48
1:A:2175:MET:HG3	1:A:2218:TYR:HD1	1.78	0.48
1:A:3105:ARG:HD3	1:B:227:ARG:HH22	1.78	0.48
1:B:3281:GLU:O	1:B:3283:LEU:N	2.47	0.48
1:C:2107:LEU:HD21	1:C:2267:GLY:HA3	1.94	0.48
1:D:1166:LEU:C	1:D:1168:ALA:H	2.17	0.48
1:D:3101:PRO:O	1:D:3104:ALA:HB3	2.13	0.48
1:D:3171:MET:C	1:D:3173:GLN:N	2.66	0.48
1:E:1073:THR:HG22	3:E:1400:ANP:PA	2.54	0.48
1:E:1166:LEU:C	1:E:1168:ALA:H	2.16	0.48
1:E:1176:ARG:HA	1:E:1218:TYR:CE1	2.48	0.48
1:E:3100:ASP:O	1:E:3101:PRO:C	2.52	0.48
1:F:2107:LEU:HD21	1:F:2267:GLY:HA3	1.95	0.48
1:G:278:GLY:HA3	1:G:284:ILE:HD12	1.95	0.48
1:G:2173:GLN:C	1:G:2175:MET:H	2.15	0.48
1:G:2264:TYR:H	1:G:2264:TYR:HD2	1.61	0.48
1:G:3326:LEU:O	1:G:3327:LEU:HG	2.13	0.48
1:A:2073:THR:HG23	1:A:2077:LEU:HD13	1.95	0.48
1:B:2114:LEU:HD22	1:B:2115:LEU:H	1.78	0.48
1:B:2175:MET:HG3	1:B:2218:TYR:HD1	1.78	0.48
1:B:3143:VAL:HG21	1:B:3191:PHE:CD1	2.49	0.48
1:D:2175:MET:HG3	1:D:2218:TYR:HD1	1.79	0.48
1:E:112:ASP:HA	1:E:1030:GLY:N	2.28	0.48
1:E:319:ILE:O	1:E:323:VAL:HG23	2.13	0.48
1:G:2114:LEU:HD22	1:G:2115:LEU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2146:VAL:HA	1:H:2149:LEU:HD23	1.96	0.48
1:H:2264:TYR:H	1:H:2264:TYR:HD2	1.61	0.48
1:B:1016:GLN:O	1:B:1020:GLN:HB2	2.13	0.48
1:C:1319:ILE:O	1:C:1323:VAL:HG23	2.13	0.48
1:C:3064:ILE:O	1:C:3192:ILE:HA	2.13	0.48
1:C:3178:LEU:O	1:C:3182:LEU:HG	2.14	0.48
1:C:3249:ASN:OD1	1:C:3251:ILE:HG22	2.13	0.48
1:F:278:GLY:HA3	1:F:284:ILE:HD12	1.96	0.48
1:F:1053:ALA:HB2	1:F:1251:ILE:CG2	2.43	0.48
1:F:3171:MET:C	1:F:3173:GLN:N	2.65	0.48
1:G:48:ASP:HB3	1:G:54:GLY:HA2	1.95	0.48
1:H:73:THR:HG23	1:H:77:LEU:HD13	1.95	0.48
1:B:3145:SER:O	1:B:3147:ALA:N	2.46	0.48
1:C:221:VAL:HA	1:C:248:LYS:O	2.13	0.48
1:D:278:GLY:HA3	1:D:284:ILE:HD12	1.96	0.48
1:G:118:GLN:NE2	1:G:1249:ASN:H	2.11	0.48
1:G:1166:LEU:O	1:G:1168:ALA:N	2.46	0.48
1:H:2175:MET:HG3	1:H:2218:TYR:HD1	1.78	0.48
1:A:1176:ARG:HA	1:A:1218:TYR:CE1	2.48	0.48
1:A:1316:ALA:O	1:A:1319:ILE:N	2.47	0.48
1:A:3100:ASP:O	1:A:3101:PRO:C	2.52	0.48
1:B:1166:LEU:O	1:B:1168:ALA:N	2.47	0.48
1:B:3171:MET:C	1:B:3173:GLN:N	2.66	0.48
1:C:3065:TYR:HE2	1:C:3224:ASP:CG	2.17	0.48
1:E:3078:GLN:HG3	1:E:3268:ILE:HG13	1.96	0.48
1:E:3311:ASP:HB3	1:F:286:LYS:HZ2	1.78	0.48
1:F:1065:TYR:C	1:F:1065:TYR:HD1	2.17	0.48
1:G:2107:LEU:HD21	1:G:2267:GLY:HA3	1.95	0.48
1:H:185:SER:HB2	1:H:187:THR:OG1	2.12	0.48
1:H:1176:ARG:HA	1:H:1218:TYR:CE1	2.49	0.48
1:A:1114:LEU:HB3	1:A:2029:LEU:HD12	1.96	0.48
1:A:3178:LEU:O	1:A:3182:LEU:HG	2.13	0.48
1:B:1145:SER:O	1:B:1146:VAL:C	2.52	0.48
1:B:1316:ALA:O	1:B:1319:ILE:N	2.46	0.48
1:B:2300:GLN:OE1	1:C:2304:ASN:HB3	2.13	0.48
1:C:1016:GLN:O	1:C:1020:GLN:HB2	2.14	0.48
1:D:1219:ALA:O	1:D:1248:LYS:NZ	2.46	0.48
1:D:3171:MET:O	1:D:3173:GLN:N	2.47	0.48
1:E:3171:MET:O	1:E:3173:GLN:N	2.47	0.48
1:F:101:PRO:HG3	1:F:1255:PHE:O	2.13	0.48
1:F:1166:LEU:O	1:F:1168:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1319:ILE:O	1:F:1323:VAL:HG23	2.14	0.48
1:F:3101:PRO:O	1:F:3104:ALA:HB3	2.14	0.48
1:G:3171:MET:C	1:G:3173:GLN:N	2.66	0.48
1:H:3174:ALA:O	1:H:3178:LEU:HD12	2.14	0.48
1:A:3065:TYR:HE2	1:A:3224:ASP:CG	2.17	0.48
1:B:2111:ILE:HD13	1:B:2111:ILE:HA	1.74	0.48
1:C:101:PRO:HG3	1:C:1255:PHE:O	2.13	0.48
1:E:3171:MET:C	1:E:3173:GLN:N	2.66	0.48
1:G:1137:ALA:O	1:G:2010:LEU:HD13	2.12	0.48
1:H:3291:TYR:HE1	1:H:3302:LYS:HA	1.78	0.48
1:A:3171:MET:O	1:A:3173:GLN:N	2.47	0.48
1:B:185:SER:HB2	1:B:187:THR:OG1	2.14	0.48
1:B:3084:GLN:HG2	1:B:3110:ASP:H	1.79	0.48
1:C:3073:THR:O	1:C:3076:THR:OG1	2.26	0.48
1:D:48:ASP:HB3	1:D:54:GLY:HA2	1.95	0.48
1:E:1065:TYR:C	1:E:1065:TYR:HD1	2.17	0.48
1:F:3281:GLU:O	1:F:3283:LEU:N	2.47	0.48
1:G:71:GLY:HA2	3:G:400:ANP:H5'1	1.96	0.48
1:H:48:ASP:HB3	1:H:54:GLY:HA2	1.96	0.48
1:H:75:LEU:O	1:H:75:LEU:HD23	2.14	0.48
1:B:1166:LEU:C	1:B:1168:ALA:H	2.17	0.47
1:B:2065:TYR:HE1	1:B:2224:ASP:CG	2.17	0.47
1:C:1327:LEU:C	1:C:1328:LEU:HD12	2.34	0.47
1:D:1166:LEU:O	1:D:1168:ALA:N	2.46	0.47
1:E:3287:ALA:HB3	1:E:3290:TRP:HB2	1.96	0.47
1:G:3171:MET:O	1:G:3173:GLN:N	2.47	0.47
1:H:3064:ILE:O	1:H:3192:ILE:HA	2.14	0.47
1:C:2146:VAL:HA	1:C:2149:LEU:HD23	1.94	0.47
1:D:2118:GLN:NE2	1:D:3249:ASN:H	2.08	0.47
1:E:1316:ALA:O	1:E:1319:ILE:N	2.48	0.47
1:F:72:LYS:HE3	3:F:400:ANP:O1B	2.14	0.47
1:G:1016:GLN:O	1:G:1020:GLN:HB2	2.13	0.47
1:G:3291:TYR:HE1	1:G:3302:LYS:HA	1.79	0.47
1:H:3298:ILE:HG13	1:H:3299:GLY:N	2.29	0.47
1:A:3264:TYR:CE1	3:A:3400:ANP:H1'	2.49	0.47
1:B:278:GLY:HA3	1:B:284:ILE:HD12	1.94	0.47
1:B:3171:MET:O	1:B:3173:GLN:N	2.47	0.47
1:C:2114:LEU:HD22	1:C:2115:LEU:H	1.79	0.47
1:F:1300:GLN:H	1:G:3300:GLN:HE22	1.59	0.47
1:G:3178:LEU:O	1:G:3182:LEU:HG	2.14	0.47
1:H:1166:LEU:C	1:H:1168:ALA:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:GLN:HE22	1:D:3300:GLN:N	2.10	0.47
1:A:2060:ARG:HB3	1:A:2220:SER:OG	2.15	0.47
1:A:2114:LEU:HD22	1:A:2115:LEU:H	1.80	0.47
1:A:3145:SER:O	1:A:3147:ALA:N	2.48	0.47
1:B:1150:THR:HA	1:B:1151:PRO:HD3	1.59	0.47
1:B:3287:ALA:HB3	1:B:3290:TRP:HB2	1.97	0.47
1:C:156:GLU:HG2	1:C:1176:ARG:CG	2.43	0.47
1:D:3065:TYR:HE2	1:D:3224:ASP:CG	2.18	0.47
1:D:3178:LEU:O	1:D:3182:LEU:HG	2.14	0.47
1:E:3048:ASP:N	1:E:3048:ASP:OD1	2.48	0.47
1:F:3065:TYR:HE2	1:F:3224:ASP:CG	2.18	0.47
1:G:64:ILE:HG12	1:G:223:LEU:HB2	1.97	0.47
1:G:2146:VAL:HA	1:G:2149:LEU:HD23	1.96	0.47
1:G:3037:VAL:HG21	1:G:3251:ILE:HD11	1.97	0.47
1:H:2114:LEU:HD22	1:H:2115:LEU:H	1.79	0.47
1:A:319:ILE:O	1:A:323:VAL:HG23	2.14	0.47
1:A:2178:LEU:HD23	1:A:2182:LEU:HD11	1.96	0.47
1:B:2064:ILE:O	1:B:2192:ILE:HA	2.15	0.47
1:C:227:ARG:HH22	1:D:3105:ARG:HD3	1.79	0.47
1:C:1053:ALA:HB2	1:C:1251:ILE:CG2	2.43	0.47
1:E:1166:LEU:O	1:E:1168:ALA:N	2.47	0.47
1:E:3065:TYR:HE2	1:E:3224:ASP:CG	2.17	0.47
1:F:1166:LEU:C	1:F:1168:ALA:H	2.17	0.47
1:F:1316:ALA:O	1:F:1319:ILE:N	2.47	0.47
1:G:157:GLY:O	1:G:158:GLU:HG3	2.15	0.47
1:G:1327:LEU:C	1:G:1328:LEU:HD12	2.34	0.47
1:G:2178:LEU:HD23	1:G:2182:LEU:HD11	1.96	0.47
1:H:1114:LEU:O	1:H:2028:ARG:HA	2.13	0.47
1:H:3048:ASP:N	1:H:3048:ASP:OD1	2.47	0.47
1:H:3178:LEU:O	1:H:3182:LEU:HG	2.14	0.47
1:A:1146:VAL:CG1	1:A:1211:GLY:HA3	2.41	0.47
1:B:1144:ASP:HA	1:B:1145:SER:HB3	1.97	0.47
1:C:3287:ALA:HB3	1:C:3290:TRP:HB2	1.97	0.47
1:F:48:ASP:HB3	1:F:54:GLY:HA2	1.96	0.47
1:F:2111:ILE:HA	1:F:2111:ILE:HD13	1.72	0.47
1:G:1176:ARG:HA	1:G:1218:TYR:CE1	2.48	0.47
1:H:2129:CYS:HB2	1:H:2178:LEU:HD11	1.96	0.47
1:A:1162:SER:O	1:A:1164:MET:N	2.48	0.47
1:A:3114:LEU:O	1:A:3114:LEU:HD13	2.15	0.47
1:A:3145:SER:C	1:A:3147:ALA:N	2.68	0.47
1:B:114:LEU:O	1:B:1028:ARG:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:O	1:C:75:LEU:HD23	2.15	0.47
1:C:1305:ALA:O	1:C:1306:THR:O	2.32	0.47
1:C:2178:LEU:HD23	1:C:2182:LEU:HD11	1.97	0.47
1:D:1176:ARG:HA	1:D:1218:TYR:CE1	2.48	0.47
1:D:3064:ILE:O	1:D:3192:ILE:HA	2.14	0.47
1:D:3174:ALA:O	1:D:3178:LEU:HD12	2.15	0.47
1:E:3300:GLN:HE22	1:H:1300:GLN:N	2.09	0.47
1:F:75:LEU:O	1:F:75:LEU:HD23	2.14	0.47
1:F:1016:GLN:O	1:F:1020:GLN:HB2	2.15	0.47
1:F:1145:SER:O	1:F:1146:VAL:C	2.53	0.47
1:F:2060:ARG:HB3	1:F:2220:SER:OG	2.14	0.47
1:F:3048:ASP:OD1	1:F:3048:ASP:N	2.48	0.47
1:F:3145:SER:O	1:F:3147:ALA:N	2.48	0.47
1:G:3010:LEU:O	1:G:3014:LEU:HG	2.15	0.47
1:G:3078:GLN:HG3	1:G:3268:ILE:HG13	1.97	0.47
1:G:3174:ALA:O	1:G:3178:LEU:HD12	2.14	0.47
1:H:1166:LEU:O	1:H:1168:ALA:N	2.47	0.47
1:H:1319:ILE:O	1:H:1323:VAL:HG23	2.14	0.47
1:H:2156:GLU:HA	1:H:3172:SER:OG	2.14	0.47
1:A:278:GLY:HA3	1:A:284:ILE:HD12	1.95	0.47
1:B:1065:TYR:C	1:B:1065:TYR:HD1	2.17	0.47
1:B:2146:VAL:HA	1:B:2149:LEU:HD23	1.95	0.47
1:C:160:GLY:O	1:C:162:SER:N	2.48	0.47
1:D:75:LEU:O	1:D:75:LEU:HD23	2.15	0.47
1:E:3178:LEU:O	1:E:3182:LEU:HG	2.15	0.47
1:G:135:SER:OG	1:G:1013:ALA:HB1	2.14	0.47
1:H:319:ILE:O	1:H:323:VAL:HG23	2.14	0.47
1:H:3010:LEU:O	1:H:3014:LEU:HG	2.15	0.47
1:A:3291:TYR:HE1	1:A:3302:LYS:HA	1.78	0.47
1:C:278:GLY:HA3	1:C:284:ILE:HD12	1.96	0.47
1:C:3171:MET:C	1:C:3173:GLN:N	2.67	0.47
1:C:3174:ALA:O	1:C:3178:LEU:HD12	2.15	0.47
1:D:1316:ALA:O	1:D:1319:ILE:N	2.48	0.47
1:D:3073:THR:O	1:D:3076:THR:OG1	2.28	0.47
1:E:1137:ALA:O	1:E:2010:LEU:HD13	2.15	0.47
1:F:3174:ALA:O	1:F:3178:LEU:HD12	2.14	0.47
1:H:2118:GLN:NE2	1:H:3249:ASN:H	2.10	0.47
1:B:75:LEU:HD23	1:B:75:LEU:O	2.15	0.47
1:C:3037:VAL:HG21	1:C:3251:ILE:HD11	1.97	0.47
1:D:1145:SER:O	1:D:1146:VAL:C	2.53	0.47
1:D:2114:LEU:HD22	1:D:2115:LEU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3298:ILE:HG13	1:E:3299:GLY:N	2.28	0.47
1:F:115:LEU:HA	1:F:1027:MET:O	2.15	0.47
1:F:2065:TYR:HE1	1:F:2224:ASP:CG	2.18	0.47
1:F:3056:LEU:HA	1:F:3057:PRO:HD3	1.65	0.47
1:G:157:GLY:HA2	1:G:1172:SER:HB2	1.96	0.47
1:H:3114:LEU:HD13	1:H:3114:LEU:O	2.15	0.47
1:A:1193:ASN:HD21	1:A:1209:THR:C	2.19	0.46
1:B:3174:ALA:O	1:B:3178:LEU:HD12	2.14	0.46
1:C:3291:TYR:HE1	1:C:3302:LYS:HA	1.79	0.46
1:C:3298:ILE:HG13	1:C:3299:GLY:N	2.29	0.46
1:D:73:THR:HG23	1:D:77:LEU:HD13	1.95	0.46
1:D:92:PHE:O	1:D:116:CYS:HA	2.15	0.46
1:D:1144:ASP:HA	1:D:1145:SER:HB3	1.97	0.46
1:D:2178:LEU:HD23	1:D:2182:LEU:HD11	1.96	0.46
1:E:278:GLY:HA3	1:E:284:ILE:HD12	1.96	0.46
1:F:69:SER:N	3:F:400:ANP:O1B	2.48	0.46
1:F:2129:CYS:HB2	1:F:2178:LEU:HD11	1.96	0.46
1:A:3287:ALA:HB3	1:A:3290:TRP:HB2	1.97	0.46
1:B:64:ILE:HG12	1:B:223:LEU:HB2	1.97	0.46
1:B:3075:LEU:O	1:B:3075:LEU:HD23	2.15	0.46
1:B:3326:LEU:O	1:B:3327:LEU:HG	2.15	0.46
1:F:125:ALA:C	1:F:127:GLU:H	2.17	0.46
1:H:2073:THR:HG23	1:H:2077:LEU:HD13	1.96	0.46
1:H:3171:MET:O	1:H:3173:GLN:N	2.47	0.46
1:A:1050:ALA:HB1	1:A:1256:LYS:HB3	1.98	0.46
1:B:2060:ARG:HB3	1:B:2220:SER:OG	2.15	0.46
1:C:3134:ARG:HD2	1:F:177:LYS:HD2	1.97	0.46
1:D:3114:LEU:O	1:D:3114:LEU:HD13	2.14	0.46
1:E:112:ASP:HA	1:E:1030:GLY:HA3	1.98	0.46
1:E:2300:GLN:HE22	1:H:2299:GLY:CA	2.22	0.46
1:E:3174:ALA:O	1:E:3178:LEU:HD12	2.14	0.46
1:F:64:ILE:HG12	1:F:223:LEU:HB2	1.96	0.46
1:G:2118:GLN:NE2	1:G:3249:ASN:H	2.12	0.46
1:H:3037:VAL:HG21	1:H:3251:ILE:HD11	1.98	0.46
1:A:1065:TYR:C	1:A:1065:TYR:HD1	2.18	0.46
1:A:1150:THR:HA	1:A:1151:PRO:HD3	1.60	0.46
1:A:3010:LEU:O	1:A:3014:LEU:HG	2.15	0.46
1:A:3174:ALA:O	1:A:3178:LEU:HD12	2.16	0.46
1:B:90:CYS:HG	1:B:140:VAL:HG13	1.79	0.46
1:D:64:ILE:HG12	1:D:223:LEU:HB2	1.96	0.46
1:D:1170:MET:O	1:D:1170:MET:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2064:ILE:O	1:D:2192:ILE:HA	2.15	0.46
1:D:3145:SER:O	1:D:3147:ALA:N	2.49	0.46
1:E:75:LEU:HD23	1:E:75:LEU:O	2.16	0.46
1:E:118:GLN:NE2	1:E:1249:ASN:H	2.13	0.46
1:E:2178:LEU:HD23	1:E:2182:LEU:HD11	1.97	0.46
1:E:3065:TYR:HD2	1:E:3065:TYR:O	1.98	0.46
1:E:3253:ALA:HA	1:E:3254:PRO:HD3	1.82	0.46
1:E:3291:TYR:HE1	1:E:3302:LYS:HA	1.79	0.46
1:F:3109:VAL:HG12	1:F:3110:ASP:N	2.31	0.46
1:F:3114:LEU:O	1:F:3114:LEU:HD13	2.15	0.46
1:F:3178:LEU:O	1:F:3182:LEU:HG	2.14	0.46
1:H:125:ALA:C	1:H:127:GLU:H	2.18	0.46
1:H:1111:ILE:HD13	1:H:1111:ILE:HA	1.80	0.46
1:H:1144:ASP:HA	1:H:1145:SER:HB3	1.98	0.46
1:H:1145:SER:O	1:H:1146:VAL:C	2.53	0.46
1:C:2048:ASP:O	1:C:2051:LEU:HB2	2.16	0.46
1:C:2111:ILE:HD13	1:C:2111:ILE:HA	1.75	0.46
1:D:1064:ILE:HG23	1:D:1223:LEU:HB3	1.98	0.46
1:D:2129:CYS:HB2	1:D:2178:LEU:HD11	1.97	0.46
1:E:3271:TYR:O	1:E:3275:VAL:HG23	2.16	0.46
1:F:1170:MET:O	1:F:1170:MET:HG2	2.16	0.46
1:G:75:LEU:HD23	1:G:75:LEU:O	2.16	0.46
1:G:1170:MET:O	1:G:1170:MET:HG2	2.16	0.46
1:A:3326:LEU:O	1:A:3327:LEU:HG	2.15	0.46
1:B:3048:ASP:N	1:B:3048:ASP:OD1	2.47	0.46
1:B:3092:PHE:CE2	1:B:3099:LEU:HD22	2.50	0.46
1:C:3010:LEU:O	1:C:3014:LEU:HG	2.15	0.46
1:D:1065:TYR:C	1:D:1065:TYR:HD1	2.17	0.46
1:D:3037:VAL:HG21	1:D:3251:ILE:HD11	1.98	0.46
1:E:73:THR:HG23	1:E:77:LEU:HD13	1.97	0.46
1:E:2064:ILE:O	1:E:2192:ILE:HA	2.16	0.46
1:F:1144:ASP:HA	1:F:1145:SER:HB3	1.98	0.46
1:A:1016:GLN:O	1:A:1020:GLN:HB2	2.16	0.46
1:A:2048:ASP:O	1:A:2051:LEU:HB2	2.16	0.46
1:A:3078:GLN:HG3	1:A:3268:ILE:HG13	1.97	0.46
1:C:1050:ALA:HB1	1:C:1256:LYS:HB3	1.97	0.46
1:C:3171:MET:O	1:C:3173:GLN:N	2.48	0.46
1:D:1016:GLN:O	1:D:1020:GLN:HB2	2.15	0.46
1:D:3056:LEU:HA	1:D:3057:PRO:HD3	1.65	0.46
1:E:64:ILE:HG12	1:E:223:LEU:HB2	1.98	0.46
1:E:3145:SER:C	1:E:3147:ALA:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1114:LEU:O	1:G:2028:ARG:HA	2.15	0.46
1:G:3048:ASP:N	1:G:3048:ASP:OD1	2.48	0.46
1:G:3287:ALA:HB3	1:G:3290:TRP:HB2	1.97	0.46
1:H:3065:TYR:HE2	1:H:3224:ASP:CG	2.18	0.46
1:D:114:LEU:HB3	1:D:1029:LEU:HD12	1.96	0.46
1:E:1050:ALA:HB1	1:E:1256:LYS:HB3	1.98	0.46
1:E:2065:TYR:HE1	1:E:2224:ASP:CG	2.18	0.46
1:E:3010:LEU:O	1:E:3014:LEU:HG	2.16	0.46
1:F:1090:CYS:HB3	1:F:1140:VAL:HG23	1.98	0.46
1:F:2064:ILE:O	1:F:2192:ILE:HA	2.16	0.46
1:G:3281:GLU:O	1:G:3283:LEU:N	2.49	0.46
1:H:2178:LEU:HD23	1:H:2182:LEU:HD11	1.97	0.46
1:A:221:VAL:HA	1:A:248:LYS:O	2.15	0.46
1:A:1327:LEU:C	1:A:1328:LEU:HD12	2.37	0.46
1:A:3037:VAL:HG21	1:A:3251:ILE:HD11	1.97	0.46
1:A:3171:MET:C	1:A:3173:GLN:N	2.67	0.46
1:A:3300:GLN:NE2	1:D:1300:GLN:H	2.14	0.46
1:B:48:ASP:HB3	1:B:54:GLY:HA2	1.96	0.46
1:B:3145:SER:C	1:B:3147:ALA:N	2.69	0.46
1:C:1062:VAL:HB	1:C:1190:ILE:HG12	1.98	0.46
1:C:3114:LEU:O	1:C:3114:LEU:HD13	2.16	0.46
1:E:1144:ASP:HA	1:E:1145:SER:HB3	1.98	0.46
1:E:2129:CYS:HB2	1:E:2178:LEU:HD11	1.98	0.46
1:E:3090:CYS:SG	1:E:3140:VAL:CG1	3.04	0.46
1:F:2227:ARG:HG3	1:F:2240:SER:HB3	1.98	0.46
1:G:73:THR:HG23	1:G:77:LEU:HD13	1.98	0.46
1:G:1050:ALA:HB1	1:G:1256:LYS:HB3	1.98	0.46
1:G:1144:ASP:HA	1:G:1145:SER:HB3	1.98	0.46
1:H:64:ILE:HG12	1:H:223:LEU:HB2	1.97	0.46
1:B:2029:LEU:HD23	1:B:2254:PRO:HD2	1.97	0.46
1:B:3037:VAL:HG21	1:B:3251:ILE:HD11	1.98	0.46
1:C:1029:LEU:HD23	1:C:1254:PRO:HD2	1.98	0.46
1:C:2065:TYR:HE1	1:C:2224:ASP:CG	2.19	0.46
1:C:3092:PHE:CE2	1:C:3099:LEU:HD22	2.51	0.46
1:D:3010:LEU:O	1:D:3014:LEU:HG	2.16	0.46
1:E:1170:MET:O	1:E:1170:MET:HG2	2.16	0.46
1:F:1099:LEU:HB3	1:F:2255:PHE:CE1	2.51	0.46
1:F:1150:THR:HA	1:F:1151:PRO:HD3	1.62	0.46
1:F:2293:TYR:CE1	1:F:2319:ILE:HD11	2.51	0.46
1:G:1065:TYR:C	1:G:1065:TYR:HD1	2.18	0.46
1:G:3065:TYR:HE2	1:G:3224:ASP:CG	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3092:PHE:CE2	1:G:3099:LEU:HD22	2.51	0.46
1:H:221:VAL:HA	1:H:248:LYS:O	2.15	0.46
1:A:1144:ASP:HA	1:A:1145:SER:HB3	1.98	0.45
1:A:1161:ASP:OD2	1:A:1166:LEU:HD13	2.16	0.45
1:B:221:VAL:HA	1:B:248:LYS:O	2.16	0.45
1:B:1064:ILE:HG23	1:B:1223:LEU:HB3	1.99	0.45
1:C:73:THR:HG23	1:C:77:LEU:HD13	1.97	0.45
1:C:1144:ASP:HA	1:C:1145:SER:HB3	1.99	0.45
1:D:1161:ASP:CB	1:F:183:LYS:HZ1	2.02	0.45
1:D:3065:TYR:HD2	1:D:3065:TYR:O	1.99	0.45
1:D:3123:GLU:O	1:D:3124:GLN:C	2.55	0.45
1:E:1145:SER:O	1:E:1146:VAL:C	2.54	0.45
1:E:1150:THR:HA	1:E:1151:PRO:HD3	1.61	0.45
1:F:3145:SER:C	1:F:3147:ALA:N	2.70	0.45
1:G:69:SER:N	3:G:400:ANP:O1B	2.49	0.45
1:G:125:ALA:C	1:G:127:GLU:H	2.20	0.45
1:A:2129:CYS:HB2	1:A:2178:LEU:HD11	1.97	0.45
1:B:1170:MET:O	1:B:1170:MET:HG2	2.16	0.45
1:B:2178:LEU:HD23	1:B:2182:LEU:HD11	1.96	0.45
1:C:118:GLN:NE2	1:C:1249:ASN:H	2.14	0.45
1:C:2129:CYS:HB2	1:C:2178:LEU:HD11	1.97	0.45
1:E:221:VAL:HA	1:E:248:LYS:O	2.15	0.45
1:E:1327:LEU:C	1:E:1328:LEU:HD12	2.37	0.45
1:G:221:VAL:HA	1:G:248:LYS:O	2.16	0.45
1:G:3064:ILE:O	1:G:3192:ILE:HA	2.16	0.45
1:G:3145:SER:C	1:G:3147:ALA:N	2.67	0.45
1:H:2064:ILE:O	1:H:2192:ILE:HA	2.16	0.45
1:H:2065:TYR:HE1	1:H:2224:ASP:CG	2.20	0.45
1:H:2293:TYR:CE1	1:H:2319:ILE:HD11	2.52	0.45
1:A:2065:TYR:HE1	1:A:2224:ASP:CG	2.19	0.45
1:B:2129:CYS:HB2	1:B:2178:LEU:HD11	1.97	0.45
1:C:92:PHE:O	1:C:116:CYS:HA	2.16	0.45
1:C:2060:ARG:HB3	1:C:2220:SER:OG	2.17	0.45
1:D:171:MET:O	1:D:175:MET:HB2	2.17	0.45
1:E:125:ALA:C	1:E:127:GLU:H	2.20	0.45
1:E:2293:TYR:CE1	1:E:2319:ILE:HD11	2.51	0.45
1:E:3037:VAL:HG21	1:E:3251:ILE:HD11	1.98	0.45
1:F:1050:ALA:HB1	1:F:1256:LYS:HB3	1.98	0.45
1:F:2048:ASP:O	1:F:2051:LEU:HB2	2.16	0.45
1:H:3090:CYS:SG	1:H:3140:VAL:CG1	3.04	0.45
1:H:3145:SER:C	1:H:3147:ALA:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:VAL:HB	1:A:1190:ILE:HG12	1.98	0.45
1:B:3010:LEU:O	1:B:3014:LEU:HG	2.16	0.45
1:E:232:LYS:HZ3	1:F:3266:GLU:HG3	1.82	0.45
1:F:73:THR:HG23	1:F:77:LEU:HD13	1.97	0.45
1:F:1305:ALA:O	1:F:1306:THR:O	2.34	0.45
1:F:3037:VAL:HG21	1:F:3251:ILE:HD11	1.99	0.45
1:F:3327:LEU:O	1:F:3328:LEU:HD12	2.16	0.45
1:G:3123:GLU:O	1:G:3124:GLN:C	2.55	0.45
1:H:1062:VAL:HB	1:H:1190:ILE:HG12	1.98	0.45
1:H:3075:LEU:HD23	1:H:3075:LEU:O	2.17	0.45
1:H:3326:LEU:O	1:H:3327:LEU:HG	2.17	0.45
1:A:2118:GLN:NE2	1:A:3249:ASN:H	2.12	0.45
1:B:1327:LEU:C	1:B:1328:LEU:HD12	2.37	0.45
1:B:2090:CYS:CB	1:B:2140:VAL:HG13	2.47	0.45
1:B:3078:GLN:HG3	1:B:3268:ILE:HG13	1.98	0.45
1:D:1062:VAL:HB	1:D:1190:ILE:HG12	1.98	0.45
1:D:3287:ALA:HB3	1:D:3290:TRP:HB2	1.99	0.45
1:F:161:ASP:H	1:F:163:HIS:H	1.65	0.45
1:F:171:MET:O	1:F:175:MET:HB2	2.17	0.45
1:G:2287:ALA:HB3	1:G:2290:TRP:HB2	1.98	0.45
1:G:2305:ALA:O	1:G:2306:THR:C	2.55	0.45
1:H:2229:GLY:O	1:H:2230:ALA:CB	2.65	0.45
1:A:3092:PHE:CE2	1:A:3099:LEU:HD22	2.52	0.45
1:C:64:ILE:HG12	1:C:223:LEU:HB2	1.98	0.45
1:D:2060:ARG:HB3	1:D:2220:SER:OG	2.16	0.45
1:D:2227:ARG:HG3	1:D:2240:SER:HB3	1.99	0.45
1:E:3092:PHE:CE2	1:E:3099:LEU:HD22	2.52	0.45
1:F:221:VAL:HA	1:F:248:LYS:O	2.17	0.45
1:G:3271:TYR:O	1:G:3275:VAL:HG23	2.17	0.45
1:A:75:LEU:O	1:A:75:LEU:HD23	2.16	0.45
1:A:125:ALA:C	1:A:127:GLU:H	2.20	0.45
1:B:2048:ASP:O	1:B:2051:LEU:HB2	2.17	0.45
1:C:1170:MET:HG2	1:C:1170:MET:O	2.16	0.45
1:D:72:LYS:HB2	1:D:72:LYS:HE3	1.74	0.45
1:E:2171:MET:O	1:E:2175:MET:HB2	2.16	0.45
1:F:72:LYS:HE3	1:F:72:LYS:HB2	1.75	0.45
1:F:2287:ALA:HB3	1:F:2290:TRP:HB2	1.99	0.45
1:G:1145:SER:O	1:G:1146:VAL:C	2.55	0.45
1:G:3151:PRO:HG2	1:H:3151:PRO:CB	2.47	0.45
1:H:1050:ALA:HB1	1:H:1256:LYS:HB3	1.99	0.45
1:H:1064:ILE:HG23	1:H:1223:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1112:ASP:HA	1:H:2030:GLY:CA	2.47	0.45
1:B:2065:TYR:CD1	1:B:2065:TYR:C	2.90	0.45
1:B:2171:MET:O	1:B:2175:MET:HB2	2.17	0.45
1:C:1090:CYS:HB3	1:C:1140:VAL:HG23	1.99	0.45
1:D:2171:MET:O	1:D:2175:MET:HB2	2.17	0.45
1:E:171:MET:O	1:E:175:MET:HB2	2.17	0.45
1:E:1324:ARG:HA	1:E:1328:LEU:HD13	1.99	0.45
1:E:2114:LEU:HD22	1:E:2115:LEU:H	1.81	0.45
1:F:3010:LEU:O	1:F:3014:LEU:HG	2.17	0.45
1:G:1324:ARG:HA	1:G:1328:LEU:HD13	1.99	0.45
1:G:2171:MET:O	1:G:2175:MET:HB2	2.16	0.45
1:G:3132:LEU:HA	1:G:3135:SER:HB2	1.99	0.45
1:A:2287:ALA:HB3	1:A:2290:TRP:HB2	1.99	0.45
1:B:2227:ARG:HG3	1:B:2240:SER:HB3	1.97	0.45
1:B:3114:LEU:O	1:B:3114:LEU:HD13	2.17	0.45
1:C:2227:ARG:HG3	1:C:2240:SER:HB3	1.98	0.45
1:C:3065:TYR:HD2	1:C:3065:TYR:O	2.00	0.45
1:C:3132:LEU:HA	1:C:3135:SER:HB2	1.99	0.45
1:D:2287:ALA:HB3	1:D:2290:TRP:HB2	1.99	0.45
1:D:3291:TYR:HE1	1:D:3302:LYS:HA	1.81	0.45
1:E:1090:CYS:HB3	1:E:1140:VAL:HG23	1.98	0.45
1:F:1062:VAL:HB	1:F:1190:ILE:HG12	1.98	0.45
1:G:2227:ARG:HG3	1:G:2240:SER:HB3	1.99	0.45
1:H:1150:THR:HA	1:H:1151:PRO:HD3	1.61	0.45
1:H:3029:LEU:CD2	1:H:3254:PRO:HD2	2.47	0.45
1:H:3287:ALA:HB3	1:H:3290:TRP:HB2	1.98	0.45
1:B:92:PHE:O	1:B:116:CYS:HA	2.17	0.45
1:D:1067:PRO:O	1:D:1070:SER:OG	2.23	0.45
1:D:1150:THR:HA	1:D:1151:PRO:HD3	1.61	0.45
1:D:1327:LEU:C	1:D:1328:LEU:HD12	2.37	0.45
1:D:2065:TYR:HE1	1:D:2224:ASP:CG	2.20	0.45
1:D:2090:CYS:CB	1:D:2140:VAL:HG13	2.47	0.45
1:E:2060:ARG:HB3	1:E:2220:SER:OG	2.17	0.45
1:G:158:GLU:HB3	1:G:159:ILE:H	1.59	0.45
1:G:2065:TYR:HE1	1:G:2224:ASP:CG	2.20	0.45
1:G:2129:CYS:HB2	1:G:2178:LEU:HD11	1.99	0.45
1:A:3281:GLU:O	1:A:3283:LEU:N	2.50	0.44
1:E:132:LEU:HD11	1:E:1026:ILE:HD12	1.99	0.44
1:E:1062:VAL:HB	1:E:1190:ILE:HG12	1.98	0.44
1:E:1282:LYS:H	1:E:1282:LYS:HG2	1.60	0.44
1:E:3040:ILE:O	1:E:3055:GLY:HA3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2090:CYS:CB	1:F:2140:VAL:HG13	2.48	0.44
1:F:3065:TYR:HD2	1:F:3065:TYR:O	1.99	0.44
1:F:3291:TYR:HE1	1:F:3302:LYS:HA	1.82	0.44
1:G:99:LEU:HD23	1:G:1255:PHE:CZ	2.52	0.44
1:G:2253:ALA:HA	1:G:2254:PRO:HD3	1.83	0.44
1:H:1327:LEU:C	1:H:1328:LEU:HD12	2.37	0.44
1:H:2171:MET:O	1:H:2175:MET:HB2	2.17	0.44
1:H:3253:ALA:HA	1:H:3254:PRO:HD3	1.80	0.44
1:A:64:ILE:HG12	1:A:223:LEU:HB2	1.98	0.44
1:A:2293:TYR:CE1	1:A:2319:ILE:HD11	2.52	0.44
1:B:2287:ALA:HB3	1:B:2290:TRP:HB2	2.00	0.44
1:C:72:LYS:HB2	1:C:72:LYS:HE3	1.75	0.44
1:D:221:VAL:HA	1:D:248:LYS:O	2.17	0.44
1:D:2293:TYR:CE1	1:D:2319:ILE:HD11	2.52	0.44
1:E:2227:ARG:HG3	1:E:2240:SER:HB3	1.98	0.44
1:F:160:GLY:HA3	1:F:163:HIS:HA	1.99	0.44
1:G:2293:TYR:CE1	1:G:2319:ILE:HD11	2.52	0.44
1:G:3075:LEU:O	1:G:3075:LEU:HD23	2.16	0.44
1:H:1018:GLU:OE2	1:H:1024:GLY:HA2	2.17	0.44
1:H:2287:ALA:HB3	1:H:2290:TRP:HB2	1.99	0.44
1:H:3264:TYR:CE1	3:H:3400:ANP:H1'	2.52	0.44
1:B:125:ALA:C	1:B:127:GLU:H	2.19	0.44
1:B:1062:VAL:HB	1:B:1190:ILE:HG12	1.98	0.44
1:B:1066:GLY:O	1:B:1067:PRO:C	2.56	0.44
1:B:3140:VAL:HG23	1:B:3188:LEU:HB3	2.00	0.44
1:E:1064:ILE:HG23	1:E:1223:LEU:HB3	1.99	0.44
1:E:3077:LEU:HG	1:E:3080:ILE:HD12	2.00	0.44
1:F:3287:ALA:HB3	1:F:3290:TRP:HB2	1.98	0.44
1:H:69:SER:N	3:H:400:ANP:O1B	2.50	0.44
1:B:1050:ALA:HB1	1:B:1256:LYS:HB3	1.99	0.44
1:B:1090:CYS:HB3	1:B:1140:VAL:HG23	1.99	0.44
1:B:3064:ILE:O	1:B:3192:ILE:HA	2.16	0.44
1:B:3291:TYR:HE1	1:B:3302:LYS:HA	1.82	0.44
1:C:1145:SER:O	1:C:1146:VAL:C	2.54	0.44
1:C:2084:GLN:HG3	1:C:2090:CYS:SG	2.58	0.44
1:C:2171:MET:O	1:C:2175:MET:HB2	2.17	0.44
1:C:2229:GLY:O	1:C:2230:ALA:CB	2.64	0.44
1:D:2230:ALA:HA	1:D:2239:GLY:O	2.18	0.44
1:E:157:GLY:O	1:E:158:GLU:O	2.36	0.44
1:E:3075:LEU:O	1:E:3075:LEU:HD23	2.17	0.44
1:F:92:PHE:O	1:F:116:CYS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2128:ILE:HG22	1:F:2132:LEU:CD1	2.47	0.44
1:G:1062:VAL:HB	1:G:1190:ILE:HG12	2.00	0.44
1:G:1305:ALA:O	1:G:1306:THR:O	2.35	0.44
1:G:2218:TYR:HD2	1:G:2218:TYR:HA	1.73	0.44
1:H:1324:ARG:HA	1:H:1328:LEU:HD13	1.98	0.44
1:A:73:THR:HG23	1:A:77:LEU:HD13	1.98	0.44
1:A:160:GLY:C	1:A:163:HIS:HB3	2.37	0.44
1:A:3224:ASP:O	1:A:3244:VAL:HA	2.18	0.44
1:B:3185:SER:C	1:B:3187:THR:N	2.70	0.44
1:C:2253:ALA:HA	1:C:2254:PRO:HD3	1.83	0.44
1:D:157:GLY:HA3	1:D:1172:SER:CB	2.47	0.44
1:D:2305:ALA:O	1:D:2306:THR:C	2.55	0.44
1:D:3269:ASN:O	1:D:3272:GLY:N	2.51	0.44
1:E:2063:GLU:HG3	1:E:2215:LEU:HD21	1.99	0.44
1:E:2287:ALA:HB3	1:E:2290:TRP:HB2	1.99	0.44
1:E:3326:LEU:O	1:E:3327:LEU:HG	2.17	0.44
1:H:3040:ILE:O	1:H:3055:GLY:HA3	2.18	0.44
1:B:171:MET:O	1:B:175:MET:HB2	2.17	0.44
1:B:1324:ARG:HA	1:B:1328:LEU:HD13	2.00	0.44
1:C:171:MET:O	1:C:175:MET:HB2	2.18	0.44
1:C:3140:VAL:HG23	1:C:3188:LEU:HB3	1.99	0.44
1:C:3271:TYR:O	1:C:3275:VAL:HG23	2.18	0.44
1:D:2063:GLU:HG3	1:D:2215:LEU:HD21	2.00	0.44
1:F:2305:ALA:O	1:F:2306:THR:C	2.54	0.44
1:F:3313:PRO:O	1:F:3316:ALA:HB3	2.17	0.44
1:G:1090:CYS:HB3	1:G:1140:VAL:HG23	1.99	0.44
1:G:3253:ALA:HA	1:G:3254:PRO:HD3	1.81	0.44
1:H:45:LEU:HD23	1:H:270:PHE:HD1	1.82	0.44
1:H:1016:GLN:O	1:H:1020:GLN:HB2	2.17	0.44
1:A:1202:MET:O	1:B:3116:CYS:O	2.36	0.44
1:A:2229:GLY:O	1:A:2230:ALA:CB	2.65	0.44
1:A:3123:GLU:O	1:A:3124:GLN:C	2.56	0.44
1:B:115:LEU:HA	1:B:1027:MET:O	2.18	0.44
1:C:125:ALA:C	1:C:127:GLU:H	2.21	0.44
1:C:173:GLN:HB3	1:C:174:ALA:H	1.68	0.44
1:C:3077:LEU:HG	1:C:3080:ILE:HD12	2.00	0.44
1:D:3326:LEU:O	1:D:3327:LEU:HG	2.17	0.44
1:E:2048:ASP:O	1:E:2051:LEU:HB2	2.18	0.44
1:F:3090:CYS:SG	1:F:3140:VAL:CG1	3.06	0.44
1:H:92:PHE:O	1:H:116:CYS:HA	2.16	0.44
1:H:3101:PRO:O	1:H:3104:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:CD2	1:A:1028:ARG:HG2	2.48	0.44
1:A:2227:ARG:HG3	1:A:2240:SER:HB3	1.99	0.44
1:A:3293:TYR:O	1:A:3296:GLU:HB2	2.18	0.44
1:B:72:LYS:HB2	1:B:72:LYS:HE3	1.74	0.44
1:C:2064:ILE:O	1:C:2192:ILE:HA	2.17	0.44
1:C:2293:TYR:CE1	1:C:2319:ILE:HD11	2.52	0.44
1:D:3092:PHE:CE2	1:D:3099:LEU:HD22	2.53	0.44
1:E:2300:GLN:CD	1:H:2304:ASN:HB3	2.38	0.44
1:E:3114:LEU:HD13	1:E:3114:LEU:O	2.18	0.44
1:F:1327:LEU:C	1:F:1328:LEU:HD12	2.38	0.44
1:F:2230:ALA:HA	1:F:2239:GLY:O	2.18	0.44
1:F:2253:ALA:HA	1:F:2254:PRO:HD3	1.83	0.44
1:F:3224:ASP:O	1:F:3244:VAL:HA	2.18	0.44
1:G:92:PHE:O	1:G:116:CYS:HA	2.17	0.44
1:G:2229:GLY:O	1:G:2230:ALA:CB	2.66	0.44
1:H:1282:LYS:H	1:H:1282:LYS:HG2	1.58	0.44
1:H:2128:ILE:HG22	1:H:2132:LEU:CD1	2.48	0.44
1:A:2090:CYS:CB	1:A:2140:VAL:HG13	2.47	0.44
1:A:2223:LEU:HD12	1:A:2223:LEU:HA	1.85	0.44
1:B:3300:GLN:NE2	1:C:1300:GLN:H	2.15	0.44
1:C:3029:LEU:CD2	1:C:3254:PRO:HD2	2.47	0.44
1:C:3040:ILE:O	1:C:3055:GLY:HA3	2.18	0.44
1:C:3048:ASP:OD1	1:C:3048:ASP:N	2.50	0.44
1:E:90:CYS:HG	1:E:140:VAL:HG13	1.82	0.44
1:G:1064:ILE:HG23	1:G:1223:LEU:HB3	2.00	0.44
1:G:2233:GLU:HG3	1:G:2238:VAL:HG11	2.00	0.44
1:H:2060:ARG:HB3	1:H:2220:SER:OG	2.17	0.44
1:H:2090:CYS:CB	1:H:2140:VAL:HG13	2.48	0.44
1:A:3056:LEU:HA	1:A:3057:PRO:HD3	1.66	0.43
1:A:3090:CYS:SG	1:A:3140:VAL:CG1	3.06	0.43
1:B:2293:TYR:CE1	1:B:2319:ILE:HD11	2.52	0.43
1:B:3029:LEU:CD2	1:B:3254:PRO:HD2	2.48	0.43
1:C:2233:GLU:HG3	1:C:2238:VAL:HG11	2.00	0.43
1:D:3140:VAL:HG23	1:D:3188:LEU:HB3	1.99	0.43
1:E:2300:GLN:HE21	1:H:2300:GLN:N	2.16	0.43
1:E:3076:THR:O	1:E:3080:ILE:HG13	2.18	0.43
1:E:3101:PRO:O	1:E:3104:ALA:HB3	2.17	0.43
1:F:2300:GLN:H	1:G:2300:GLN:NE2	2.16	0.43
1:G:2048:ASP:O	1:G:2051:LEU:HB2	2.18	0.43
1:G:2060:ARG:HB3	1:G:2220:SER:OG	2.17	0.43
1:G:3029:LEU:CD2	1:G:3254:PRO:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3065:TYR:HD2	1:G:3065:TYR:O	2.01	0.43
1:G:3090:CYS:SG	1:G:3140:VAL:CG1	3.06	0.43
1:H:1153:ALA:O	1:H:1157:GLY:O	2.36	0.43
1:A:1161:ASP:C	1:A:1163:HIS:N	2.70	0.43
1:A:1300:GLN:N	1:D:3300:GLN:NE2	2.64	0.43
1:A:3048:ASP:OD1	1:A:3048:ASP:N	2.51	0.43
1:A:3132:LEU:HA	1:A:3135:SER:HB2	2.00	0.43
1:A:3218:TYR:HD2	1:A:3218:TYR:HA	1.66	0.43
1:A:3271:TYR:O	1:A:3275:VAL:HG23	2.19	0.43
1:B:2305:ALA:O	1:B:2306:THR:C	2.57	0.43
1:C:2128:ILE:HG22	1:C:2132:LEU:CD1	2.47	0.43
1:C:3051:LEU:HD23	1:C:3051:LEU:HA	1.84	0.43
1:D:1050:ALA:HB1	1:D:1256:LYS:HB3	2.00	0.43
1:D:1305:ALA:O	1:D:1306:THR:O	2.35	0.43
1:G:171:MET:O	1:G:175:MET:HB2	2.17	0.43
1:G:2111:ILE:HD13	1:G:2111:ILE:HA	1.75	0.43
1:G:2230:ALA:HA	1:G:2239:GLY:O	2.18	0.43
1:H:231:VAL:HB	1:H:239:GLY:HA3	2.00	0.43
1:H:3140:VAL:HG23	1:H:3188:LEU:HB3	2.01	0.43
1:A:3072:LYS:CE	3:A:3400:ANP:O1B	2.59	0.43
1:B:3300:GLN:HE22	1:C:1299:GLY:HA2	1.83	0.43
1:C:2305:ALA:O	1:C:2306:THR:C	2.57	0.43
1:C:3123:GLU:O	1:C:3124:GLN:C	2.57	0.43
1:C:3326:LEU:O	1:C:3327:LEU:HG	2.17	0.43
1:D:2233:GLU:HG3	1:D:2238:VAL:HG11	2.01	0.43
1:E:92:PHE:O	1:E:116:CYS:HA	2.17	0.43
1:E:3132:LEU:HA	1:E:3135:SER:HB2	2.00	0.43
1:E:3281:GLU:O	1:E:3283:LEU:N	2.51	0.43
1:F:3029:LEU:CD2	1:F:3254:PRO:HD2	2.47	0.43
1:F:3171:MET:C	1:F:3173:GLN:H	2.21	0.43
1:F:3264:TYR:CE1	3:F:3400:ANP:H1'	2.53	0.43
1:H:3109:VAL:HG12	1:H:3110:ASP:N	2.33	0.43
1:B:73:THR:HG23	1:B:77:LEU:HD13	1.99	0.43
1:B:1018:GLU:OE2	1:B:1024:GLY:HA2	2.18	0.43
1:B:1090:CYS:SG	1:B:1140:VAL:HG22	2.59	0.43
1:B:3224:ASP:O	1:B:3244:VAL:HA	2.18	0.43
1:C:66:GLY:O	1:C:72:LYS:HE2	2.18	0.43
1:C:164:MET:C	1:C:166:LEU:N	2.71	0.43
1:D:1154:GLU:HG2	1:D:1159:ILE:HA	2.00	0.43
1:G:2128:ILE:HG22	1:G:2132:LEU:CD1	2.48	0.43
1:A:3065:TYR:HD2	1:A:3065:TYR:O	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3140:VAL:HG23	1:A:3188:LEU:HB3	2.00	0.43
1:B:2218:TYR:HD2	1:B:2218:TYR:HA	1.73	0.43
1:B:3327:LEU:O	1:B:3328:LEU:HD12	2.17	0.43
1:C:1066:GLY:O	1:C:1067:PRO:C	2.56	0.43
1:C:3177:LYS:HE3	1:F:173:GLN:NE2	2.34	0.43
1:C:3281:GLU:O	1:C:3283:LEU:N	2.52	0.43
1:D:1066:GLY:O	1:D:1067:PRO:C	2.57	0.43
1:D:1072:LYS:HB3	1:D:1225:ILE:HG21	2.00	0.43
1:D:2128:ILE:HG22	1:D:2132:LEU:CD1	2.49	0.43
1:D:3185:SER:C	1:D:3187:THR:N	2.71	0.43
1:F:1048:ASP:HB3	1:F:1054:GLY:HA2	2.01	0.43
1:F:2171:MET:O	1:F:2175:MET:HB2	2.17	0.43
1:G:2122:GLY:O	1:G:2125:ALA:HB3	2.18	0.43
1:G:3151:PRO:CB	1:H:3151:PRO:HG2	2.48	0.43
1:G:3185:SER:C	1:G:3187:THR:N	2.71	0.43
1:H:1048:ASP:HB3	1:H:1054:GLY:HA2	2.00	0.43
1:A:1090:CYS:HB3	1:A:1140:VAL:HG23	1.99	0.43
1:B:3144:ASP:OD1	1:B:3145:SER:HB2	2.19	0.43
1:C:1067:PRO:O	1:C:1070:SER:OG	2.24	0.43
1:C:2063:GLU:HG3	1:C:2215:LEU:HD21	1.99	0.43
1:D:231:VAL:HB	1:D:239:GLY:HA3	2.00	0.43
1:D:1090:CYS:HB3	1:D:1140:VAL:HG23	2.00	0.43
1:D:2229:GLY:O	1:D:2230:ALA:CB	2.66	0.43
1:E:72:LYS:HB2	1:E:72:LYS:HE3	1.73	0.43
1:E:1048:ASP:HB3	1:E:1054:GLY:HA2	2.01	0.43
1:E:1114:LEU:O	1:E:2028:ARG:HA	2.19	0.43
1:E:1300:GLN:H	1:H:3300:GLN:HE21	1.54	0.43
1:F:3092:PHE:CE2	1:F:3099:LEU:HD22	2.54	0.43
1:F:3123:GLU:O	1:F:3124:GLN:C	2.56	0.43
1:G:1056:LEU:HA	1:G:1057:PRO:HD2	1.81	0.43
1:A:2171:MET:O	1:A:2175:MET:HB2	2.18	0.43
1:B:1066:GLY:HA2	1:B:1067:PRO:HD2	1.85	0.43
1:B:2063:GLU:HG3	1:B:2215:LEU:HD21	2.01	0.43
1:B:2300:GLN:HE21	1:C:2300:GLN:CB	2.31	0.43
1:C:3185:SER:C	1:C:3187:THR:N	2.72	0.43
1:E:1072:LYS:HB3	1:E:1225:ILE:HG21	2.01	0.43
1:F:1097:HIS:CD2	1:F:2248:LYS:HG3	2.53	0.43
1:G:2063:GLU:HG3	1:G:2215:LEU:HD21	2.01	0.43
1:G:2064:ILE:O	1:G:2192:ILE:HA	2.19	0.43
1:G:3114:LEU:O	1:G:3114:LEU:HD13	2.17	0.43
1:H:1090:CYS:HB3	1:H:1140:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:MET:O	1:A:175:MET:HB2	2.19	0.43
1:B:1048:ASP:HB3	1:B:1054:GLY:HA2	2.01	0.43
1:B:3132:LEU:HA	1:B:3135:SER:HB2	2.00	0.43
1:C:100:ASP:HB3	1:C:103:TYR:HB3	2.01	0.43
1:C:1040:ILE:HD13	1:C:1040:ILE:HA	1.91	0.43
1:D:2048:ASP:O	1:D:2051:LEU:HB2	2.19	0.43
1:D:3145:SER:C	1:D:3147:ALA:N	2.72	0.43
1:E:118:GLN:HE21	1:E:1254:PRO:HB3	1.84	0.43
1:E:2233:GLU:HG3	1:E:2238:VAL:HG11	2.00	0.43
1:G:100:ASP:HB3	1:G:103:TYR:HB3	2.01	0.43
1:H:3281:GLU:O	1:H:3283:LEU:N	2.51	0.43
1:A:1305:ALA:O	1:A:1306:THR:O	2.37	0.43
1:A:2305:ALA:O	1:A:2306:THR:C	2.56	0.43
1:B:100:ASP:HB3	1:B:103:TYR:HB3	2.01	0.43
1:B:3051:LEU:HD23	1:B:3051:LEU:HA	1.84	0.43
1:B:3056:LEU:HA	1:B:3057:PRO:HD3	1.63	0.43
1:E:1300:GLN:HE22	1:H:3300:GLN:N	2.11	0.43
1:E:3232:LYS:NZ	1:H:1235:GLU:HG2	2.34	0.43
1:F:2223:LEU:HD12	1:F:2223:LEU:HA	1.83	0.43
1:F:3073:THR:O	1:F:3076:THR:OG1	2.30	0.43
1:G:3101:PRO:O	1:G:3104:ALA:HB3	2.18	0.43
1:G:3140:VAL:HG23	1:G:3188:LEU:HB3	2.00	0.43
1:A:1209:THR:O	1:A:1209:THR:CG2	2.63	0.43
1:A:1324:ARG:HA	1:A:1328:LEU:HD13	2.01	0.43
1:A:3040:ILE:O	1:A:3055:GLY:HA3	2.19	0.43
1:A:3084:GLN:O	1:B:226:ARG:HD3	2.18	0.43
1:B:2254:PRO:HB2	1:B:2255:PHE:CD2	2.54	0.43
1:B:3293:TYR:O	1:B:3296:GLU:HB2	2.19	0.43
1:C:3101:PRO:O	1:C:3104:ALA:HB3	2.19	0.43
1:C:3253:ALA:HA	1:C:3254:PRO:HD3	1.80	0.43
1:D:3313:PRO:O	1:D:3316:ALA:HB3	2.19	0.43
1:E:1090:CYS:SG	1:E:1140:VAL:HG22	2.58	0.43
1:E:2128:ILE:HG22	1:E:2132:LEU:CD1	2.49	0.43
1:F:1040:ILE:HD13	1:F:1040:ILE:HA	1.92	0.43
1:F:1064:ILE:HG23	1:F:1223:LEU:HB3	2.01	0.43
1:G:116:CYS:O	1:G:1026:ILE:HA	2.19	0.43
1:H:3224:ASP:O	1:H:3244:VAL:HA	2.19	0.43
1:H:3268:ILE:HG22	1:H:3269:ASN:N	2.33	0.43
1:A:1161:ASP:HA	1:A:1166:LEU:HD12	2.01	0.42
1:A:2253:ALA:HA	1:A:2254:PRO:HD3	1.83	0.42
1:B:2065:TYR:O	1:B:2065:TYR:HD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2118:GLN:NE2	1:C:3249:ASN:H	2.11	0.42
1:D:3072:LYS:CE	3:D:3400:ANP:O1B	2.60	0.42
1:D:3224:ASP:O	1:D:3244:VAL:HA	2.19	0.42
1:E:3144:ASP:OD1	1:E:3145:SER:HB2	2.19	0.42
1:F:2065:TYR:C	1:F:2065:TYR:CD1	2.92	0.42
1:G:72:LYS:HE3	1:G:72:LYS:HB2	1.74	0.42
1:G:90:CYS:HG	1:G:140:VAL:HG13	1.80	0.42
1:H:1066:GLY:O	1:H:1067:PRO:C	2.57	0.42
1:H:2048:ASP:O	1:H:2051:LEU:HB2	2.19	0.42
1:H:3132:LEU:HA	1:H:3135:SER:HB2	2.01	0.42
1:H:3293:TYR:O	1:H:3296:GLU:HB2	2.19	0.42
1:A:1064:ILE:HG23	1:A:1223:LEU:HB3	2.00	0.42
1:A:1090:CYS:O	1:A:1114:LEU:HD22	2.20	0.42
1:A:1163:HIS:O	1:A:1165:GLY:N	2.52	0.42
1:A:1202:MET:HA	1:A:1202:MET:CE	2.49	0.42
1:A:3185:SER:C	1:A:3187:THR:N	2.72	0.42
1:B:173:GLN:HB3	1:B:174:ALA:H	1.68	0.42
1:B:2301:GLY:O	1:B:2302:LYS:C	2.57	0.42
1:B:3040:ILE:O	1:B:3055:GLY:HA3	2.19	0.42
1:B:3271:TYR:O	1:B:3275:VAL:HG23	2.19	0.42
1:C:1090:CYS:SG	1:C:1140:VAL:HG22	2.59	0.42
1:C:3090:CYS:SG	1:C:3140:VAL:CG1	3.07	0.42
1:D:125:ALA:C	1:D:127:GLU:H	2.21	0.42
1:D:3056:LEU:CD1	1:D:3190:ILE:HD11	2.49	0.42
1:E:71:GLY:HA2	3:E:400:ANP:H5'1	2.01	0.42
1:E:2229:GLY:O	1:E:2230:ALA:CB	2.66	0.42
1:E:2253:ALA:HA	1:E:2254:PRO:HD3	1.83	0.42
1:F:107:LEU:HD23	1:F:267:GLY:HA3	2.01	0.42
1:F:231:VAL:HB	1:F:239:GLY:HA3	2.00	0.42
1:F:3056:LEU:CD1	1:F:3190:ILE:HD11	2.48	0.42
1:F:3140:VAL:HG23	1:F:3188:LEU:HB3	2.01	0.42
1:G:3040:ILE:O	1:G:3055:GLY:HA3	2.18	0.42
1:H:171:MET:O	1:H:175:MET:HB2	2.19	0.42
1:H:2230:ALA:HA	1:H:2239:GLY:O	2.19	0.42
1:A:92:PHE:O	1:A:116:CYS:HA	2.18	0.42
1:A:126:LEU:HA	1:A:129:CYS:SG	2.59	0.42
1:A:1161:ASP:HB3	1:A:1166:LEU:CD1	2.49	0.42
1:A:1170:MET:O	1:A:1170:MET:HG2	2.17	0.42
1:A:2128:ILE:HG22	1:A:2132:LEU:CD1	2.49	0.42
1:B:231:VAL:HB	1:B:239:GLY:HA3	2.01	0.42
1:B:2122:GLY:O	1:B:2125:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2128:ILE:HG22	1:B:2132:LEU:CD1	2.49	0.42
1:B:2229:GLY:O	1:B:2230:ALA:CB	2.65	0.42
1:C:2065:TYR:CD1	1:C:2065:TYR:C	2.92	0.42
1:C:2090:CYS:CB	1:C:2140:VAL:HG13	2.48	0.42
1:C:3269:ASN:O	1:C:3272:GLY:N	2.52	0.42
1:D:2253:ALA:HA	1:D:2254:PRO:HD3	1.83	0.42
1:D:3246:VAL:O	1:D:3246:VAL:HG12	2.19	0.42
1:D:3281:GLU:O	1:D:3283:LEU:N	2.52	0.42
1:D:3293:TYR:O	1:D:3296:GLU:HB2	2.20	0.42
1:E:1155:ILE:HG22	1:E:1156:GLU:OE2	2.19	0.42
1:F:1018:GLU:OE2	1:F:1024:GLY:HA2	2.19	0.42
1:G:3077:LEU:HG	1:G:3080:ILE:HD12	2.00	0.42
1:G:3293:TYR:O	1:G:3296:GLU:HB2	2.19	0.42
1:H:156:GLU:HG3	1:H:1176:ARG:CG	2.49	0.42
1:H:268:ILE:HG22	1:H:269:ASN:N	2.33	0.42
1:H:2218:TYR:HD2	1:H:2218:TYR:HA	1.73	0.42
1:H:2227:ARG:HG3	1:H:2240:SER:HB3	1.99	0.42
1:H:2233:GLU:HG3	1:H:2238:VAL:HG11	2.01	0.42
1:A:2233:GLU:HG3	1:A:2238:VAL:HG11	2.01	0.42
1:B:2233:GLU:HG3	1:B:2238:VAL:HG11	2.01	0.42
1:C:118:GLN:HE21	1:C:1249:ASN:H	1.67	0.42
1:C:1048:ASP:HB3	1:C:1054:GLY:HA2	2.01	0.42
1:D:253:ALA:HA	1:D:254:PRO:HD3	1.94	0.42
1:D:3144:ASP:OD1	1:D:3145:SER:HB2	2.19	0.42
1:F:1253:ALA:HA	1:F:1254:PRO:HD3	1.90	0.42
1:F:3306:THR:C	1:F:3308:TRP:H	2.23	0.42
1:F:3326:LEU:O	1:F:3327:LEU:HG	2.19	0.42
1:G:115:LEU:HA	1:G:1027:MET:O	2.19	0.42
1:G:3051:LEU:HD23	1:G:3051:LEU:HA	1.85	0.42
1:G:3269:ASN:O	1:G:3272:GLY:N	2.52	0.42
1:H:2063:GLU:HG3	1:H:2215:LEU:HD21	2.01	0.42
1:H:2275:VAL:HG21	1:H:2306:THR:HA	2.01	0.42
1:A:1066:GLY:O	1:A:1067:PRO:C	2.58	0.42
1:A:1123:GLU:HG3	1:A:1170:MET:HG3	2.02	0.42
1:A:3171:MET:C	1:A:3173:GLN:H	2.23	0.42
1:A:3253:ALA:HA	1:A:3254:PRO:HD3	1.78	0.42
1:C:2230:ALA:HA	1:C:2239:GLY:O	2.18	0.42
1:D:100:ASP:HB3	1:D:103:TYR:HB3	2.01	0.42
1:D:3051:LEU:HD23	1:D:3051:LEU:HA	1.86	0.42
1:E:2100:ASP:HA	1:E:2101:PRO:HD2	1.92	0.42
1:E:3268:ILE:HG22	1:E:3269:ASN:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3269:ASN:O	1:E:3272:GLY:N	2.53	0.42
1:F:1072:LYS:HB3	1:F:1225:ILE:HG21	2.01	0.42
1:F:3056:LEU:HD12	1:F:3190:ILE:HD11	2.01	0.42
1:H:92:PHE:CE2	1:H:94:ASP:HB2	2.55	0.42
1:H:3065:TYR:HD2	1:H:3065:TYR:O	2.01	0.42
1:A:3075:LEU:O	1:A:3075:LEU:HD23	2.20	0.42
1:A:3101:PRO:O	1:A:3104:ALA:HB3	2.20	0.42
1:B:2230:ALA:HA	1:B:2239:GLY:O	2.20	0.42
1:B:3123:GLU:O	1:B:3124:GLN:C	2.57	0.42
1:C:76:THR:O	1:C:79:VAL:HG22	2.19	0.42
1:C:2223:LEU:HD12	1:C:2223:LEU:HA	1.86	0.42
1:C:2287:ALA:HB3	1:C:2290:TRP:HB2	2.00	0.42
1:D:1018:GLU:OE2	1:D:1024:GLY:HA2	2.19	0.42
1:D:1090:CYS:SG	1:D:1140:VAL:HG22	2.59	0.42
1:D:2029:LEU:HD23	1:D:2254:PRO:HD2	2.01	0.42
1:D:2254:PRO:HB2	1:D:2255:PHE:CD2	2.55	0.42
1:F:100:ASP:HB3	1:F:103:TYR:HB3	2.01	0.42
1:F:3185:SER:C	1:F:3187:THR:N	2.70	0.42
1:G:101:PRO:HG3	1:G:1255:PHE:O	2.19	0.42
1:G:1145:SER:HB2	1:G:1192:ILE:HB	2.02	0.42
1:H:3077:LEU:HG	1:H:3080:ILE:HD12	2.02	0.42
1:A:231:VAL:HB	1:A:239:GLY:HA3	2.01	0.42
1:A:1193:ASN:ND2	1:A:1209:THR:CA	2.83	0.42
1:A:2064:ILE:O	1:A:2192:ILE:HA	2.19	0.42
1:A:2125:ALA:HA	1:A:2128:ILE:HD12	2.02	0.42
1:A:3029:LEU:CD2	1:A:3254:PRO:HD2	2.49	0.42
1:B:2264:TYR:N	1:B:2264:TYR:CD2	2.88	0.42
1:C:3145:SER:C	1:C:3147:ALA:N	2.69	0.42
1:C:3224:ASP:O	1:C:3244:VAL:HA	2.19	0.42
1:D:3029:LEU:CD2	1:D:3254:PRO:HD2	2.47	0.42
1:D:3090:CYS:SG	1:D:3140:VAL:CG1	3.08	0.42
1:D:3271:TYR:O	1:D:3275:VAL:HG23	2.19	0.42
1:E:126:LEU:HA	1:E:129:CYS:SG	2.60	0.42
1:E:2300:GLN:OE1	1:H:2304:ASN:HB3	2.20	0.42
1:E:3140:VAL:HG23	1:E:3188:LEU:HB3	2.02	0.42
1:E:3224:ASP:O	1:E:3244:VAL:HA	2.20	0.42
1:E:3299:GLY:HA2	1:H:1300:GLN:HE22	1.85	0.42
1:E:3311:ASP:OD2	1:F:286:LYS:NZ	2.53	0.42
1:F:2063:GLU:HG3	1:F:2215:LEU:HD21	2.01	0.42
1:G:76:THR:O	1:G:79:VAL:HG22	2.19	0.42
1:H:97:HIS:NE2	1:H:1248:LYS:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:253:ALA:HA	1:H:254:PRO:HD3	1.94	0.42
1:H:1123:GLU:HG3	1:H:1170:MET:HG3	2.02	0.42
1:A:1208:THR:HG21	1:A:1222:ARG:NH2	2.35	0.42
1:B:3109:VAL:HG12	1:B:3110:ASP:N	2.35	0.42
1:C:1018:GLU:OE2	1:C:1024:GLY:HA2	2.19	0.42
1:D:3044:SER:HA	1:D:3273:GLU:OE1	2.20	0.42
1:E:3123:GLU:O	1:E:3124:GLN:C	2.58	0.42
1:F:3132:LEU:HA	1:F:3135:SER:HB2	2.02	0.42
1:G:3171:MET:C	1:G:3173:GLN:H	2.22	0.42
1:H:76:THR:O	1:H:79:VAL:HG22	2.20	0.42
1:H:2065:TYR:CD1	1:H:2065:TYR:C	2.94	0.42
1:A:1219:ALA:O	1:A:1248:LYS:NZ	2.45	0.42
1:A:2218:TYR:HD2	1:A:2218:TYR:HA	1.74	0.42
1:B:3090:CYS:SG	1:B:3140:VAL:CG1	3.08	0.42
1:B:3232:LYS:HZ2	1:C:1235:GLU:HG2	1.84	0.42
1:C:1072:LYS:HB3	1:C:1225:ILE:HG21	2.00	0.42
1:C:1324:ARG:HA	1:C:1328:LEU:HD13	2.02	0.42
1:D:2073:THR:HA	1:D:2076:THR:HB	2.02	0.42
1:E:3218:TYR:HD2	1:E:3218:TYR:HA	1.66	0.42
1:E:3327:LEU:O	1:E:3328:LEU:HD12	2.20	0.42
1:F:1123:GLU:HG3	1:F:1170:MET:HG3	2.01	0.42
1:G:114:LEU:HD22	1:G:114:LEU:HA	1.92	0.42
1:A:107:LEU:HD23	1:A:267:GLY:HA3	2.01	0.42
1:A:1090:CYS:SG	1:A:1140:VAL:HG22	2.60	0.42
1:A:3306:THR:C	1:A:3308:TRP:H	2.22	0.42
1:B:92:PHE:CE2	1:B:94:ASP:HB2	2.55	0.42
1:B:3077:LEU:HG	1:B:3080:ILE:HD12	2.02	0.42
1:C:2014:LEU:C	1:C:2016:GLN:H	2.22	0.42
1:D:92:PHE:CE2	1:D:94:ASP:HB2	2.54	0.42
1:D:3232:LYS:HA	1:D:3236:ASN:O	2.20	0.42
1:E:111:ILE:HD13	1:E:111:ILE:HA	1.90	0.42
1:E:173:GLN:HB3	1:E:174:ALA:H	1.68	0.42
1:E:2118:GLN:NE2	1:E:3249:ASN:H	2.13	0.42
1:E:2275:VAL:HG21	1:E:2306:THR:HA	2.02	0.42
1:F:75:LEU:HD23	1:F:75:LEU:C	2.40	0.42
1:F:92:PHE:CE2	1:F:94:ASP:HB2	2.55	0.42
1:F:157:GLY:O	1:F:158:GLU:O	2.38	0.42
1:F:2065:TYR:O	1:F:2065:TYR:HD1	2.03	0.42
1:F:3040:ILE:O	1:F:3055:GLY:HA3	2.20	0.42
1:F:3051:LEU:HD23	1:F:3051:LEU:HA	1.88	0.42
1:H:66:GLY:O	1:H:72:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:LYS:HB2	1:H:72:LYS:HE3	1.74	0.42
1:H:118:GLN:NE2	1:H:1249:ASN:H	2.17	0.42
1:H:126:LEU:HA	1:H:129:CYS:SG	2.60	0.42
1:H:3092:PHE:CE2	1:H:3099:LEU:HD22	2.55	0.42
1:H:3123:GLU:O	1:H:3124:GLN:C	2.57	0.42
1:A:76:THR:O	1:A:79:VAL:HG22	2.20	0.41
1:A:92:PHE:CE2	1:A:94:ASP:HB2	2.54	0.41
1:A:2230:ALA:HA	1:A:2239:GLY:O	2.20	0.41
1:B:65:TYR:HD2	1:B:223:LEU:O	2.03	0.41
1:B:66:GLY:O	1:B:72:LYS:HE2	2.20	0.41
1:B:2100:ASP:HA	1:B:2101:PRO:HD2	1.92	0.41
1:C:92:PHE:CE2	1:C:94:ASP:HB2	2.55	0.41
1:C:107:LEU:HD23	1:C:267:GLY:HA3	2.01	0.41
1:C:2073:THR:HA	1:C:2076:THR:HB	2.02	0.41
1:D:66:GLY:O	1:D:72:LYS:HE2	2.20	0.41
1:D:1324:ARG:HA	1:D:1328:LEU:HD13	2.01	0.41
1:D:3040:ILE:O	1:D:3055:GLY:HA3	2.19	0.41
1:E:231:VAL:HB	1:E:239:GLY:HA3	2.02	0.41
1:E:2305:ALA:O	1:E:2306:THR:C	2.57	0.41
1:F:114:LEU:O	1:F:1028:ARG:HA	2.21	0.41
1:F:1219:ALA:O	1:F:1248:LYS:NZ	2.45	0.41
1:F:1324:ARG:HA	1:F:1328:LEU:HD13	2.02	0.41
1:F:2229:GLY:O	1:F:2230:ALA:CB	2.65	0.41
1:G:107:LEU:HD23	1:G:267:GLY:HA3	2.01	0.41
1:G:1066:GLY:O	1:G:1067:PRO:C	2.57	0.41
1:G:1090:CYS:O	1:G:1114:LEU:HD22	2.19	0.41
1:H:150:THR:OG1	1:H:1217:PHE:CE2	2.72	0.41
1:H:173:GLN:HB3	1:H:174:ALA:H	1.66	0.41
1:H:2305:ALA:O	1:H:2306:THR:C	2.57	0.41
1:A:1048:ASP:HB3	1:A:1054:GLY:HA2	2.01	0.41
1:A:1204:GLY:O	1:A:1205:ASN:CB	2.68	0.41
1:A:2124:GLN:O	1:A:2128:ILE:HG13	2.20	0.41
1:A:2254:PRO:HB2	1:A:2255:PHE:CD2	2.55	0.41
1:A:3144:ASP:OD1	1:A:3145:SER:HB2	2.20	0.41
1:B:1072:LYS:HB3	1:B:1225:ILE:HG21	2.02	0.41
1:B:1133:ALA:C	1:B:1135:SER:H	2.24	0.41
1:B:1300:GLN:OE1	1:C:3304:ASN:HB3	2.20	0.41
1:B:2140:VAL:HA	1:B:2188:LEU:O	2.20	0.41
1:B:3056:LEU:CD1	1:B:3190:ILE:HD11	2.50	0.41
1:D:2111:ILE:HD13	1:D:2111:ILE:HA	1.74	0.41
1:E:2230:ALA:HA	1:E:2239:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2233:GLU:HG3	1:F:2238:VAL:HG11	2.01	0.41
1:F:2300:GLN:H	1:G:2300:GLN:HE22	1.67	0.41
1:G:93:ILE:HB	1:G:143:VAL:HA	2.02	0.41
1:G:1072:LYS:HB3	1:G:1225:ILE:HG21	2.01	0.41
1:H:3185:SER:C	1:H:3187:THR:N	2.72	0.41
1:A:1193:ASN:ND2	1:A:1209:THR:C	2.74	0.41
1:B:2223:LEU:HD12	1:B:2223:LEU:HA	1.85	0.41
1:B:3171:MET:C	1:B:3173:GLN:H	2.23	0.41
1:C:229:GLY:O	1:C:230:ALA:HB2	2.21	0.41
1:C:231:VAL:HB	1:C:239:GLY:HA3	2.01	0.41
1:C:2122:GLY:O	1:C:2125:ALA:HB3	2.19	0.41
1:C:2254:PRO:HB2	1:C:2255:PHE:CD2	2.55	0.41
1:D:1048:ASP:HB3	1:D:1054:GLY:HA2	2.00	0.41
1:D:2065:TYR:CD1	1:D:2065:TYR:C	2.94	0.41
1:E:57:PRO:CG	1:E:251:ILE:HG12	2.50	0.41
1:E:3056:LEU:HA	1:E:3057:PRO:HD3	1.69	0.41
1:F:66:GLY:O	1:F:72:LYS:HE2	2.21	0.41
1:F:114:LEU:HD22	1:F:114:LEU:HA	1.93	0.41
1:F:3269:ASN:O	1:F:3272:GLY:N	2.52	0.41
1:G:1048:ASP:HB3	1:G:1054:GLY:HA2	2.02	0.41
1:G:1123:GLU:HG3	1:G:1170:MET:HG3	2.02	0.41
1:G:1133:ALA:C	1:G:1135:SER:H	2.24	0.41
1:G:2254:PRO:HB2	1:G:2255:PHE:CD2	2.55	0.41
1:G:3056:LEU:HA	1:G:3057:PRO:HD3	1.68	0.41
1:G:3072:LYS:HD2	1:G:3193:ASN:O	2.20	0.41
1:G:3264:TYR:CE1	3:G:3400:ANP:H1'	2.56	0.41
1:H:97:HIS:HB3	1:H:1247:VAL:HB	2.01	0.41
1:H:1170:MET:O	1:H:1170:MET:HG2	2.18	0.41
1:H:1305:ALA:O	1:H:1306:THR:O	2.38	0.41
1:H:2122:GLY:O	1:H:2125:ALA:HB3	2.21	0.41
1:H:3218:TYR:HD2	1:H:3218:TYR:HA	1.66	0.41
1:A:1111:ILE:HG23	1:A:2029:LEU:HD13	2.02	0.41
1:A:3232:LYS:HA	1:A:3236:ASN:O	2.20	0.41
1:B:107:LEU:HD23	1:B:267:GLY:HA3	2.00	0.41
1:C:1123:GLU:HG3	1:C:1170:MET:HG3	2.02	0.41
1:C:2264:TYR:N	1:C:2264:TYR:CD2	2.88	0.41
1:C:3064:ILE:CG1	1:C:3223:LEU:HB2	2.38	0.41
1:D:3044:SER:HG	1:D:3045:LEU:H	1.66	0.41
1:E:66:GLY:O	1:E:72:LYS:HE2	2.21	0.41
1:E:3151:PRO:HB3	1:F:3166:LEU:N	2.35	0.41
1:F:57:PRO:CG	1:F:251:ILE:HG12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1066:GLY:O	1:F:1067:PRO:C	2.59	0.41
1:F:2140:VAL:HA	1:F:2188:LEU:O	2.19	0.41
1:G:57:PRO:CG	1:G:251:ILE:HG12	2.50	0.41
1:G:2264:TYR:CD2	1:G:2264:TYR:N	2.89	0.41
1:G:3274:LEU:O	1:G:3275:VAL:C	2.59	0.41
1:H:1090:CYS:O	1:H:1114:LEU:HD22	2.20	0.41
1:H:1253:ALA:HA	1:H:1254:PRO:HD3	1.89	0.41
1:A:2111:ILE:HD13	1:A:2111:ILE:HA	1.75	0.41
1:A:2301:GLY:O	1:A:2302:LYS:C	2.59	0.41
1:B:111:ILE:HD13	1:B:111:ILE:HA	1.90	0.41
1:B:3065:TYR:HD2	1:B:3065:TYR:O	2.03	0.41
1:C:114:LEU:HD22	1:C:114:LEU:HA	1.92	0.41
1:C:3293:TYR:O	1:C:3296:GLU:HB2	2.21	0.41
1:D:126:LEU:HA	1:D:129:CYS:SG	2.61	0.41
1:D:1062:VAL:O	1:D:1190:ILE:HA	2.21	0.41
1:D:2140:VAL:HA	1:D:2188:LEU:O	2.20	0.41
1:E:100:ASP:HB3	1:E:103:TYR:HB3	2.02	0.41
1:E:107:LEU:HD23	1:E:267:GLY:HA3	2.02	0.41
1:E:1123:GLU:HG3	1:E:1170:MET:HG3	2.03	0.41
1:E:1133:ALA:C	1:E:1135:SER:H	2.24	0.41
1:E:2254:PRO:HB2	1:E:2255:PHE:CD2	2.56	0.41
1:F:71:GLY:N	3:F:400:ANP:C5'	2.84	0.41
1:G:1018:GLU:OE2	1:G:1024:GLY:HA2	2.20	0.41
1:G:2065:TYR:CD1	1:G:2065:TYR:C	2.93	0.41
1:G:3224:ASP:O	1:G:3244:VAL:HA	2.21	0.41
1:H:2254:PRO:HB2	1:H:2255:PHE:CD2	2.55	0.41
1:H:3144:ASP:OD1	1:H:3145:SER:HB2	2.20	0.41
1:A:2122:GLY:O	1:A:2125:ALA:HB3	2.21	0.41
1:B:135:SER:OG	1:B:1013:ALA:HB1	2.20	0.41
1:B:1305:ALA:O	1:B:1306:THR:O	2.38	0.41
1:B:2057:PRO:O	1:B:2188:LEU:HD13	2.21	0.41
1:C:75:LEU:HD23	1:C:75:LEU:C	2.40	0.41
1:C:3056:LEU:CD1	1:C:3190:ILE:HD11	2.50	0.41
1:D:1146:VAL:CG1	1:D:1211:GLY:HA3	2.50	0.41
1:D:3077:LEU:HG	1:D:3080:ILE:HD12	2.01	0.41
1:D:3109:VAL:HG12	1:D:3110:ASP:N	2.35	0.41
1:E:1300:GLN:HE22	1:H:3299:GLY:CA	2.26	0.41
1:E:2084:GLN:HG3	1:E:2090:CYS:SG	2.60	0.41
1:E:2264:TYR:N	1:E:2264:TYR:CD2	2.88	0.41
1:E:3042:THR:OG1	1:E:3048:ASP:OD1	2.27	0.41
1:F:2254:PRO:HB2	1:F:2255:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2300:GLN:NE2	1:G:2300:GLN:H	2.18	0.41
1:G:1040:ILE:HD13	1:G:1040:ILE:HA	1.92	0.41
1:H:1173:GLN:C	1:H:1175:MET:H	2.23	0.41
1:H:1219:ALA:O	1:H:1248:LYS:NZ	2.45	0.41
1:H:3271:TYR:O	1:H:3275:VAL:HG23	2.20	0.41
1:A:229:GLY:O	1:A:230:ALA:HB2	2.21	0.41
1:A:2063:GLU:HG3	1:A:2215:LEU:HD21	2.01	0.41
1:A:2264:TYR:N	1:A:2264:TYR:CD2	2.89	0.41
1:A:3269:ASN:O	1:A:3272:GLY:N	2.53	0.41
1:B:57:PRO:CG	1:B:251:ILE:HG12	2.51	0.41
1:B:1300:GLN:HE22	1:C:3300:GLN:H	1.66	0.41
1:C:93:ILE:HB	1:C:143:VAL:HA	2.03	0.41
1:C:93:ILE:HG13	1:C:143:VAL:HG13	2.01	0.41
1:C:141:ILE:HB	1:C:189:LEU:HG	2.03	0.41
1:C:2254:PRO:O	1:C:2255:PHE:HB2	2.21	0.41
1:D:107:LEU:HD23	1:D:267:GLY:HA3	2.01	0.41
1:E:1090:CYS:O	1:E:1114:LEU:HD22	2.20	0.41
1:E:2014:LEU:C	1:E:2016:GLN:H	2.24	0.41
1:E:2090:CYS:CB	1:E:2140:VAL:HG13	2.48	0.41
1:E:3293:TYR:O	1:E:3296:GLU:HB2	2.21	0.41
1:F:224:ASP:HB3	1:F:245:LYS:HB3	2.02	0.41
1:F:1014:LEU:C	1:F:1016:GLN:N	2.74	0.41
1:F:2264:TYR:N	1:F:2264:TYR:CD2	2.88	0.41
1:F:2300:GLN:HE21	1:G:2300:GLN:HB3	1.85	0.41
1:F:3144:ASP:OD1	1:F:3145:SER:HB2	2.20	0.41
1:G:3010:LEU:C	1:G:3012:ALA:H	2.24	0.41
1:G:3313:PRO:O	1:G:3316:ALA:HB3	2.20	0.41
1:H:1040:ILE:HD13	1:H:1040:ILE:HA	1.91	0.41
1:A:100:ASP:HB3	1:A:103:TYR:HB3	2.02	0.41
1:A:3274:LEU:O	1:A:3275:VAL:C	2.59	0.41
1:A:3327:LEU:O	1:A:3328:LEU:HD12	2.20	0.41
1:B:93:ILE:HG13	1:B:143:VAL:HG13	2.02	0.41
1:B:2142:VAL:HG22	1:B:2190:ILE:HB	2.02	0.41
1:C:57:PRO:CG	1:C:251:ILE:HG12	2.51	0.41
1:C:1090:CYS:O	1:C:1114:LEU:HD22	2.21	0.41
1:C:2301:GLY:O	1:C:2302:LYS:C	2.59	0.41
1:C:3010:LEU:C	1:C:3012:ALA:H	2.24	0.41
1:C:3144:ASP:OD1	1:C:3145:SER:HB2	2.21	0.41
1:D:2122:GLY:O	1:D:2125:ALA:HB3	2.21	0.41
1:E:76:THR:O	1:E:79:VAL:HG22	2.21	0.41
1:E:3105:ARG:HH11	1:F:227:ARG:HH22	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3171:MET:C	1:E:3173:GLN:H	2.22	0.41
1:F:1097:HIS:NE2	1:F:2248:LYS:HG3	2.36	0.41
1:H:141:ILE:HB	1:H:189:LEU:HG	2.03	0.41
1:A:57:PRO:CG	1:A:251:ILE:HG12	2.50	0.41
1:A:66:GLY:O	1:A:72:LYS:HE2	2.20	0.41
1:A:71:GLY:HA2	3:A:400:ANP:H5'1	2.03	0.41
1:A:75:LEU:HD23	1:A:75:LEU:C	2.42	0.41
1:A:178:LEU:O	1:A:182:LEU:HG	2.21	0.41
1:A:2057:PRO:O	1:A:2188:LEU:HD13	2.21	0.41
1:A:2065:TYR:C	1:A:2065:TYR:CD1	2.93	0.41
1:A:3306:THR:C	1:A:3308:TRP:N	2.75	0.41
1:B:1006:LYS:HG3	1:B:1007:GLN:H	1.86	0.41
1:B:2014:LEU:C	1:B:2016:GLN:H	2.23	0.41
1:B:2275:VAL:HG21	1:B:2306:THR:HA	2.02	0.41
1:B:3274:LEU:O	1:B:3275:VAL:C	2.59	0.41
1:C:99:LEU:HD23	1:C:1255:PHE:CZ	2.56	0.41
1:C:1006:LYS:HG3	1:C:1007:GLN:H	1.86	0.41
1:C:1064:ILE:HG23	1:C:1223:LEU:HB3	2.02	0.41
1:C:2122:GLY:O	1:C:2123:GLU:C	2.59	0.41
1:C:2125:ALA:HA	1:C:2128:ILE:HD12	2.03	0.41
1:C:3274:LEU:O	1:C:3275:VAL:C	2.59	0.41
1:C:3306:THR:C	1:C:3308:TRP:H	2.24	0.41
1:C:3327:LEU:O	1:C:3328:LEU:HD12	2.20	0.41
1:D:57:PRO:CG	1:D:251:ILE:HG12	2.51	0.41
1:D:2264:TYR:N	1:D:2264:TYR:CD2	2.88	0.41
1:D:3076:THR:O	1:D:3080:ILE:HG13	2.20	0.41
1:E:158:GLU:O	1:E:159:ILE:O	2.39	0.41
1:E:1006:LYS:HG3	1:E:1007:GLN:H	1.86	0.41
1:E:1111:ILE:HD13	1:E:1111:ILE:HA	1.81	0.41
1:E:2073:THR:HA	1:E:2076:THR:HB	2.03	0.41
1:E:2111:ILE:HD13	1:E:2111:ILE:HA	1.74	0.41
1:E:3056:LEU:CD1	1:E:3190:ILE:HD11	2.51	0.41
1:E:3185:SER:C	1:E:3187:THR:N	2.72	0.41
1:E:3232:LYS:HA	1:E:3236:ASN:O	2.21	0.41
1:F:3010:LEU:C	1:F:3012:ALA:H	2.25	0.41
1:F:3232:LYS:HA	1:F:3236:ASN:O	2.20	0.41
1:G:224:ASP:HB3	1:G:245:LYS:HB3	2.03	0.41
1:G:231:VAL:HB	1:G:239:GLY:HA3	2.01	0.41
1:G:1090:CYS:SG	1:G:1140:VAL:HG22	2.60	0.41
1:G:2072:LYS:HE3	1:G:2193:ASN:O	2.20	0.41
1:G:2072:LYS:HE2	1:G:2192:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3044:SER:HB3	1:G:3047:LEU:HB2	2.03	0.41
1:G:3246:VAL:O	1:G:3246:VAL:HG12	2.20	0.41
1:H:75:LEU:HD23	1:H:75:LEU:C	2.41	0.41
1:H:144:ASP:HA	1:H:145:SER:HA	1.84	0.41
1:H:178:LEU:O	1:H:182:LEU:HG	2.21	0.41
1:H:224:ASP:HB3	1:H:245:LYS:HB3	2.03	0.41
1:H:1133:ALA:C	1:H:1135:SER:H	2.23	0.41
1:H:3090:CYS:SG	1:H:3140:VAL:HG12	2.61	0.41
1:H:3232:LYS:HA	1:H:3236:ASN:O	2.20	0.41
1:A:3010:LEU:C	1:A:3012:ALA:H	2.24	0.41
1:B:93:ILE:HB	1:B:143:VAL:HA	2.03	0.41
1:B:1040:ILE:HD13	1:B:1040:ILE:HA	1.92	0.41
1:B:1090:CYS:O	1:B:1114:LEU:HD22	2.21	0.41
1:B:2065:TYR:C	1:B:2065:TYR:HD1	2.24	0.41
1:C:3075:LEU:O	1:C:3075:LEU:HD23	2.21	0.41
1:D:93:ILE:HG13	1:D:143:VAL:HG13	2.03	0.41
1:D:141:ILE:HB	1:D:189:LEU:HG	2.03	0.41
1:D:1090:CYS:O	1:D:1114:LEU:HD22	2.20	0.41
1:E:1040:ILE:HD13	1:E:1040:ILE:HA	1.93	0.41
1:E:1066:GLY:O	1:E:1067:PRO:C	2.59	0.41
1:E:2140:VAL:HA	1:E:2188:LEU:O	2.21	0.41
1:E:2142:VAL:HG22	1:E:2190:ILE:HB	2.04	0.41
1:F:111:ILE:HD13	1:F:111:ILE:HA	1.88	0.41
1:F:229:GLY:O	1:F:230:ALA:HB2	2.21	0.41
1:F:2073:THR:HA	1:F:2076:THR:HB	2.03	0.41
1:G:118:GLN:HE21	1:G:1249:ASN:H	1.68	0.41
1:G:3327:LEU:O	1:G:3328:LEU:HD12	2.21	0.41
1:H:3313:PRO:O	1:H:3316:ALA:HB3	2.21	0.41
1:A:3151:PRO:HG2	1:B:3151:PRO:CG	2.45	0.40
1:B:76:THR:O	1:B:79:VAL:HG22	2.21	0.40
1:B:3284:ILE:HG23	1:B:3292:SER:O	2.21	0.40
1:C:144:ASP:HA	1:C:145:SER:HA	1.81	0.40
1:C:178:LEU:O	1:C:182:LEU:HG	2.22	0.40
1:C:1133:ALA:C	1:C:1135:SER:H	2.24	0.40
1:C:3171:MET:C	1:C:3173:GLN:H	2.23	0.40
1:D:1133:ALA:C	1:D:1135:SER:H	2.24	0.40
1:D:2301:GLY:O	1:D:2302:LYS:C	2.60	0.40
1:E:75:LEU:HD23	1:E:75:LEU:C	2.42	0.40
1:E:1062:VAL:O	1:E:1190:ILE:HA	2.21	0.40
1:E:1219:ALA:O	1:E:1248:LYS:NZ	2.45	0.40
1:F:2091:ALA:HA	1:F:2115:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2125:ALA:HA	1:F:2128:ILE:HD12	2.03	0.40
1:F:2254:PRO:O	1:F:2255:PHE:HB2	2.20	0.40
1:G:2301:GLY:O	1:G:2302:LYS:C	2.59	0.40
1:H:100:ASP:HB3	1:H:103:TYR:HB3	2.02	0.40
1:H:2072:LYS:HE2	1:H:2192:ILE:HG22	2.03	0.40
1:H:2308:TRP:CE3	1:H:2309:LEU:HD23	2.56	0.40
1:B:2084:GLN:HG3	1:B:2090:CYS:SG	2.61	0.40
1:C:2065:TYR:HD1	1:C:2065:TYR:O	2.03	0.40
1:C:3232:LYS:HA	1:C:3236:ASN:O	2.21	0.40
1:C:3269:ASN:O	1:C:3270:PHE:C	2.60	0.40
1:D:76:THR:O	1:D:79:VAL:HG22	2.20	0.40
1:D:224:ASP:HB3	1:D:245:LYS:HB3	2.03	0.40
1:D:1123:GLU:HG3	1:D:1170:MET:HG3	2.02	0.40
1:D:1173:GLN:C	1:D:1175:MET:H	2.25	0.40
1:D:2064:ILE:HG12	1:D:2223:LEU:HB2	2.03	0.40
1:E:224:ASP:HB3	1:E:245:LYS:HB3	2.04	0.40
1:E:1063:GLU:OE1	1:E:1222:ARG:HD3	2.22	0.40
1:E:2065:TYR:C	1:E:2065:TYR:CD1	2.94	0.40
1:E:2223:LEU:HD12	1:E:2223:LEU:HA	1.85	0.40
1:E:3010:LEU:C	1:E:3012:ALA:H	2.25	0.40
1:F:135:SER:OG	1:F:1013:ALA:HB1	2.21	0.40
1:F:1145:SER:HB2	1:F:1192:ILE:HB	2.02	0.40
1:F:2218:TYR:HD2	1:F:2218:TYR:HA	1.73	0.40
1:G:112:ASP:HA	1:G:1030:GLY:H	1.86	0.40
1:G:2090:CYS:CB	1:G:2140:VAL:HG13	2.47	0.40
1:G:2125:ALA:HA	1:G:2128:ILE:HD12	2.04	0.40
1:G:3056:LEU:CD1	1:G:3190:ILE:HD11	2.51	0.40
1:H:57:PRO:CG	1:H:251:ILE:HG12	2.51	0.40
1:H:65:TYR:HD2	1:H:223:LEU:O	2.04	0.40
1:H:1056:LEU:HA	1:H:1057:PRO:HD2	1.80	0.40
1:H:1090:CYS:SG	1:H:1140:VAL:HG22	2.61	0.40
1:H:1145:SER:HB2	1:H:1192:ILE:HB	2.03	0.40
1:H:2064:ILE:HG12	1:H:2223:LEU:HB2	2.03	0.40
1:H:3056:LEU:CD1	1:H:3190:ILE:HD11	2.52	0.40
1:A:141:ILE:HB	1:A:189:LEU:HG	2.03	0.40
1:A:1072:LYS:HB3	1:A:1225:ILE:HG21	2.04	0.40
1:A:2014:LEU:C	1:A:2016:GLN:H	2.24	0.40
1:B:1062:VAL:O	1:B:1190:ILE:HA	2.21	0.40
1:B:3232:LYS:HA	1:B:3236:ASN:O	2.20	0.40
1:B:3246:VAL:O	1:B:3246:VAL:HG12	2.21	0.40
1:C:2140:VAL:HA	1:C:2188:LEU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1100:ASP:HA	1:D:1101:PRO:HD2	1.98	0.40
1:D:3132:LEU:HA	1:D:3135:SER:HB2	2.01	0.40
1:E:92:PHE:CE2	1:E:94:ASP:HB2	2.56	0.40
1:E:112:ASP:HA	1:E:1030:GLY:CA	2.51	0.40
1:E:1300:GLN:N	1:H:3300:GLN:HE22	2.11	0.40
1:F:90:CYS:HG	1:F:140:VAL:HG13	1.84	0.40
1:F:161:ASP:H	1:F:163:HIS:N	2.19	0.40
1:F:1066:GLY:HA2	1:F:1067:PRO:HD2	1.89	0.40
1:F:1090:CYS:SG	1:F:1140:VAL:HG22	2.61	0.40
1:F:2014:LEU:C	1:F:2016:GLN:H	2.24	0.40
1:F:2084:GLN:HG3	1:F:2090:CYS:SG	2.61	0.40
1:F:2122:GLY:O	1:F:2123:GLU:C	2.58	0.40
1:G:1150:THR:HA	1:G:1151:PRO:HD3	1.60	0.40
1:G:2142:VAL:HG22	1:G:2190:ILE:HB	2.03	0.40
1:G:2223:LEU:HD12	1:G:2223:LEU:HA	1.86	0.40
1:G:3232:LYS:HA	1:G:3236:ASN:O	2.21	0.40
1:H:1014:LEU:C	1:H:1016:GLN:N	2.75	0.40
1:A:1074:THR:N	3:A:1400:ANP:O1A	2.50	0.40
1:A:3284:ILE:HG23	1:A:3292:SER:O	2.22	0.40
1:C:1254:PRO:HB2	1:C:1255:PHE:CD2	2.57	0.40
1:D:2142:VAL:HG22	1:D:2190:ILE:HB	2.03	0.40
1:E:3306:THR:C	1:E:3308:TRP:H	2.25	0.40
1:F:76:THR:O	1:F:79:VAL:HG22	2.20	0.40
1:F:1090:CYS:O	1:F:1114:LEU:HD22	2.21	0.40
1:H:111:ILE:HD13	1:H:111:ILE:HA	1.87	0.40
1:H:1114:LEU:HD12	1:H:2029:LEU:CD1	2.52	0.40
1:H:2057:PRO:O	1:H:2188:LEU:HD13	2.22	0.40
1:H:2264:TYR:CD2	1:H:2264:TYR:N	2.89	0.40
1:H:2301:GLY:O	1:H:2302:LYS:C	2.60	0.40
1:H:3171:MET:C	1:H:3173:GLN:H	2.23	0.40
1:A:1173:GLN:C	1:A:1175:MET:H	2.25	0.40
1:A:2122:GLY:O	1:A:2123:GLU:C	2.59	0.40
1:A:3077:LEU:HG	1:A:3080:ILE:HD12	2.03	0.40
1:B:126:LEU:HA	1:B:129:CYS:SG	2.61	0.40
1:B:2125:ALA:HA	1:B:2128:ILE:HD12	2.04	0.40
1:C:135:SER:OG	1:C:1013:ALA:HB1	2.21	0.40
1:D:1006:LYS:HG3	1:D:1007:GLN:H	1.86	0.40
1:E:2103:TYR:HE1	1:E:2265:GLY:H	1.70	0.40
1:E:2125:ALA:HA	1:E:2128:ILE:HD12	2.03	0.40
1:E:3274:LEU:O	1:E:3275:VAL:C	2.60	0.40
1:F:3075:LEU:O	1:F:3075:LEU:HD23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:PHE:CE2	1:G:94:ASP:HB2	2.56	0.40
1:G:2073:THR:HA	1:G:2076:THR:HB	2.02	0.40
1:G:2275:VAL:HG21	1:G:2306:THR:HA	2.03	0.40
1:G:3220:SER:O	1:G:3221:VAL:HG23	2.22	0.40

All (1) 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:A:1161:ASP:OD1	1:C:1314:GLU:OE2[4_456]	2.05	0.15

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1172/1357 (86%)	923 (79%)	191 (16%)	58 (5%)	2 23
1	B	1139/1357 (84%)	915 (80%)	172 (15%)	52 (5%)	2 24
1	C	1155/1357 (85%)	919 (80%)	178 (15%)	58 (5%)	2 23
1	D	1155/1357 (85%)	923 (80%)	179 (16%)	53 (5%)	2 24
1	E	1141/1357 (84%)	910 (80%)	178 (16%)	53 (5%)	2 24
1	F	1155/1357 (85%)	913 (79%)	188 (16%)	54 (5%)	2 24
1	G	1145/1357 (84%)	914 (80%)	179 (16%)	52 (4%)	2 24
1	H	1151/1357 (85%)	914 (79%)	180 (16%)	57 (5%)	2 23
All	All	9213/10856 (85%)	7331 (80%)	1445 (16%)	437 (5%)	2 24

All (437) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	LYS

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Mol	Chain	Res	Type
1	A	99	LEU
1	A	238	VAL
1	A	1099	LEU
1	A	1146	VAL
1	A	1173	GLN
1	A	1203	PHE
1	A	1282	LYS
1	A	2099	LEU
1	A	2173	GLN
1	A	3033	ARG
1	A	3099	LEU
1	A	3213	ASN
1	A	3214	ALA
1	A	3230	ALA
1	B	88	LYS
1	B	99	LEU
1	B	157	GLY
1	B	163	HIS
1	B	238	VAL
1	B	1099	LEU
1	B	1146	VAL
1	B	1173	GLN
1	B	1282	LYS
1	B	2099	LEU
1	B	2173	GLN
1	B	3033	ARG
1	B	3099	LEU
1	B	3213	ASN
1	B	3214	ALA
1	B	3230	ALA
1	C	88	LYS
1	C	99	LEU
1	C	238	VAL
1	C	1099	LEU
1	C	1146	VAL
1	C	1173	GLN
1	C	1282	LYS
1	C	2099	LEU
1	C	2173	GLN
1	C	3033	ARG
1	C	3099	LEU
1	C	3213	ASN

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Mol	Chain	Res	Type
1	C	3214	ALA
1	C	3230	ALA
1	D	88	LYS
1	D	99	LEU
1	D	159	ILE
1	D	238	VAL
1	D	1099	LEU
1	D	1146	VAL
1	D	1159	ILE
1	D	1173	GLN
1	D	1282	LYS
1	D	2099	LEU
1	D	2173	GLN
1	D	3033	ARG
1	D	3099	LEU
1	D	3213	ASN
1	D	3214	ALA
1	D	3230	ALA
1	E	88	LYS
1	E	99	LEU
1	E	158	GLU
1	E	163	HIS
1	E	238	VAL
1	E	1099	LEU
1	E	1146	VAL
1	E	1173	GLN
1	E	1282	LYS
1	E	2099	LEU
1	E	2173	GLN
1	E	3033	ARG
1	E	3099	LEU
1	E	3213	ASN
1	E	3214	ALA
1	E	3230	ALA
1	F	88	LYS
1	F	99	LEU
1	F	158	GLU
1	F	238	VAL
1	F	1099	LEU
1	F	1146	VAL
1	F	1159	ILE
1	F	1161	ASP

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Mol	Chain	Res	Type
1	F	1173	GLN
1	F	1282	LYS
1	F	2099	LEU
1	F	2173	GLN
1	F	3033	ARG
1	F	3099	LEU
1	F	3213	ASN
1	F	3214	ALA
1	F	3230	ALA
1	G	88	LYS
1	G	99	LEU
1	G	163	HIS
1	G	238	VAL
1	G	1099	LEU
1	G	1146	VAL
1	G	1173	GLN
1	G	1282	LYS
1	G	2099	LEU
1	G	2173	GLN
1	G	3033	ARG
1	G	3099	LEU
1	G	3213	ASN
1	G	3214	ALA
1	G	3230	ALA
1	H	88	LYS
1	H	99	LEU
1	H	238	VAL
1	H	1099	LEU
1	H	1146	VAL
1	H	1163	HIS
1	H	1164	MET
1	H	1173	GLN
1	H	1282	LYS
1	H	2099	LEU
1	H	2173	GLN
1	H	3033	ARG
1	H	3099	LEU
1	H	3213	ASN
1	H	3214	ALA
1	H	3230	ALA
1	A	136	GLY
1	A	173	GLN

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Mol	Chain	Res	Type
1	A	1163	HIS
1	A	1167	ALA
1	A	1195	ILE
1	A	2230	ALA
1	A	3282	LYS
1	A	3307	ALA
1	B	136	GLY
1	B	173	GLN
1	B	1167	ALA
1	B	2230	ALA
1	B	3282	LYS
1	B	3306	THR
1	B	3307	ALA
1	C	136	GLY
1	C	159	ILE
1	C	161	ASP
1	C	165	GLY
1	C	173	GLN
1	C	1159	ILE
1	C	1164	MET
1	C	1165	GLY
1	C	1167	ALA
1	C	2230	ALA
1	C	3282	LYS
1	C	3307	ALA
1	D	136	GLY
1	D	173	GLN
1	D	1167	ALA
1	D	2230	ALA
1	D	3282	LYS
1	D	3306	THR
1	D	3307	ALA
1	E	136	GLY
1	E	173	GLN
1	E	1167	ALA
1	E	2230	ALA
1	E	3282	LYS
1	E	3306	THR
1	E	3307	ALA
1	F	136	GLY
1	F	173	GLN
1	F	1164	MET

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Mol	Chain	Res	Type
1	F	1167	ALA
1	F	2230	ALA
1	F	3282	LYS
1	F	3307	ALA
1	G	136	GLY
1	G	173	GLN
1	G	1167	ALA
1	G	2230	ALA
1	G	3282	LYS
1	G	3307	ALA
1	H	136	GLY
1	H	173	GLN
1	H	1160	GLY
1	H	1167	ALA
1	H	2230	ALA
1	H	3282	LYS
1	H	3306	THR
1	H	3307	ALA
1	A	126	LEU
1	A	264	TYR
1	A	1067	PRO
1	A	1160	GLY
1	A	1162	SER
1	A	2294	LYS
1	A	3011	ALA
1	A	3172	SER
1	A	3186	ASN
1	A	3303	ALA
1	A	3306	THR
1	B	126	LEU
1	B	264	TYR
1	B	1067	PRO
1	B	2294	LYS
1	B	3011	ALA
1	B	3186	ASN
1	B	3303	ALA
1	C	126	LEU
1	C	264	TYR
1	C	1067	PRO
1	C	2294	LYS
1	C	3011	ALA
1	C	3172	SER

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Mol	Chain	Res	Type
1	C	3186	ASN
1	C	3303	ALA
1	C	3306	THR
1	D	126	LEU
1	D	163	HIS
1	D	264	TYR
1	D	1067	PRO
1	D	1306	THR
1	D	2294	LYS
1	D	3011	ALA
1	D	3186	ASN
1	D	3303	ALA
1	E	126	LEU
1	E	264	TYR
1	E	1067	PRO
1	E	2294	LYS
1	E	3186	ASN
1	E	3303	ALA
1	F	126	LEU
1	F	264	TYR
1	F	1067	PRO
1	F	2294	LYS
1	F	3011	ALA
1	F	3172	SER
1	F	3186	ASN
1	F	3303	ALA
1	F	3306	THR
1	G	126	LEU
1	G	264	TYR
1	G	1067	PRO
1	G	2294	LYS
1	G	3011	ALA
1	G	3172	SER
1	G	3186	ASN
1	G	3303	ALA
1	G	3306	THR
1	H	126	LEU
1	H	264	TYR
1	H	1067	PRO
1	H	1306	THR
1	H	2294	LYS
1	H	3011	ALA

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Mol	Chain	Res	Type
1	H	3172	SER
1	H	3186	ASN
1	H	3303	ALA
1	A	164	MET
1	A	172	SER
1	A	174	ALA
1	A	1205	ASN
1	A	1306	THR
1	A	1320	GLU
1	A	3014	LEU
1	A	3072	LYS
1	A	3167	ALA
1	B	174	ALA
1	B	1306	THR
1	B	3014	LEU
1	B	3072	LYS
1	B	3146	VAL
1	B	3167	ALA
1	B	3172	SER
1	C	172	SER
1	C	174	ALA
1	C	1306	THR
1	C	3014	LEU
1	C	3072	LYS
1	C	3167	ALA
1	D	174	ALA
1	D	1164	MET
1	D	1320	GLU
1	D	3014	LEU
1	D	3072	LYS
1	D	3167	ALA
1	D	3172	SER
1	E	174	ALA
1	E	1306	THR
1	E	1320	GLU
1	E	3011	ALA
1	E	3014	LEU
1	E	3072	LYS
1	E	3167	ALA
1	E	3172	SER
1	F	163	HIS
1	F	172	SER

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Mol	Chain	Res	Type
1	F	174	ALA
1	F	1306	THR
1	F	1320	GLU
1	F	3014	LEU
1	F	3072	LYS
1	F	3167	ALA
1	G	172	SER
1	G	174	ALA
1	G	1306	THR
1	G	3014	LEU
1	G	3072	LYS
1	G	3167	ALA
1	H	163	HIS
1	H	172	SER
1	H	174	ALA
1	H	1158	GLU
1	H	3014	LEU
1	H	3072	LYS
1	H	3167	ALA
1	A	230	ALA
1	A	1252	ALA
1	A	3146	VAL
1	B	172	SER
1	B	1252	ALA
1	B	1320	GLU
1	B	3088	LYS
1	B	3173	GLN
1	C	118	GLN
1	C	163	HIS
1	C	230	ALA
1	C	1252	ALA
1	C	1320	GLU
1	C	2187	THR
1	C	3146	VAL
1	C	3173	GLN
1	D	118	GLN
1	D	172	SER
1	D	230	ALA
1	D	3146	VAL
1	D	3173	GLN
1	E	118	GLN
1	E	172	SER

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Mol	Chain	Res	Type
1	E	230	ALA
1	E	1252	ALA
1	E	2187	THR
1	E	3088	LYS
1	E	3146	VAL
1	E	3173	GLN
1	F	118	GLN
1	F	230	ALA
1	G	118	GLN
1	G	158	GLU
1	G	230	ALA
1	G	1252	ALA
1	G	1320	GLU
1	G	2187	THR
1	G	3146	VAL
1	G	3173	GLN
1	H	165	GLY
1	H	230	ALA
1	H	1252	ALA
1	H	1320	GLU
1	H	3088	LYS
1	H	3146	VAL
1	H	3173	GLN
1	A	118	GLN
1	A	2252	ALA
1	A	3088	LYS
1	A	3173	GLN
1	B	118	GLN
1	B	230	ALA
1	B	2187	THR
1	C	2252	ALA
1	C	3088	LYS
1	D	1252	ALA
1	D	2187	THR
1	D	3088	LYS
1	E	2252	ALA
1	F	1252	ALA
1	F	2174	ALA
1	F	3146	VAL
1	F	3173	GLN
1	G	2252	ALA
1	G	3088	LYS

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Mol	Chain	Res	Type
1	H	118	GLN
1	H	1174	ALA
1	H	2252	ALA
1	A	1057	PRO
1	B	1057	PRO
1	C	1155	ILE
1	D	1057	PRO
1	E	1057	PRO
1	E	2026	ILE
1	F	1057	PRO
1	G	1057	PRO
1	H	1057	PRO
1	H	3067	PRO
1	A	212	GLY
1	A	2026	ILE
1	B	212	GLY
1	C	212	GLY
1	C	1057	PRO
1	D	212	GLY
1	D	2026	ILE
1	D	3067	PRO
1	E	212	GLY
1	E	3067	PRO
1	F	212	GLY
1	G	212	GLY
1	G	2026	ILE
1	H	212	GLY
1	A	313	PRO
1	A	3067	PRO
1	B	2026	ILE
1	B	3067	PRO
1	C	313	PRO
1	C	2026	ILE
1	F	159	ILE
1	F	2026	ILE
1	F	3067	PRO
1	H	2026	ILE
1	A	3102	ILE
1	A	3212	GLY
1	B	313	PRO
1	B	3212	GLY
1	C	3067	PRO

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Mol	Chain	Res	Type
1	C	3212	GLY
1	D	313	PRO
1	D	3212	GLY
1	E	313	PRO
1	E	3102	ILE
1	E	3212	GLY
1	F	313	PRO
1	F	3212	GLY
1	G	313	PRO
1	G	3067	PRO
1	G	3212	GLY
1	H	313	PRO
1	H	3102	ILE
1	H	3212	GLY
1	A	1200	GLY
1	B	3102	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	930/1065 (87%)	813 (87%)	117 (13%)	4	22
1	B	908/1065 (85%)	801 (88%)	107 (12%)	5	23
1	C	917/1065 (86%)	805 (88%)	112 (12%)	5	23
1	D	917/1065 (86%)	810 (88%)	107 (12%)	5	23
1	E	910/1065 (85%)	801 (88%)	109 (12%)	5	23
1	F	917/1065 (86%)	812 (88%)	105 (12%)	5	24
1	G	911/1065 (86%)	800 (88%)	111 (12%)	5	23
1	H	916/1065 (86%)	806 (88%)	110 (12%)	5	23
All	All	7326/8520 (86%)	6448 (88%)	878 (12%)	5	23

All (878) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	45	LEU
1	A	65	TYR
1	A	72	LYS
1	A	73	THR
1	A	113	ASN
1	A	114	LEU
1	A	116	CYS
1	A	117	SER
1	A	140	VAL
1	A	143	VAL
1	A	149	LEU
1	A	159	ILE
1	A	163	HIS
1	A	164	MET
1	A	173	GLN
1	A	189	LEU
1	A	194	GLN
1	A	223	LEU
1	A	238	VAL
1	A	277	LEU
1	A	1006	LYS
1	A	1023	LYS
1	A	1033	ARG
1	A	1035	MET
1	A	1036	ASP
1	A	1045	LEU
1	A	1065	TYR
1	A	1070	SER
1	A	1073	THR
1	A	1078	GLN
1	A	1079	VAL
1	A	1116	CYS
1	A	1123	GLU
1	A	1141	ILE
1	A	1149	LEU
1	A	1150	THR
1	A	1152	LYS
1	A	1156	GLU
1	A	1159	ILE
1	A	1161	ASP
1	A	1170	MET
1	A	1173	GLN

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Mol	Chain	Res	Type
1	A	1176	ARG
1	A	1192	ILE
1	A	1201	VAL
1	A	1207	GLU
1	A	1210	THR
1	A	1221	VAL
1	A	1231	VAL
1	A	1247	VAL
1	A	1270	PHE
1	A	1277	LEU
1	A	1282	LYS
1	A	1284	ILE
1	A	1296	GLU
1	A	1312	ASN
1	A	1314	GLU
1	A	1317	LYS
1	A	2016	GLN
1	A	2023	LYS
1	A	2025	SER
1	A	2036	ASP
1	A	2045	LEU
1	A	2065	TYR
1	A	2073	THR
1	A	2076	THR
1	A	2078	GLN
1	A	2089	THR
1	A	2090	CYS
1	A	2130	ASP
1	A	2140	VAL
1	A	2149	LEU
1	A	2152	LYS
1	A	2166	LEU
1	A	2223	LEU
1	A	2235	GLU
1	A	2236	ASN
1	A	2247	VAL
1	A	2264	TYR
1	A	2296	GLU
1	A	2311	ASP
1	A	2312	ASN
1	A	2315	THR
1	A	3006	LYS

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Mol	Chain	Res	Type
1	A	3032	ASP
1	A	3036	ASP
1	A	3045	LEU
1	A	3048	ASP
1	A	3065	TYR
1	A	3068	GLU
1	A	3072	LYS
1	A	3077	LEU
1	A	3089	THR
1	A	3099	LEU
1	A	3107	LEU
1	A	3112	ASP
1	A	3114	LEU
1	A	3127	GLU
1	A	3135	SER
1	A	3143	VAL
1	A	3166	LEU
1	A	3173	GLN
1	A	3184	GLN
1	A	3186	ASN
1	A	3189	LEU
1	A	3218	TYR
1	A	3223	LEU
1	A	3236	ASN
1	A	3237	VAL
1	A	3247	VAL
1	A	3254	PRO
1	A	3270	PHE
1	A	3274	LEU
1	A	3296	GLU
1	A	3311	ASP
1	A	3326	LEU
1	B	37	VAL
1	B	45	LEU
1	B	65	TYR
1	B	72	LYS
1	B	73	THR
1	B	113	ASN
1	B	114	LEU
1	B	116	CYS
1	B	117	SER
1	B	140	VAL

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Mol	Chain	Res	Type
1	B	143	VAL
1	B	149	LEU
1	B	156	GLU
1	B	163	HIS
1	B	164	MET
1	B	173	GLN
1	B	189	LEU
1	B	194	GLN
1	B	223	LEU
1	B	238	VAL
1	B	277	LEU
1	B	1006	LYS
1	B	1023	LYS
1	B	1033	ARG
1	B	1035	MET
1	B	1036	ASP
1	B	1045	LEU
1	B	1065	TYR
1	B	1073	THR
1	B	1078	GLN
1	B	1079	VAL
1	B	1116	CYS
1	B	1123	GLU
1	B	1141	ILE
1	B	1149	LEU
1	B	1150	THR
1	B	1152	LYS
1	B	1170	MET
1	B	1173	GLN
1	B	1176	ARG
1	B	1192	ILE
1	B	1221	VAL
1	B	1231	VAL
1	B	1247	VAL
1	B	1270	PHE
1	B	1277	LEU
1	B	1282	LYS
1	B	1284	ILE
1	B	1296	GLU
1	B	1312	ASN
1	B	1314	GLU
1	B	1317	LYS

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Mol	Chain	Res	Type
1	B	2016	GLN
1	B	2023	LYS
1	B	2025	SER
1	B	2036	ASP
1	B	2045	LEU
1	B	2065	TYR
1	B	2073	THR
1	B	2076	THR
1	B	2078	GLN
1	B	2089	THR
1	B	2090	CYS
1	B	2130	ASP
1	B	2140	VAL
1	B	2149	LEU
1	B	2152	LYS
1	B	2166	LEU
1	B	2223	LEU
1	B	2235	GLU
1	B	2236	ASN
1	B	2247	VAL
1	B	2264	TYR
1	B	2296	GLU
1	B	2311	ASP
1	B	2312	ASN
1	B	2315	THR
1	B	3006	LYS
1	B	3032	ASP
1	B	3036	ASP
1	B	3045	LEU
1	B	3048	ASP
1	B	3065	TYR
1	B	3068	GLU
1	B	3072	LYS
1	B	3077	LEU
1	B	3099	LEU
1	B	3107	LEU
1	B	3114	LEU
1	B	3127	GLU
1	B	3135	SER
1	B	3143	VAL
1	B	3166	LEU
1	B	3173	GLN

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Mol	Chain	Res	Type
1	B	3184	GLN
1	B	3186	ASN
1	B	3189	LEU
1	B	3223	LEU
1	B	3236	ASN
1	B	3237	VAL
1	B	3247	VAL
1	B	3254	PRO
1	B	3270	PHE
1	B	3274	LEU
1	B	3296	GLU
1	B	3311	ASP
1	B	3326	LEU
1	C	37	VAL
1	C	45	LEU
1	C	65	TYR
1	C	72	LYS
1	C	73	THR
1	C	113	ASN
1	C	114	LEU
1	C	116	CYS
1	C	117	SER
1	C	140	VAL
1	C	143	VAL
1	C	149	LEU
1	C	159	ILE
1	C	162	SER
1	C	164	MET
1	C	173	GLN
1	C	189	LEU
1	C	194	GLN
1	C	223	LEU
1	C	238	VAL
1	C	277	LEU
1	C	1006	LYS
1	C	1023	LYS
1	C	1033	ARG
1	C	1035	MET
1	C	1036	ASP
1	C	1045	LEU
1	C	1065	TYR
1	C	1073	THR

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Mol	Chain	Res	Type
1	C	1078	GLN
1	C	1079	VAL
1	C	1116	CYS
1	C	1123	GLU
1	C	1141	ILE
1	C	1150	THR
1	C	1152	LYS
1	C	1158	GLU
1	C	1159	ILE
1	C	1164	MET
1	C	1170	MET
1	C	1173	GLN
1	C	1176	ARG
1	C	1192	ILE
1	C	1221	VAL
1	C	1231	VAL
1	C	1247	VAL
1	C	1270	PHE
1	C	1277	LEU
1	C	1282	LYS
1	C	1284	ILE
1	C	1296	GLU
1	C	1312	ASN
1	C	1314	GLU
1	C	1317	LYS
1	C	2016	GLN
1	C	2023	LYS
1	C	2025	SER
1	C	2036	ASP
1	C	2045	LEU
1	C	2065	TYR
1	C	2073	THR
1	C	2076	THR
1	C	2078	GLN
1	C	2089	THR
1	C	2090	CYS
1	C	2130	ASP
1	C	2140	VAL
1	C	2149	LEU
1	C	2152	LYS
1	C	2156	GLU
1	C	2166	LEU

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Mol	Chain	Res	Type
1	C	2223	LEU
1	C	2235	GLU
1	C	2236	ASN
1	C	2247	VAL
1	C	2264	TYR
1	C	2296	GLU
1	C	2311	ASP
1	C	2312	ASN
1	C	2315	THR
1	C	3006	LYS
1	C	3032	ASP
1	C	3036	ASP
1	C	3045	LEU
1	C	3048	ASP
1	C	3065	TYR
1	C	3068	GLU
1	C	3072	LYS
1	C	3077	LEU
1	C	3099	LEU
1	C	3107	LEU
1	C	3112	ASP
1	C	3114	LEU
1	C	3127	GLU
1	C	3135	SER
1	C	3143	VAL
1	C	3166	LEU
1	C	3173	GLN
1	C	3184	GLN
1	C	3186	ASN
1	C	3189	LEU
1	C	3218	TYR
1	C	3223	LEU
1	C	3236	ASN
1	C	3237	VAL
1	C	3247	VAL
1	C	3254	PRO
1	C	3270	PHE
1	C	3274	LEU
1	C	3296	GLU
1	C	3311	ASP
1	C	3326	LEU
1	D	37	VAL

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Mol	Chain	Res	Type
1	D	45	LEU
1	D	65	TYR
1	D	72	LYS
1	D	73	THR
1	D	113	ASN
1	D	114	LEU
1	D	116	CYS
1	D	117	SER
1	D	140	VAL
1	D	143	VAL
1	D	149	LEU
1	D	161	ASP
1	D	164	MET
1	D	173	GLN
1	D	189	LEU
1	D	194	GLN
1	D	223	LEU
1	D	238	VAL
1	D	277	LEU
1	D	1006	LYS
1	D	1023	LYS
1	D	1033	ARG
1	D	1035	MET
1	D	1036	ASP
1	D	1045	LEU
1	D	1065	TYR
1	D	1073	THR
1	D	1078	GLN
1	D	1079	VAL
1	D	1116	CYS
1	D	1123	GLU
1	D	1141	ILE
1	D	1149	LEU
1	D	1150	THR
1	D	1152	LYS
1	D	1164	MET
1	D	1170	MET
1	D	1173	GLN
1	D	1176	ARG
1	D	1192	ILE
1	D	1221	VAL
1	D	1231	VAL

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Mol	Chain	Res	Type
1	D	1247	VAL
1	D	1270	PHE
1	D	1277	LEU
1	D	1282	LYS
1	D	1284	ILE
1	D	1296	GLU
1	D	1312	ASN
1	D	1314	GLU
1	D	1317	LYS
1	D	2016	GLN
1	D	2023	LYS
1	D	2025	SER
1	D	2036	ASP
1	D	2045	LEU
1	D	2065	TYR
1	D	2073	THR
1	D	2076	THR
1	D	2078	GLN
1	D	2089	THR
1	D	2090	CYS
1	D	2130	ASP
1	D	2140	VAL
1	D	2149	LEU
1	D	2152	LYS
1	D	2166	LEU
1	D	2223	LEU
1	D	2235	GLU
1	D	2236	ASN
1	D	2247	VAL
1	D	2264	TYR
1	D	2296	GLU
1	D	2311	ASP
1	D	2312	ASN
1	D	2315	THR
1	D	3006	LYS
1	D	3032	ASP
1	D	3036	ASP
1	D	3045	LEU
1	D	3048	ASP
1	D	3065	TYR
1	D	3068	GLU
1	D	3072	LYS

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Mol	Chain	Res	Type
1	D	3077	LEU
1	D	3089	THR
1	D	3099	LEU
1	D	3107	LEU
1	D	3114	LEU
1	D	3127	GLU
1	D	3135	SER
1	D	3143	VAL
1	D	3166	LEU
1	D	3173	GLN
1	D	3184	GLN
1	D	3186	ASN
1	D	3189	LEU
1	D	3223	LEU
1	D	3236	ASN
1	D	3237	VAL
1	D	3247	VAL
1	D	3270	PHE
1	D	3274	LEU
1	D	3296	GLU
1	D	3311	ASP
1	D	3326	LEU
1	E	37	VAL
1	E	45	LEU
1	E	65	TYR
1	E	72	LYS
1	E	73	THR
1	E	113	ASN
1	E	114	LEU
1	E	116	CYS
1	E	117	SER
1	E	140	VAL
1	E	143	VAL
1	E	149	LEU
1	E	156	GLU
1	E	158	GLU
1	E	159	ILE
1	E	162	SER
1	E	164	MET
1	E	173	GLN
1	E	189	LEU
1	E	194	GLN

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Mol	Chain	Res	Type
1	E	223	LEU
1	E	238	VAL
1	E	277	LEU
1	E	1006	LYS
1	E	1023	LYS
1	E	1033	ARG
1	E	1035	MET
1	E	1036	ASP
1	E	1045	LEU
1	E	1065	TYR
1	E	1073	THR
1	E	1078	GLN
1	E	1079	VAL
1	E	1116	CYS
1	E	1123	GLU
1	E	1141	ILE
1	E	1149	LEU
1	E	1150	THR
1	E	1152	LYS
1	E	1170	MET
1	E	1173	GLN
1	E	1176	ARG
1	E	1192	ILE
1	E	1221	VAL
1	E	1231	VAL
1	E	1247	VAL
1	E	1270	PHE
1	E	1277	LEU
1	E	1282	LYS
1	E	1284	ILE
1	E	1296	GLU
1	E	1312	ASN
1	E	1314	GLU
1	E	1317	LYS
1	E	2016	GLN
1	E	2023	LYS
1	E	2025	SER
1	E	2036	ASP
1	E	2045	LEU
1	E	2065	TYR
1	E	2073	THR
1	E	2076	THR

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Mol	Chain	Res	Type
1	E	2078	GLN
1	E	2089	THR
1	E	2090	CYS
1	E	2130	ASP
1	E	2140	VAL
1	E	2149	LEU
1	E	2152	LYS
1	E	2166	LEU
1	E	2223	LEU
1	E	2235	GLU
1	E	2236	ASN
1	E	2247	VAL
1	E	2264	TYR
1	E	2296	GLU
1	E	2311	ASP
1	E	2312	ASN
1	E	2315	THR
1	E	3006	LYS
1	E	3032	ASP
1	E	3036	ASP
1	E	3045	LEU
1	E	3048	ASP
1	E	3065	TYR
1	E	3068	GLU
1	E	3072	LYS
1	E	3077	LEU
1	E	3099	LEU
1	E	3107	LEU
1	E	3112	ASP
1	E	3114	LEU
1	E	3127	GLU
1	E	3135	SER
1	E	3143	VAL
1	E	3166	LEU
1	E	3173	GLN
1	E	3184	GLN
1	E	3186	ASN
1	E	3189	LEU
1	E	3223	LEU
1	E	3236	ASN
1	E	3237	VAL
1	E	3247	VAL

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Mol	Chain	Res	Type
1	E	3254	PRO
1	E	3270	PHE
1	E	3274	LEU
1	E	3296	GLU
1	E	3311	ASP
1	F	37	VAL
1	F	45	LEU
1	F	65	TYR
1	F	72	LYS
1	F	73	THR
1	F	113	ASN
1	F	114	LEU
1	F	116	CYS
1	F	117	SER
1	F	140	VAL
1	F	143	VAL
1	F	149	LEU
1	F	173	GLN
1	F	189	LEU
1	F	194	GLN
1	F	223	LEU
1	F	238	VAL
1	F	277	LEU
1	F	1006	LYS
1	F	1023	LYS
1	F	1033	ARG
1	F	1035	MET
1	F	1036	ASP
1	F	1045	LEU
1	F	1065	TYR
1	F	1073	THR
1	F	1078	GLN
1	F	1079	VAL
1	F	1116	CYS
1	F	1123	GLU
1	F	1141	ILE
1	F	1149	LEU
1	F	1150	THR
1	F	1152	LYS
1	F	1161	ASP
1	F	1170	MET
1	F	1173	GLN

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Mol	Chain	Res	Type
1	F	1176	ARG
1	F	1221	VAL
1	F	1231	VAL
1	F	1247	VAL
1	F	1270	PHE
1	F	1277	LEU
1	F	1282	LYS
1	F	1284	ILE
1	F	1296	GLU
1	F	1312	ASN
1	F	1314	GLU
1	F	1317	LYS
1	F	2016	GLN
1	F	2023	LYS
1	F	2025	SER
1	F	2036	ASP
1	F	2045	LEU
1	F	2065	TYR
1	F	2073	THR
1	F	2076	THR
1	F	2078	GLN
1	F	2089	THR
1	F	2090	CYS
1	F	2130	ASP
1	F	2140	VAL
1	F	2149	LEU
1	F	2152	LYS
1	F	2166	LEU
1	F	2223	LEU
1	F	2235	GLU
1	F	2236	ASN
1	F	2247	VAL
1	F	2264	TYR
1	F	2296	GLU
1	F	2311	ASP
1	F	2312	ASN
1	F	2315	THR
1	F	3006	LYS
1	F	3032	ASP
1	F	3036	ASP
1	F	3045	LEU
1	F	3048	ASP

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Mol	Chain	Res	Type
1	F	3065	TYR
1	F	3068	GLU
1	F	3072	LYS
1	F	3077	LEU
1	F	3099	LEU
1	F	3107	LEU
1	F	3112	ASP
1	F	3114	LEU
1	F	3127	GLU
1	F	3135	SER
1	F	3143	VAL
1	F	3166	LEU
1	F	3173	GLN
1	F	3184	GLN
1	F	3186	ASN
1	F	3189	LEU
1	F	3223	LEU
1	F	3236	ASN
1	F	3237	VAL
1	F	3247	VAL
1	F	3254	PRO
1	F	3270	PHE
1	F	3274	LEU
1	F	3296	GLU
1	F	3311	ASP
1	F	3326	LEU
1	G	37	VAL
1	G	45	LEU
1	G	65	TYR
1	G	72	LYS
1	G	73	THR
1	G	113	ASN
1	G	114	LEU
1	G	116	CYS
1	G	117	SER
1	G	140	VAL
1	G	143	VAL
1	G	149	LEU
1	G	159	ILE
1	G	162	SER
1	G	163	HIS
1	G	173	GLN

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Mol	Chain	Res	Type
1	G	189	LEU
1	G	194	GLN
1	G	223	LEU
1	G	238	VAL
1	G	277	LEU
1	G	1006	LYS
1	G	1023	LYS
1	G	1033	ARG
1	G	1035	MET
1	G	1036	ASP
1	G	1045	LEU
1	G	1065	TYR
1	G	1073	THR
1	G	1078	GLN
1	G	1079	VAL
1	G	1116	CYS
1	G	1123	GLU
1	G	1141	ILE
1	G	1149	LEU
1	G	1150	THR
1	G	1152	LYS
1	G	1170	MET
1	G	1173	GLN
1	G	1176	ARG
1	G	1192	ILE
1	G	1221	VAL
1	G	1231	VAL
1	G	1247	VAL
1	G	1270	PHE
1	G	1277	LEU
1	G	1282	LYS
1	G	1284	ILE
1	G	1296	GLU
1	G	1312	ASN
1	G	1314	GLU
1	G	1317	LYS
1	G	2016	GLN
1	G	2023	LYS
1	G	2025	SER
1	G	2036	ASP
1	G	2045	LEU
1	G	2065	TYR

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Mol	Chain	Res	Type
1	G	2073	THR
1	G	2076	THR
1	G	2078	GLN
1	G	2079	VAL
1	G	2089	THR
1	G	2090	CYS
1	G	2130	ASP
1	G	2140	VAL
1	G	2149	LEU
1	G	2152	LYS
1	G	2166	LEU
1	G	2223	LEU
1	G	2235	GLU
1	G	2236	ASN
1	G	2247	VAL
1	G	2264	TYR
1	G	2296	GLU
1	G	2311	ASP
1	G	2312	ASN
1	G	2315	THR
1	G	3006	LYS
1	G	3032	ASP
1	G	3036	ASP
1	G	3045	LEU
1	G	3048	ASP
1	G	3065	TYR
1	G	3068	GLU
1	G	3072	LYS
1	G	3077	LEU
1	G	3089	THR
1	G	3099	LEU
1	G	3107	LEU
1	G	3112	ASP
1	G	3114	LEU
1	G	3127	GLU
1	G	3135	SER
1	G	3143	VAL
1	G	3166	LEU
1	G	3173	GLN
1	G	3184	GLN
1	G	3186	ASN
1	G	3189	LEU

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Mol	Chain	Res	Type
1	G	3218	TYR
1	G	3223	LEU
1	G	3236	ASN
1	G	3237	VAL
1	G	3247	VAL
1	G	3254	PRO
1	G	3270	PHE
1	G	3274	LEU
1	G	3296	GLU
1	G	3311	ASP
1	G	3326	LEU
1	H	37	VAL
1	H	45	LEU
1	H	65	TYR
1	H	72	LYS
1	H	73	THR
1	H	113	ASN
1	H	114	LEU
1	H	116	CYS
1	H	117	SER
1	H	140	VAL
1	H	143	VAL
1	H	149	LEU
1	H	158	GLU
1	H	159	ILE
1	H	164	MET
1	H	173	GLN
1	H	189	LEU
1	H	194	GLN
1	H	223	LEU
1	H	238	VAL
1	H	277	LEU
1	H	1006	LYS
1	H	1023	LYS
1	H	1033	ARG
1	H	1035	MET
1	H	1036	ASP
1	H	1045	LEU
1	H	1065	TYR
1	H	1073	THR
1	H	1078	GLN
1	H	1079	VAL

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Mol	Chain	Res	Type
1	H	1116	CYS
1	H	1123	GLU
1	H	1141	ILE
1	H	1149	LEU
1	H	1150	THR
1	H	1152	LYS
1	H	1162	SER
1	H	1163	HIS
1	H	1170	MET
1	H	1173	GLN
1	H	1176	ARG
1	H	1192	ILE
1	H	1221	VAL
1	H	1231	VAL
1	H	1247	VAL
1	H	1270	PHE
1	H	1277	LEU
1	H	1282	LYS
1	H	1284	ILE
1	H	1296	GLU
1	H	1312	ASN
1	H	1314	GLU
1	H	1317	LYS
1	H	2016	GLN
1	H	2023	LYS
1	H	2025	SER
1	H	2036	ASP
1	H	2045	LEU
1	H	2065	TYR
1	H	2073	THR
1	H	2076	THR
1	H	2078	GLN
1	H	2089	THR
1	H	2090	CYS
1	H	2130	ASP
1	H	2140	VAL
1	H	2149	LEU
1	H	2152	LYS
1	H	2166	LEU
1	H	2223	LEU
1	H	2235	GLU
1	H	2236	ASN

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Mol	Chain	Res	Type
1	H	2247	VAL
1	H	2264	TYR
1	H	2296	GLU
1	H	2311	ASP
1	H	2312	ASN
1	H	2315	THR
1	H	3006	LYS
1	H	3032	ASP
1	H	3036	ASP
1	H	3045	LEU
1	H	3048	ASP
1	H	3065	TYR
1	H	3068	GLU
1	H	3072	LYS
1	H	3077	LEU
1	H	3099	LEU
1	H	3107	LEU
1	H	3112	ASP
1	H	3114	LEU
1	H	3127	GLU
1	H	3135	SER
1	H	3143	VAL
1	H	3166	LEU
1	H	3173	GLN
1	H	3184	GLN
1	H	3186	ASN
1	H	3189	LEU
1	H	3223	LEU
1	H	3236	ASN
1	H	3237	VAL
1	H	3247	VAL
1	H	3254	PRO
1	H	3270	PHE
1	H	3274	LEU
1	H	3296	GLU
1	H	3311	ASP
1	H	3326	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS

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Mol	Chain	Res	Type
1	A	118	GLN
1	A	173	GLN
1	A	181	ASN
1	A	1193	ASN
1	A	1213	ASN
1	A	1300	GLN
1	A	2020	GLN
1	A	2118	GLN
1	A	2181	ASN
1	A	2236	ASN
1	A	2300	GLN
1	A	3124	GLN
1	A	3181	ASN
1	A	3300	GLN
1	A	3304	ASN
1	B	97	HIS
1	B	118	GLN
1	B	173	GLN
1	B	181	ASN
1	B	1118	GLN
1	B	1300	GLN
1	B	2118	GLN
1	B	2181	ASN
1	B	2236	ASN
1	B	2300	GLN
1	B	3124	GLN
1	B	3181	ASN
1	B	3300	GLN
1	B	3304	ASN
1	C	97	HIS
1	C	118	GLN
1	C	173	GLN
1	C	181	ASN
1	C	1118	GLN
1	C	1300	GLN
1	C	2020	GLN
1	C	2118	GLN
1	C	2181	ASN
1	C	2236	ASN
1	C	2300	GLN
1	C	3124	GLN
1	C	3181	ASN

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Mol	Chain	Res	Type
1	C	3300	GLN
1	C	3304	ASN
1	D	173	GLN
1	D	181	ASN
1	D	1118	GLN
1	D	1300	GLN
1	D	2118	GLN
1	D	2181	ASN
1	D	2236	ASN
1	D	2300	GLN
1	D	3124	GLN
1	D	3181	ASN
1	D	3300	GLN
1	D	3304	ASN
1	E	97	HIS
1	E	118	GLN
1	E	173	GLN
1	E	181	ASN
1	E	1118	GLN
1	E	1300	GLN
1	E	2118	GLN
1	E	2181	ASN
1	E	2236	ASN
1	E	2300	GLN
1	E	3124	GLN
1	E	3181	ASN
1	E	3300	GLN
1	E	3304	ASN
1	F	97	HIS
1	F	118	GLN
1	F	173	GLN
1	F	181	ASN
1	F	1163	HIS
1	F	1213	ASN
1	F	1300	GLN
1	F	2020	GLN
1	F	2118	GLN
1	F	2181	ASN
1	F	2236	ASN
1	F	2300	GLN
1	F	3113	ASN
1	F	3124	GLN

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Mol	Chain	Res	Type
1	F	3181	ASN
1	F	3300	GLN
1	F	3304	ASN
1	G	97	HIS
1	G	118	GLN
1	G	173	GLN
1	G	181	ASN
1	G	1118	GLN
1	G	1300	GLN
1	G	2118	GLN
1	G	2181	ASN
1	G	2236	ASN
1	G	2300	GLN
1	G	3124	GLN
1	G	3181	ASN
1	G	3300	GLN
1	G	3304	ASN
1	H	97	HIS
1	H	118	GLN
1	H	173	GLN
1	H	181	ASN
1	H	1213	ASN
1	H	1300	GLN
1	H	2020	GLN
1	H	2118	GLN
1	H	2181	ASN
1	H	2236	ASN
1	H	2300	GLN
1	H	3124	GLN
1	H	3181	ASN
1	H	3300	GLN
1	H	3304	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 64 ligands modelled in this entry, 32 are monoatomic - leaving 32 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ANP	B	2400	-	29,33,33	2.01	8 (27%)	31,52,52	2.00	7 (22%)
3	ANP	D	400	-	29,33,33	2.07	11 (37%)	31,52,52	1.85	8 (25%)
3	ANP	G	2400	-	29,33,33	2.06	8 (27%)	31,52,52	1.99	7 (22%)
3	ANP	B	3400	-	29,33,33	1.95	7 (24%)	31,52,52	2.43	9 (29%)
3	ANP	E	2400	-	29,33,33	2.07	9 (31%)	31,52,52	1.99	7 (22%)
3	ANP	F	400	-	29,33,33	1.95	8 (27%)	31,52,52	1.85	7 (22%)
3	ANP	C	2400	-	29,33,33	1.96	7 (24%)	31,52,52	1.99	7 (22%)
3	ANP	C	1400	-	29,33,33	2.11	8 (27%)	31,52,52	2.02	8 (25%)
3	ANP	D	3400	-	29,33,33	1.99	8 (27%)	31,52,52	2.37	8 (25%)
3	ANP	E	1400	-	29,33,33	2.05	9 (31%)	31,52,52	1.99	7 (22%)
3	ANP	D	1400	-	29,33,33	1.99	7 (24%)	31,52,52	1.97	8 (25%)
3	ANP	H	2400	-	29,33,33	2.01	11 (37%)	31,52,52	1.99	7 (22%)
3	ANP	A	400	-	29,33,33	2.07	9 (31%)	31,52,52	1.84	7 (22%)
3	ANP	H	3400	-	29,33,33	2.07	8 (27%)	31,52,52	2.44	9 (29%)
3	ANP	C	3400	-	29,33,33	2.14	8 (27%)	31,52,52	2.30	9 (29%)
3	ANP	G	1400	-	29,33,33	2.01	7 (24%)	31,52,52	1.95	8 (25%)
3	ANP	E	400	-	29,33,33	2.00	9 (31%)	31,52,52	1.86	8 (25%)
3	ANP	G	400	-	29,33,33	1.99	7 (24%)	31,52,52	1.89	7 (22%)
3	ANP	E	3400	2	29,33,33	1.81	8 (27%)	31,52,52	2.40	10 (32%)
3	ANP	A	3400	-	29,33,33	1.96	7 (24%)	31,52,52	2.35	9 (29%)
3	ANP	G	3400	-	29,33,33	2.11	8 (27%)	31,52,52	2.32	8 (25%)
3	ANP	F	1400	-	29,33,33	2.10	9 (31%)	31,52,52	2.01	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ANP	C	400	-	29,33,33	1.85	7 (24%)	31,52,52	1.91	7 (22%)
3	ANP	F	3400	-	29,33,33	1.98	10 (34%)	31,52,52	2.34	9 (29%)
3	ANP	H	400	-	29,33,33	1.96	8 (27%)	31,52,52	1.84	7 (22%)
3	ANP	A	1400	-	29,33,33	1.95	10 (34%)	31,52,52	1.96	7 (22%)
3	ANP	F	2400	-	29,33,33	1.91	9 (31%)	31,52,52	1.99	7 (22%)
3	ANP	B	1400	-	29,33,33	2.00	7 (24%)	31,52,52	2.02	7 (22%)
3	ANP	B	400	-	29,33,33	2.01	8 (27%)	31,52,52	1.83	9 (29%)
3	ANP	H	1400	-	29,33,33	2.09	8 (27%)	31,52,52	1.91	8 (25%)
3	ANP	D	2400	-	29,33,33	2.02	8 (27%)	31,52,52	1.98	7 (22%)
3	ANP	A	2400	-	29,33,33	2.04	8 (27%)	31,52,52	2.01	7 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	B	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	D	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	G	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	B	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	E	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	F	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	C	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	C	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	D	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	E	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	D	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	H	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	A	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	H	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	C	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	G	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	E	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	G	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	E	3400	2	1/1/7/8	7/14/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	G	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	F	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	C	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	F	3400	-	1/1/7/8	7/14/38/38	0/3/3/3
3	ANP	H	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	A	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	F	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	B	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	B	400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	H	1400	-	1/1/7/8	10/14/38/38	0/3/3/3
3	ANP	D	2400	-	1/1/7/8	9/14/38/38	0/3/3/3
3	ANP	A	2400	-	1/1/7/8	9/14/38/38	0/3/3/3

All (264) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3400	ANP	PG-N3B	5.90	1.78	1.63
3	H	3400	ANP	PG-N3B	5.54	1.77	1.63
3	G	3400	ANP	PG-N3B	5.49	1.77	1.63
3	C	3400	ANP	PB-N3B	5.45	1.77	1.63
3	G	3400	ANP	PB-N3B	5.33	1.77	1.63
3	H	1400	ANP	PG-N3B	5.30	1.77	1.63
3	H	3400	ANP	PB-N3B	5.27	1.77	1.63
3	G	2400	ANP	PG-N3B	5.27	1.77	1.63
3	B	1400	ANP	PG-N3B	5.25	1.77	1.63
3	C	1400	ANP	PG-N3B	5.23	1.77	1.63
3	D	3400	ANP	PG-N3B	5.20	1.76	1.63
3	D	2400	ANP	PG-N3B	5.20	1.76	1.63
3	A	2400	ANP	PG-N3B	5.17	1.76	1.63
3	E	2400	ANP	PG-N3B	5.16	1.76	1.63
3	B	2400	ANP	PG-N3B	5.14	1.76	1.63
3	H	2400	ANP	PG-N3B	5.06	1.76	1.63
3	G	400	ANP	PG-N3B	5.06	1.76	1.63
3	F	1400	ANP	PG-N3B	5.05	1.76	1.63
3	D	400	ANP	PB-N3B	5.05	1.76	1.63
3	E	400	ANP	PG-N3B	5.04	1.76	1.63
3	B	3400	ANP	PG-N3B	5.03	1.76	1.63
3	B	400	ANP	PG-N3B	5.00	1.76	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	ANP	PB-N3B	4.99	1.76	1.63
3	C	2400	ANP	PG-N3B	4.99	1.76	1.63
3	D	400	ANP	PG-N3B	4.96	1.76	1.63
3	D	1400	ANP	PG-N3B	4.95	1.76	1.63
3	C	1400	ANP	PB-N3B	4.93	1.76	1.63
3	H	400	ANP	PG-N3B	4.91	1.76	1.63
3	H	1400	ANP	PB-N3B	4.90	1.76	1.63
3	E	1400	ANP	PG-N3B	4.90	1.76	1.63
3	E	2400	ANP	PB-N3B	4.86	1.76	1.63
3	A	400	ANP	PG-N3B	4.86	1.76	1.63
3	A	2400	ANP	PB-N3B	4.83	1.76	1.63
3	F	1400	ANP	PB-N3B	4.83	1.76	1.63
3	F	2400	ANP	PG-N3B	4.81	1.75	1.63
3	E	1400	ANP	PB-N3B	4.80	1.75	1.63
3	G	1400	ANP	PG-N3B	4.80	1.75	1.63
3	F	3400	ANP	PB-N3B	4.78	1.75	1.63
3	G	2400	ANP	PB-N3B	4.77	1.75	1.63
3	E	400	ANP	PB-N3B	4.77	1.75	1.63
3	G	400	ANP	PB-N3B	4.74	1.75	1.63
3	B	2400	ANP	PB-N3B	4.73	1.75	1.63
3	F	400	ANP	PG-N3B	4.73	1.75	1.63
3	B	3400	ANP	PB-N3B	4.71	1.75	1.63
3	H	2400	ANP	PB-N3B	4.70	1.75	1.63
3	D	2400	ANP	PB-N3B	4.69	1.75	1.63
3	A	1400	ANP	PG-N3B	4.66	1.75	1.63
3	E	3400	ANP	PG-N3B	4.63	1.75	1.63
3	F	3400	ANP	PG-N3B	4.61	1.75	1.63
3	C	400	ANP	PG-N3B	4.61	1.75	1.63
3	D	1400	ANP	PB-N3B	4.59	1.75	1.63
3	B	1400	ANP	PB-N3B	4.58	1.75	1.63
3	C	2400	ANP	PB-N3B	4.55	1.75	1.63
3	G	1400	ANP	PB-N3B	4.52	1.75	1.63
3	H	400	ANP	PB-N3B	4.49	1.75	1.63
3	F	2400	ANP	PB-N3B	4.42	1.74	1.63
3	F	400	ANP	PB-N3B	4.40	1.74	1.63
3	B	400	ANP	PB-N3B	4.29	1.74	1.63
3	A	3400	ANP	PG-N3B	4.28	1.74	1.63
3	A	1400	ANP	PB-N3B	4.27	1.74	1.63
3	A	3400	ANP	PB-N3B	4.27	1.74	1.63
3	D	3400	ANP	PB-N3B	4.17	1.74	1.63
3	E	3400	ANP	PB-N3B	4.15	1.74	1.63
3	C	400	ANP	PB-N3B	3.96	1.73	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3400	ANP	PG-O1G	3.94	1.52	1.46
3	G	3400	ANP	PG-O1G	3.92	1.52	1.46
3	C	1400	ANP	PG-O1G	3.77	1.52	1.46
3	C	3400	ANP	PG-O1G	3.73	1.52	1.46
3	G	1400	ANP	PG-O1G	3.73	1.52	1.46
3	C	1400	ANP	PB-O1B	3.70	1.52	1.46
3	G	2400	ANP	PB-O1B	3.70	1.52	1.46
3	A	400	ANP	PG-O1G	3.69	1.52	1.46
3	F	1400	ANP	PG-O1G	3.66	1.52	1.46
3	E	1400	ANP	PG-O1G	3.64	1.51	1.46
3	D	3400	ANP	PG-O1G	3.61	1.51	1.46
3	A	2400	ANP	PG-O1G	3.58	1.51	1.46
3	H	1400	ANP	PB-O1B	3.57	1.51	1.46
3	A	3400	ANP	C5-C4	3.55	1.50	1.40
3	H	1400	ANP	PG-O1G	3.55	1.51	1.46
3	E	400	ANP	PG-O1G	3.50	1.51	1.46
3	F	3400	ANP	PG-O1G	3.48	1.51	1.46
3	B	1400	ANP	PG-O1G	3.47	1.51	1.46
3	H	3400	ANP	PG-O1G	3.46	1.51	1.46
3	B	3400	ANP	C2-N3	3.46	1.37	1.32
3	E	2400	ANP	PG-O1G	3.43	1.51	1.46
3	B	3400	ANP	PG-O1G	3.43	1.51	1.46
3	D	3400	ANP	C5-C4	3.42	1.50	1.40
3	B	2400	ANP	PG-O1G	3.42	1.51	1.46
3	B	1400	ANP	PB-O1B	3.41	1.51	1.46
3	B	400	ANP	PB-O1B	3.41	1.51	1.46
3	D	1400	ANP	PB-O1B	3.40	1.51	1.46
3	E	2400	ANP	PB-O1B	3.40	1.51	1.46
3	F	1400	ANP	PB-O1B	3.39	1.51	1.46
3	G	1400	ANP	PB-O1B	3.39	1.51	1.46
3	B	400	ANP	PG-O1G	3.38	1.51	1.46
3	G	3400	ANP	C5-C4	3.38	1.49	1.40
3	C	3400	ANP	C5-C4	3.37	1.49	1.40
3	A	2400	ANP	PB-O1B	3.36	1.51	1.46
3	H	400	ANP	PG-O1G	3.36	1.51	1.46
3	E	3400	ANP	PG-O1G	3.35	1.51	1.46
3	C	2400	ANP	PG-O1G	3.35	1.51	1.46
3	D	400	ANP	PB-O1B	3.34	1.51	1.46
3	A	1400	ANP	PB-O1B	3.32	1.51	1.46
3	D	2400	ANP	PG-O1G	3.32	1.51	1.46
3	B	2400	ANP	PB-O1B	3.32	1.51	1.46
3	G	400	ANP	PG-O1G	3.30	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	3400	ANP	C2-N3	3.30	1.37	1.32
3	H	2400	ANP	PG-O1G	3.30	1.51	1.46
3	H	2400	ANP	PB-O1B	3.29	1.51	1.46
3	A	400	ANP	PB-O3A	3.28	1.63	1.59
3	G	2400	ANP	PG-O1G	3.28	1.51	1.46
3	B	400	ANP	C5-C4	3.25	1.49	1.40
3	D	400	ANP	PG-O1G	3.25	1.51	1.46
3	D	1400	ANP	PG-O1G	3.22	1.51	1.46
3	A	1400	ANP	PG-O1G	3.20	1.51	1.46
3	F	400	ANP	C5-C4	3.20	1.49	1.40
3	D	2400	ANP	PB-O1B	3.17	1.51	1.46
3	H	1400	ANP	C5-C4	3.17	1.49	1.40
3	D	400	ANP	C5-C4	3.16	1.49	1.40
3	E	1400	ANP	PB-O1B	3.15	1.51	1.46
3	F	1400	ANP	PB-O3A	3.15	1.63	1.59
3	F	400	ANP	PG-O1G	3.15	1.51	1.46
3	F	2400	ANP	PG-O1G	3.13	1.51	1.46
3	C	3400	ANP	C2-N3	3.12	1.37	1.32
3	F	3400	ANP	C5-C4	3.10	1.49	1.40
3	E	2400	ANP	C5-C4	3.09	1.49	1.40
3	C	1400	ANP	PB-O3A	3.09	1.63	1.59
3	C	400	ANP	PB-O1B	3.09	1.51	1.46
3	F	1400	ANP	C5-C4	3.09	1.49	1.40
3	G	2400	ANP	C5-C4	3.09	1.49	1.40
3	H	3400	ANP	C5-C4	3.08	1.49	1.40
3	A	3400	ANP	C2-N3	3.07	1.37	1.32
3	D	1400	ANP	C5-C4	3.07	1.49	1.40
3	G	400	ANP	PB-O1B	3.07	1.51	1.46
3	B	3400	ANP	C5-C4	3.06	1.49	1.40
3	H	2400	ANP	C5-C4	3.03	1.48	1.40
3	H	400	ANP	PB-O1B	3.02	1.50	1.46
3	E	1400	ANP	C5-C4	3.02	1.48	1.40
3	B	1400	ANP	C5-C4	3.01	1.48	1.40
3	C	400	ANP	C5-C4	3.00	1.48	1.40
3	H	3400	ANP	C2-N3	3.00	1.36	1.32
3	A	400	ANP	C5-C4	3.00	1.48	1.40
3	G	400	ANP	C5-C4	2.99	1.48	1.40
3	D	2400	ANP	C5-C4	2.99	1.48	1.40
3	C	2400	ANP	C5-C4	2.98	1.48	1.40
3	C	2400	ANP	PB-O1B	2.98	1.50	1.46
3	F	2400	ANP	C5-C4	2.98	1.48	1.40
3	A	400	ANP	PB-O1B	2.98	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	400	ANP	PB-O1B	2.97	1.50	1.46
3	A	2400	ANP	C5-C4	2.96	1.48	1.40
3	E	400	ANP	PB-O1B	2.96	1.50	1.46
3	E	1400	ANP	PB-O3A	2.96	1.62	1.59
3	C	1400	ANP	C5-C4	2.95	1.48	1.40
3	G	1400	ANP	C5-C4	2.93	1.48	1.40
3	D	400	ANP	PB-O3A	2.90	1.62	1.59
3	B	2400	ANP	C5-C4	2.88	1.48	1.40
3	A	1400	ANP	C5-C4	2.88	1.48	1.40
3	H	400	ANP	C5-C4	2.87	1.48	1.40
3	C	400	ANP	PG-O1G	2.84	1.50	1.46
3	G	3400	ANP	PB-O1B	2.83	1.50	1.46
3	A	1400	ANP	PB-O3A	2.82	1.62	1.59
3	F	2400	ANP	PB-O1B	2.79	1.50	1.46
3	G	1400	ANP	PB-O3A	2.79	1.62	1.59
3	E	400	ANP	C5-C4	2.79	1.48	1.40
3	F	1400	ANP	C2-N3	2.74	1.36	1.32
3	E	3400	ANP	C2-N3	2.74	1.36	1.32
3	E	3400	ANP	C5-C4	2.74	1.48	1.40
3	F	400	ANP	PB-O3A	2.71	1.62	1.59
3	D	2400	ANP	PB-O3A	2.69	1.62	1.59
3	G	3400	ANP	C2-N3	2.69	1.36	1.32
3	D	1400	ANP	PB-O3A	2.65	1.62	1.59
3	F	3400	ANP	C2-N3	2.64	1.36	1.32
3	E	400	ANP	PB-O3A	2.63	1.62	1.59
3	D	3400	ANP	C6-C5	2.60	1.52	1.43
3	C	3400	ANP	C6-C5	2.59	1.52	1.43
3	F	3400	ANP	PB-O2B	-2.58	1.49	1.56
3	F	3400	ANP	PB-O1B	2.58	1.50	1.46
3	A	3400	ANP	PB-O2B	-2.57	1.49	1.56
3	H	1400	ANP	PB-O3A	2.57	1.62	1.59
3	G	2400	ANP	C2-N3	2.57	1.36	1.32
3	E	2400	ANP	PB-O3A	2.57	1.62	1.59
3	E	1400	ANP	C2-N3	2.53	1.36	1.32
3	A	400	ANP	C2-N3	2.52	1.36	1.32
3	G	1400	ANP	C2-N3	2.52	1.36	1.32
3	B	2400	ANP	PB-O3A	2.51	1.62	1.59
3	C	3400	ANP	PB-O1B	2.51	1.50	1.46
3	F	3400	ANP	O4'-C1'	2.50	1.44	1.41
3	H	1400	ANP	C2-N3	2.50	1.36	1.32
3	A	1400	ANP	C2-N3	2.50	1.36	1.32
3	E	2400	ANP	C2-N3	2.50	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1400	ANP	C2-N3	2.49	1.36	1.32
3	C	2400	ANP	C2-N3	2.49	1.36	1.32
3	B	400	ANP	PB-O3A	2.49	1.62	1.59
3	H	400	ANP	PB-O3A	2.49	1.62	1.59
3	H	3400	ANP	C6-C5	2.48	1.52	1.43
3	F	400	ANP	C2-N3	2.48	1.36	1.32
3	D	2400	ANP	C2-N3	2.47	1.36	1.32
3	A	2400	ANP	PB-O3A	2.46	1.62	1.59
3	H	400	ANP	C2-N3	2.44	1.36	1.32
3	A	400	ANP	PG-O2G	-2.43	1.50	1.56
3	G	400	ANP	C2-N3	2.43	1.36	1.32
3	A	3400	ANP	C6-C5	2.42	1.52	1.43
3	C	400	ANP	C2-N3	2.41	1.36	1.32
3	D	1400	ANP	C2-N3	2.38	1.35	1.32
3	A	2400	ANP	C2-N3	2.37	1.35	1.32
3	E	3400	ANP	PB-O1B	2.36	1.49	1.46
3	B	2400	ANP	C2-N3	2.36	1.35	1.32
3	B	400	ANP	C2-N3	2.36	1.35	1.32
3	H	2400	ANP	C2-N3	2.34	1.35	1.32
3	F	2400	ANP	C2-N3	2.34	1.35	1.32
3	B	1400	ANP	C2-N3	2.34	1.35	1.32
3	C	400	ANP	PG-O2G	-2.31	1.50	1.56
3	G	400	ANP	PG-O2G	-2.31	1.50	1.56
3	E	400	ANP	C2-N3	2.31	1.35	1.32
3	B	3400	ANP	PB-O2B	-2.30	1.50	1.56
3	B	400	ANP	PG-O2G	-2.30	1.50	1.56
3	G	2400	ANP	PB-O3A	2.26	1.61	1.59
3	B	3400	ANP	C6-C5	2.24	1.51	1.43
3	D	400	ANP	C2-N3	2.24	1.35	1.32
3	H	3400	ANP	PB-O1B	2.22	1.49	1.46
3	D	3400	ANP	PB-O2B	-2.22	1.50	1.56
3	E	3400	ANP	C6-C5	2.21	1.51	1.43
3	F	3400	ANP	C6-C5	2.20	1.51	1.43
3	H	2400	ANP	PB-O3A	2.19	1.61	1.59
3	F	1400	ANP	PG-O2G	-2.16	1.50	1.56
3	G	2400	ANP	PG-O3G	-2.15	1.51	1.56
3	E	400	ANP	PG-O2G	-2.15	1.51	1.56
3	E	400	ANP	PG-O3G	-2.14	1.51	1.56
3	G	3400	ANP	C6-C5	2.14	1.51	1.43
3	E	2400	ANP	PG-O3G	-2.14	1.51	1.56
3	B	1400	ANP	PB-O2B	-2.14	1.51	1.56
3	F	2400	ANP	PG-O2G	-2.14	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	400	ANP	PG-O2G	-2.13	1.51	1.56
3	F	2400	ANP	PB-O3A	2.12	1.61	1.59
3	F	1400	ANP	C6-C5	2.11	1.51	1.43
3	F	3400	ANP	PG-O2G	-2.11	1.51	1.56
3	E	2400	ANP	O4'-C1'	2.10	1.44	1.41
3	A	400	ANP	PG-O3G	-2.10	1.51	1.56
3	D	400	ANP	O4'-C1'	2.10	1.44	1.41
3	H	2400	ANP	PB-O2B	-2.08	1.51	1.56
3	A	1400	ANP	C6-C5	2.08	1.51	1.43
3	A	1400	ANP	PG-O2G	-2.07	1.51	1.56
3	E	3400	ANP	PB-O2B	-2.07	1.51	1.56
3	D	400	ANP	PG-O3G	-2.07	1.51	1.56
3	D	3400	ANP	PG-O2G	-2.06	1.51	1.56
3	D	2400	ANP	O4'-C1'	2.06	1.44	1.41
3	F	400	ANP	PG-O2G	-2.05	1.51	1.56
3	C	1400	ANP	PG-O3G	-2.05	1.51	1.56
3	G	3400	ANP	O4'-C1'	2.05	1.43	1.41
3	H	3400	ANP	PB-O2B	-2.04	1.51	1.56
3	C	2400	ANP	PB-O3A	2.04	1.61	1.59
3	E	1400	ANP	C6-C5	2.04	1.50	1.43
3	H	2400	ANP	O4'-C1'	2.04	1.43	1.41
3	D	400	ANP	PB-O2B	-2.03	1.51	1.56
3	E	1400	ANP	PB-O2B	-2.03	1.51	1.56
3	C	3400	ANP	PB-O2B	-2.03	1.51	1.56
3	H	2400	ANP	PG-O3G	-2.03	1.51	1.56
3	A	2400	ANP	PG-O3G	-2.02	1.51	1.56
3	F	2400	ANP	PB-O2B	-2.02	1.51	1.56
3	H	2400	ANP	PG-O2G	-2.02	1.51	1.56
3	H	1400	ANP	C6-C5	2.01	1.50	1.43
3	D	400	ANP	PG-O2G	-2.01	1.51	1.56
3	B	2400	ANP	PB-O2B	-2.00	1.51	1.56
3	A	1400	ANP	PG-O3G	-2.00	1.51	1.56

All (247) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	3400	ANP	O1G-PG-N3B	-7.84	100.23	111.77
3	F	3400	ANP	O1G-PG-N3B	-7.45	100.81	111.77
3	H	3400	ANP	O1G-PG-N3B	-7.29	101.03	111.77
3	A	3400	ANP	O1G-PG-N3B	-7.10	101.32	111.77
3	G	3400	ANP	O1G-PG-N3B	-7.08	101.34	111.77
3	E	3400	ANP	O1G-PG-N3B	-7.02	101.44	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3400	ANP	O1G-PG-N3B	-6.82	101.72	111.77
3	C	3400	ANP	O1G-PG-N3B	-6.58	102.08	111.77
3	H	3400	ANP	C4-C5-N7	-5.13	104.06	109.40
3	A	2400	ANP	O1G-PG-N3B	-4.92	104.53	111.77
3	A	3400	ANP	C4-C5-N7	-4.88	104.32	109.40
3	B	2400	ANP	O1G-PG-N3B	-4.86	104.61	111.77
3	F	1400	ANP	O1G-PG-N3B	-4.82	104.67	111.77
3	B	1400	ANP	O1G-PG-N3B	-4.80	104.71	111.77
3	H	2400	ANP	O1G-PG-N3B	-4.77	104.74	111.77
3	G	2400	ANP	O1G-PG-N3B	-4.77	104.75	111.77
3	B	3400	ANP	C4-C5-N7	-4.76	104.44	109.40
3	G	3400	ANP	O1B-PB-N3B	-4.75	104.77	111.77
3	E	2400	ANP	O1G-PG-N3B	-4.75	104.78	111.77
3	D	2400	ANP	O1G-PG-N3B	-4.73	104.81	111.77
3	F	2400	ANP	O1G-PG-N3B	-4.73	104.81	111.77
3	C	2400	ANP	O1G-PG-N3B	-4.72	104.81	111.77
3	E	3400	ANP	O1B-PB-N3B	-4.72	104.81	111.77
3	E	3400	ANP	C4-C5-N7	-4.72	104.48	109.40
3	D	3400	ANP	O1B-PB-N3B	-4.68	104.88	111.77
3	E	1400	ANP	O1G-PG-N3B	-4.66	104.91	111.77
3	H	3400	ANP	O2B-PB-O1B	4.63	119.62	109.92
3	C	1400	ANP	O1G-PG-N3B	-4.61	104.97	111.77
3	E	3400	ANP	O2B-PB-O1B	4.57	119.51	109.92
3	D	3400	ANP	C4-C5-N7	-4.50	104.71	109.40
3	F	2400	ANP	O2B-PB-O1B	4.49	119.34	109.92
3	C	3400	ANP	O2B-PB-O1B	4.46	119.27	109.92
3	E	2400	ANP	O2B-PB-O1B	4.44	119.23	109.92
3	C	2400	ANP	O2B-PB-O1B	4.43	119.22	109.92
3	D	2400	ANP	O2B-PB-O1B	4.41	119.17	109.92
3	C	3400	ANP	C4-C5-N7	-4.41	104.80	109.40
3	B	2400	ANP	O2B-PB-O1B	4.40	119.15	109.92
3	A	2400	ANP	O2B-PB-O1B	4.35	119.03	109.92
3	D	400	ANP	O1G-PG-N3B	-4.35	105.37	111.77
3	C	400	ANP	O2B-PB-O1B	4.32	118.97	109.92
3	G	400	ANP	O1G-PG-N3B	-4.31	105.42	111.77
3	A	400	ANP	O1G-PG-N3B	-4.29	105.45	111.77
3	G	2400	ANP	O2B-PB-O1B	4.29	118.92	109.92
3	D	1400	ANP	O1G-PG-N3B	-4.29	105.45	111.77
3	C	1400	ANP	C3'-C2'-C1'	4.27	107.41	100.98
3	A	1400	ANP	O2B-PB-O1B	4.25	118.84	109.92
3	A	3400	ANP	O1B-PB-N3B	-4.25	105.51	111.77
3	H	2400	ANP	O2B-PB-O1B	4.24	118.81	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1400	ANP	O2B-PB-O1B	4.23	118.79	109.92
3	F	400	ANP	O2B-PB-O1B	4.22	118.77	109.92
3	D	1400	ANP	O2B-PB-O1B	4.22	118.76	109.92
3	C	3400	ANP	O1B-PB-N3B	-4.21	105.56	111.77
3	D	3400	ANP	O2B-PB-O1B	4.21	118.74	109.92
3	C	400	ANP	O1G-PG-N3B	-4.19	105.59	111.77
3	B	1400	ANP	O2B-PB-O1B	4.17	118.67	109.92
3	G	400	ANP	O2B-PB-O1B	4.15	118.63	109.92
3	G	3400	ANP	C4-C5-N7	-4.15	105.07	109.40
3	F	1400	ANP	C3'-C2'-C1'	4.15	107.23	100.98
3	F	1400	ANP	O2B-PB-O1B	4.14	118.60	109.92
3	G	1400	ANP	C3'-C2'-C1'	4.14	107.21	100.98
3	H	1400	ANP	O1G-PG-N3B	-4.13	105.69	111.77
3	A	1400	ANP	C3'-C2'-C1'	4.12	107.18	100.98
3	B	1400	ANP	C3'-C2'-C1'	4.12	107.18	100.98
3	F	3400	ANP	O2B-PB-O1B	4.07	118.46	109.92
3	F	3400	ANP	C4-C5-N7	-4.07	105.16	109.40
3	G	1400	ANP	O2B-PB-O1B	4.07	118.45	109.92
3	H	1400	ANP	O2B-PB-O1B	4.06	118.44	109.92
3	B	2400	ANP	C3'-C2'-C1'	4.05	107.08	100.98
3	G	1400	ANP	O1G-PG-N3B	-4.03	105.84	111.77
3	A	2400	ANP	C3'-C2'-C1'	4.02	107.03	100.98
3	A	1400	ANP	O1G-PG-N3B	-4.01	105.86	111.77
3	B	3400	ANP	O2B-PB-O1B	4.00	118.32	109.92
3	F	3400	ANP	O1B-PB-N3B	-4.00	105.89	111.77
3	F	2400	ANP	C3'-C2'-C1'	3.98	106.97	100.98
3	E	400	ANP	O1G-PG-N3B	-3.97	105.93	111.77
3	C	1400	ANP	O3A-PB-N3B	3.95	117.54	106.59
3	D	2400	ANP	C3'-C2'-C1'	3.95	106.92	100.98
3	E	2400	ANP	C3'-C2'-C1'	3.94	106.91	100.98
3	C	1400	ANP	O2B-PB-O1B	3.94	118.18	109.92
3	H	2400	ANP	C3'-C2'-C1'	3.93	106.90	100.98
3	H	3400	ANP	O1B-PB-N3B	-3.92	105.99	111.77
3	B	400	ANP	O1G-PG-N3B	-3.92	106.00	111.77
3	G	1400	ANP	O3A-PB-N3B	3.91	117.44	106.59
3	C	2400	ANP	C3'-C2'-C1'	3.91	106.86	100.98
3	F	400	ANP	O1G-PG-N3B	-3.89	106.04	111.77
3	D	1400	ANP	C3'-C2'-C1'	3.87	106.81	100.98
3	G	2400	ANP	C3'-C2'-C1'	3.87	106.81	100.98
3	E	400	ANP	O2B-PB-O1B	3.86	118.02	109.92
3	H	400	ANP	O1G-PG-N3B	-3.86	106.08	111.77
3	H	400	ANP	C3'-C2'-C1'	3.86	106.78	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1400	ANP	O3A-PB-N3B	3.85	117.28	106.59
3	F	400	ANP	C3'-C2'-C1'	3.85	106.77	100.98
3	C	400	ANP	C3'-C2'-C1'	3.84	106.76	100.98
3	A	1400	ANP	O3A-PB-N3B	3.83	117.22	106.59
3	F	2400	ANP	N3-C2-N1	-3.81	122.72	128.68
3	G	2400	ANP	O3A-PB-N3B	3.81	117.16	106.59
3	B	400	ANP	O2B-PB-O1B	3.80	117.89	109.92
3	H	1400	ANP	C3'-C2'-C1'	3.80	106.70	100.98
3	F	1400	ANP	O3A-PB-N3B	3.80	117.13	106.59
3	G	3400	ANP	O2B-PB-O1B	3.79	117.87	109.92
3	H	400	ANP	O2B-PB-O1B	3.79	117.86	109.92
3	D	400	ANP	O2B-PB-O1B	3.79	117.86	109.92
3	G	400	ANP	C3'-C2'-C1'	3.77	106.66	100.98
3	E	400	ANP	C3'-C2'-C1'	3.77	106.65	100.98
3	H	1400	ANP	O3A-PB-N3B	3.76	117.03	106.59
3	A	400	ANP	O2B-PB-O1B	3.74	117.75	109.92
3	H	2400	ANP	N3-C2-N1	-3.73	122.84	128.68
3	A	2400	ANP	N3-C2-N1	-3.73	122.85	128.68
3	A	3400	ANP	O2B-PB-O1B	3.73	117.73	109.92
3	E	1400	ANP	C3'-C2'-C1'	3.72	106.58	100.98
3	E	3400	ANP	PB-O3A-PA	-3.70	119.59	132.62
3	A	400	ANP	C3'-C2'-C1'	3.69	106.54	100.98
3	D	1400	ANP	O3A-PB-N3B	3.69	116.83	106.59
3	E	1400	ANP	N3-C2-N1	-3.68	122.92	128.68
3	E	2400	ANP	N3-C2-N1	-3.67	122.94	128.68
3	C	2400	ANP	O3A-PB-N3B	3.67	116.77	106.59
3	C	2400	ANP	N3-C2-N1	-3.67	122.95	128.68
3	B	400	ANP	C3'-C2'-C1'	3.64	106.47	100.98
3	F	2400	ANP	O3A-PB-N3B	3.64	116.70	106.59
3	H	2400	ANP	O3A-PB-N3B	3.64	116.70	106.59
3	B	2400	ANP	N3-C2-N1	-3.64	122.99	128.68
3	H	2400	ANP	O1B-PB-N3B	-3.64	106.42	111.77
3	G	2400	ANP	N3-C2-N1	-3.63	123.01	128.68
3	C	1400	ANP	N3-C2-N1	-3.60	123.05	128.68
3	A	2400	ANP	O3A-PB-N3B	3.60	116.56	106.59
3	D	1400	ANP	N3-C2-N1	-3.59	123.06	128.68
3	B	3400	ANP	O1B-PB-N3B	-3.58	106.50	111.77
3	D	400	ANP	C3'-C2'-C1'	3.58	106.37	100.98
3	B	2400	ANP	O3A-PB-N3B	3.57	116.50	106.59
3	B	1400	ANP	N3-C2-N1	-3.57	123.09	128.68
3	E	2400	ANP	O3A-PB-N3B	3.57	116.50	106.59
3	D	2400	ANP	N3-C2-N1	-3.57	123.10	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400	ANP	N3-C2-N1	-3.56	123.11	128.68
3	E	400	ANP	N3-C2-N1	-3.56	123.11	128.68
3	G	1400	ANP	N3-C2-N1	-3.55	123.12	128.68
3	E	1400	ANP	O3A-PB-N3B	3.51	116.33	106.59
3	A	400	ANP	N3-C2-N1	-3.51	123.19	128.68
3	C	1400	ANP	O1B-PB-N3B	-3.51	106.60	111.77
3	H	400	ANP	N3-C2-N1	-3.51	123.19	128.68
3	A	1400	ANP	N3-C2-N1	-3.51	123.19	128.68
3	F	1400	ANP	N3-C2-N1	-3.50	123.21	128.68
3	D	2400	ANP	O3A-PB-N3B	3.50	116.29	106.59
3	C	400	ANP	N3-C2-N1	-3.50	123.22	128.68
3	H	1400	ANP	N3-C2-N1	-3.48	123.24	128.68
3	E	2400	ANP	O1B-PB-N3B	-3.46	106.67	111.77
3	A	2400	ANP	O1B-PB-N3B	-3.45	106.69	111.77
3	B	1400	ANP	O1B-PB-N3B	-3.44	106.71	111.77
3	A	3400	ANP	O2G-PG-O3G	3.44	116.80	107.64
3	E	1400	ANP	O1B-PB-N3B	-3.44	106.71	111.77
3	B	3400	ANP	PB-O3A-PA	-3.42	120.56	132.62
3	D	400	ANP	N3-C2-N1	-3.42	123.34	128.68
3	D	2400	ANP	O1B-PB-N3B	-3.41	106.74	111.77
3	G	2400	ANP	O1B-PB-N3B	-3.41	106.75	111.77
3	B	2400	ANP	O1B-PB-N3B	-3.40	106.76	111.77
3	C	2400	ANP	O1B-PB-N3B	-3.40	106.77	111.77
3	G	1400	ANP	O1B-PB-N3B	-3.38	106.80	111.77
3	F	1400	ANP	O1B-PB-N3B	-3.36	106.82	111.77
3	G	3400	ANP	PB-O3A-PA	-3.33	120.89	132.62
3	E	1400	ANP	C4-C5-N7	-3.32	105.94	109.40
3	A	1400	ANP	O1B-PB-N3B	-3.31	106.90	111.77
3	H	3400	ANP	PB-O3A-PA	-3.30	120.98	132.62
3	C	3400	ANP	PB-O3A-PA	-3.30	121.00	132.62
3	F	400	ANP	N3-C2-N1	-3.30	123.52	128.68
3	G	400	ANP	N3-C2-N1	-3.28	123.55	128.68
3	D	1400	ANP	O1B-PB-N3B	-3.27	106.96	111.77
3	D	3400	ANP	PB-O3A-PA	-3.26	121.13	132.62
3	E	400	ANP	C4-C5-N7	-3.22	106.05	109.40
3	F	2400	ANP	O1B-PB-N3B	-3.21	107.05	111.77
3	F	3400	ANP	PB-O3A-PA	-3.19	121.37	132.62
3	D	1400	ANP	C4-C5-N7	-3.19	106.08	109.40
3	H	3400	ANP	O2G-PG-O3G	3.17	116.08	107.64
3	F	1400	ANP	C4-C5-N7	-3.14	106.12	109.40
3	C	3400	ANP	O2G-PG-O3G	3.10	115.89	107.64
3	H	3400	ANP	N3-C2-N1	-3.10	123.84	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1400	ANP	C4-C5-N7	-3.09	106.18	109.40
3	A	3400	ANP	PB-O3A-PA	-3.08	121.75	132.62
3	H	1400	ANP	O1B-PB-N3B	-3.07	107.25	111.77
3	C	400	ANP	O3A-PB-N3B	3.07	115.10	106.59
3	A	400	ANP	C4-C5-N7	-3.03	106.24	109.40
3	F	3400	ANP	O2G-PG-O3G	3.03	115.69	107.64
3	B	3400	ANP	C3'-C2'-C1'	3.00	105.49	100.98
3	C	1400	ANP	C4-C5-N7	-2.99	106.28	109.40
3	B	1400	ANP	C4-C5-N7	-2.98	106.30	109.40
3	H	1400	ANP	C4-C5-N7	-2.96	106.31	109.40
3	G	400	ANP	C4-C5-N7	-2.96	106.31	109.40
3	G	400	ANP	O3A-PB-N3B	2.95	114.78	106.59
3	H	400	ANP	C4-C5-N7	-2.94	106.33	109.40
3	D	3400	ANP	O2G-PG-O3G	2.94	115.47	107.64
3	B	3400	ANP	O2G-PG-O3G	2.94	115.46	107.64
3	G	3400	ANP	O2G-PG-O3G	2.93	115.45	107.64
3	G	3400	ANP	N3-C2-N1	-2.88	124.17	128.68
3	E	400	ANP	O3A-PB-N3B	2.86	114.52	106.59
3	F	400	ANP	C4-C5-N7	-2.85	106.43	109.40
3	G	1400	ANP	C4-C5-N7	-2.85	106.43	109.40
3	D	400	ANP	O3A-PB-N3B	2.82	114.42	106.59
3	H	400	ANP	O3A-PB-N3B	2.82	114.41	106.59
3	C	400	ANP	C4-C5-N7	-2.81	106.47	109.40
3	F	400	ANP	O3A-PB-N3B	2.81	114.38	106.59
3	E	3400	ANP	O2G-PG-O3G	2.80	115.09	107.64
3	F	3400	ANP	N3-C2-N1	-2.75	124.37	128.68
3	D	3400	ANP	N3-C2-N1	-2.72	124.43	128.68
3	C	3400	ANP	N3-C2-N1	-2.71	124.44	128.68
3	B	400	ANP	C4-C5-N7	-2.70	106.58	109.40
3	D	3400	ANP	C3'-C2'-C1'	2.68	105.01	100.98
3	B	3400	ANP	N3-C2-N1	-2.66	124.53	128.68
3	B	400	ANP	O3A-PB-N3B	2.65	113.94	106.59
3	D	2400	ANP	C4-C5-N7	-2.64	106.64	109.40
3	A	400	ANP	O3A-PB-N3B	2.60	113.82	106.59
3	D	400	ANP	C4-C5-N7	-2.58	106.72	109.40
3	C	2400	ANP	C4-C5-N7	-2.57	106.72	109.40
3	B	2400	ANP	C4-C5-N7	-2.57	106.72	109.40
3	G	2400	ANP	C4-C5-N7	-2.55	106.74	109.40
3	E	3400	ANP	C5-C6-N6	2.53	124.20	120.35
3	A	2400	ANP	C4-C5-N7	-2.52	106.77	109.40
3	A	3400	ANP	C3'-C2'-C1'	2.50	104.74	100.98
3	H	3400	ANP	C3'-C2'-C1'	2.49	104.73	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2400	ANP	C4-C5-N7	-2.46	106.84	109.40
3	C	3400	ANP	C5-C6-N6	2.44	124.06	120.35
3	F	2400	ANP	C4-C5-N7	-2.41	106.89	109.40
3	H	2400	ANP	C4-C5-N7	-2.40	106.90	109.40
3	A	3400	ANP	N3-C2-N1	-2.36	125.00	128.68
3	H	3400	ANP	C5-C6-N6	2.35	123.92	120.35
3	D	400	ANP	O2G-PG-O3G	2.34	113.88	107.64
3	F	3400	ANP	C5-C6-N6	2.33	123.89	120.35
3	E	3400	ANP	N3-C2-N1	-2.32	125.06	128.68
3	F	400	ANP	O2G-PG-O3G	2.30	113.76	107.64
3	G	400	ANP	O2G-PG-O3G	2.28	113.70	107.64
3	E	3400	ANP	C3'-C2'-C1'	2.28	104.40	100.98
3	F	3400	ANP	C3'-C2'-C1'	2.22	104.33	100.98
3	A	400	ANP	O2G-PG-O3G	2.19	113.47	107.64
3	B	3400	ANP	C5-C6-N6	2.19	123.67	120.35
3	C	3400	ANP	C3'-C2'-C1'	2.16	104.24	100.98
3	H	1400	ANP	O2G-PG-O3G	2.16	113.38	107.64
3	E	3400	ANP	O3A-PB-N3B	2.16	112.57	106.59
3	H	400	ANP	O2G-PG-O3G	2.15	113.37	107.64
3	D	1400	ANP	O2G-PG-O3G	2.15	113.36	107.64
3	A	3400	ANP	C5-C6-N6	2.13	123.59	120.35
3	G	3400	ANP	O3A-PB-N3B	2.12	112.48	106.59
3	C	1400	ANP	O2G-PG-O3G	2.11	113.27	107.64
3	B	400	ANP	O2G-PG-O3G	2.11	113.26	107.64
3	C	400	ANP	O3'-C3'-C4'	2.09	117.09	111.05
3	G	1400	ANP	O2G-PG-O3G	2.09	113.20	107.64
3	B	400	ANP	O1B-PB-N3B	-2.05	108.75	111.77
3	E	400	ANP	O2G-PG-O3G	2.04	113.08	107.64
3	D	400	ANP	C2-N1-C6	2.04	122.24	118.75
3	B	400	ANP	C2-N1-C6	2.03	122.23	118.75
3	E	400	ANP	O3'-C3'-C4'	2.02	116.90	111.05

All (32) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	400	ANP	C4'
3	A	1400	ANP	C4'
3	A	2400	ANP	C4'
3	A	3400	ANP	C4'
3	B	400	ANP	C4'
3	B	1400	ANP	C4'
3	B	2400	ANP	C4'

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Mol	Chain	Res	Type	Atom
3	B	3400	ANP	C4'
3	C	400	ANP	C4'
3	C	1400	ANP	C4'
3	C	2400	ANP	C4'
3	C	3400	ANP	C4'
3	D	400	ANP	C4'
3	D	1400	ANP	C4'
3	D	2400	ANP	C4'
3	D	3400	ANP	C4'
3	E	400	ANP	C4'
3	E	1400	ANP	C4'
3	E	2400	ANP	C4'
3	E	3400	ANP	C4'
3	F	400	ANP	C4'
3	F	1400	ANP	C4'
3	F	2400	ANP	C4'
3	F	3400	ANP	C4'
3	G	400	ANP	C4'
3	G	1400	ANP	C4'
3	G	2400	ANP	C4'
3	G	3400	ANP	C4'
3	H	400	ANP	C4'
3	H	1400	ANP	C4'
3	H	2400	ANP	C4'
3	H	3400	ANP	C4'

All (280) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	ANP	PB-N3B-PG-O1G
3	A	400	ANP	PG-N3B-PB-O1B
3	A	400	ANP	PG-N3B-PB-O3A
3	A	400	ANP	PA-O3A-PB-O2B
3	A	400	ANP	C5'-O5'-PA-O2A
3	A	400	ANP	C5'-O5'-PA-O3A
3	A	400	ANP	C3'-C4'-C5'-O5'
3	A	1400	ANP	PB-N3B-PG-O1G
3	A	1400	ANP	PG-N3B-PB-O1B
3	A	1400	ANP	PG-N3B-PB-O3A
3	A	1400	ANP	PA-O3A-PB-O1B
3	A	1400	ANP	PA-O3A-PB-O2B
3	A	1400	ANP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	A	1400	ANP	C5'-O5'-PA-O3A
3	A	1400	ANP	C3'-C4'-C5'-O5'
3	A	2400	ANP	PB-N3B-PG-O1G
3	A	2400	ANP	PG-N3B-PB-O1B
3	A	2400	ANP	PG-N3B-PB-O3A
3	A	2400	ANP	PA-O3A-PB-O2B
3	A	2400	ANP	C5'-O5'-PA-O2A
3	A	2400	ANP	C5'-O5'-PA-O3A
3	A	2400	ANP	C4'-C5'-O5'-PA
3	A	2400	ANP	C3'-C4'-C5'-O5'
3	A	3400	ANP	PB-N3B-PG-O1G
3	A	3400	ANP	PG-N3B-PB-O1B
3	A	3400	ANP	PG-N3B-PB-O3A
3	A	3400	ANP	C5'-O5'-PA-O3A
3	B	400	ANP	PB-N3B-PG-O1G
3	B	400	ANP	PG-N3B-PB-O1B
3	B	400	ANP	PG-N3B-PB-O3A
3	B	400	ANP	PA-O3A-PB-O2B
3	B	400	ANP	C5'-O5'-PA-O2A
3	B	400	ANP	C5'-O5'-PA-O3A
3	B	400	ANP	C3'-C4'-C5'-O5'
3	B	1400	ANP	PB-N3B-PG-O1G
3	B	1400	ANP	PG-N3B-PB-O1B
3	B	1400	ANP	PG-N3B-PB-O3A
3	B	1400	ANP	PA-O3A-PB-O1B
3	B	1400	ANP	PA-O3A-PB-O2B
3	B	1400	ANP	C5'-O5'-PA-O2A
3	B	1400	ANP	C5'-O5'-PA-O3A
3	B	1400	ANP	C3'-C4'-C5'-O5'
3	B	2400	ANP	PB-N3B-PG-O1G
3	B	2400	ANP	PG-N3B-PB-O1B
3	B	2400	ANP	PG-N3B-PB-O3A
3	B	2400	ANP	PA-O3A-PB-O2B
3	B	2400	ANP	C5'-O5'-PA-O2A
3	B	2400	ANP	C5'-O5'-PA-O3A
3	B	2400	ANP	C4'-C5'-O5'-PA
3	B	2400	ANP	C3'-C4'-C5'-O5'
3	B	3400	ANP	PB-N3B-PG-O1G
3	B	3400	ANP	PG-N3B-PB-O1B
3	B	3400	ANP	PG-N3B-PB-O3A
3	B	3400	ANP	C5'-O5'-PA-O3A
3	C	400	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
3	C	400	ANP	PG-N3B-PB-O1B
3	C	400	ANP	PG-N3B-PB-O3A
3	C	400	ANP	PA-O3A-PB-O2B
3	C	400	ANP	C5'-O5'-PA-O2A
3	C	400	ANP	C5'-O5'-PA-O3A
3	C	400	ANP	C3'-C4'-C5'-O5'
3	C	1400	ANP	PB-N3B-PG-O1G
3	C	1400	ANP	PG-N3B-PB-O1B
3	C	1400	ANP	PG-N3B-PB-O3A
3	C	1400	ANP	PA-O3A-PB-O1B
3	C	1400	ANP	PA-O3A-PB-O2B
3	C	1400	ANP	C5'-O5'-PA-O2A
3	C	1400	ANP	C5'-O5'-PA-O3A
3	C	1400	ANP	C3'-C4'-C5'-O5'
3	C	2400	ANP	PB-N3B-PG-O1G
3	C	2400	ANP	PG-N3B-PB-O1B
3	C	2400	ANP	PG-N3B-PB-O3A
3	C	2400	ANP	PA-O3A-PB-O2B
3	C	2400	ANP	C5'-O5'-PA-O2A
3	C	2400	ANP	C5'-O5'-PA-O3A
3	C	2400	ANP	C4'-C5'-O5'-PA
3	C	2400	ANP	C3'-C4'-C5'-O5'
3	C	3400	ANP	PB-N3B-PG-O1G
3	C	3400	ANP	PG-N3B-PB-O1B
3	C	3400	ANP	PG-N3B-PB-O3A
3	C	3400	ANP	C5'-O5'-PA-O3A
3	D	400	ANP	PB-N3B-PG-O1G
3	D	400	ANP	PG-N3B-PB-O1B
3	D	400	ANP	PG-N3B-PB-O3A
3	D	400	ANP	PA-O3A-PB-O2B
3	D	400	ANP	C5'-O5'-PA-O2A
3	D	400	ANP	C5'-O5'-PA-O3A
3	D	400	ANP	C3'-C4'-C5'-O5'
3	D	1400	ANP	PB-N3B-PG-O1G
3	D	1400	ANP	PG-N3B-PB-O1B
3	D	1400	ANP	PG-N3B-PB-O3A
3	D	1400	ANP	PA-O3A-PB-O1B
3	D	1400	ANP	PA-O3A-PB-O2B
3	D	1400	ANP	C5'-O5'-PA-O2A
3	D	1400	ANP	C5'-O5'-PA-O3A
3	D	1400	ANP	C3'-C4'-C5'-O5'
3	D	2400	ANP	PB-N3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
3	D	2400	ANP	PG-N3B-PB-O1B
3	D	2400	ANP	PG-N3B-PB-O3A
3	D	2400	ANP	PA-O3A-PB-O2B
3	D	2400	ANP	C5'-O5'-PA-O2A
3	D	2400	ANP	C5'-O5'-PA-O3A
3	D	2400	ANP	C4'-C5'-O5'-PA
3	D	2400	ANP	C3'-C4'-C5'-O5'
3	D	3400	ANP	PB-N3B-PG-O1G
3	D	3400	ANP	PG-N3B-PB-O1B
3	D	3400	ANP	PG-N3B-PB-O3A
3	D	3400	ANP	C5'-O5'-PA-O3A
3	E	400	ANP	PB-N3B-PG-O1G
3	E	400	ANP	PG-N3B-PB-O1B
3	E	400	ANP	PG-N3B-PB-O3A
3	E	400	ANP	PA-O3A-PB-O2B
3	E	400	ANP	C5'-O5'-PA-O2A
3	E	400	ANP	C5'-O5'-PA-O3A
3	E	400	ANP	C3'-C4'-C5'-O5'
3	E	1400	ANP	PB-N3B-PG-O1G
3	E	1400	ANP	PG-N3B-PB-O1B
3	E	1400	ANP	PG-N3B-PB-O3A
3	E	1400	ANP	PA-O3A-PB-O1B
3	E	1400	ANP	PA-O3A-PB-O2B
3	E	1400	ANP	C5'-O5'-PA-O2A
3	E	1400	ANP	C5'-O5'-PA-O3A
3	E	1400	ANP	C3'-C4'-C5'-O5'
3	E	2400	ANP	PB-N3B-PG-O1G
3	E	2400	ANP	PG-N3B-PB-O1B
3	E	2400	ANP	PG-N3B-PB-O3A
3	E	2400	ANP	PA-O3A-PB-O2B
3	E	2400	ANP	C5'-O5'-PA-O2A
3	E	2400	ANP	C5'-O5'-PA-O3A
3	E	2400	ANP	C4'-C5'-O5'-PA
3	E	2400	ANP	C3'-C4'-C5'-O5'
3	E	3400	ANP	PB-N3B-PG-O1G
3	E	3400	ANP	PG-N3B-PB-O1B
3	E	3400	ANP	PG-N3B-PB-O3A
3	E	3400	ANP	C5'-O5'-PA-O3A
3	F	400	ANP	PB-N3B-PG-O1G
3	F	400	ANP	PG-N3B-PB-O1B
3	F	400	ANP	PG-N3B-PB-O3A
3	F	400	ANP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	F	400	ANP	C5'-O5'-PA-O2A
3	F	400	ANP	C5'-O5'-PA-O3A
3	F	400	ANP	C3'-C4'-C5'-O5'
3	F	1400	ANP	PB-N3B-PG-O1G
3	F	1400	ANP	PG-N3B-PB-O1B
3	F	1400	ANP	PG-N3B-PB-O3A
3	F	1400	ANP	PA-O3A-PB-O1B
3	F	1400	ANP	PA-O3A-PB-O2B
3	F	1400	ANP	C5'-O5'-PA-O2A
3	F	1400	ANP	C5'-O5'-PA-O3A
3	F	1400	ANP	C3'-C4'-C5'-O5'
3	F	2400	ANP	PB-N3B-PG-O1G
3	F	2400	ANP	PG-N3B-PB-O1B
3	F	2400	ANP	PG-N3B-PB-O3A
3	F	2400	ANP	PA-O3A-PB-O2B
3	F	2400	ANP	C5'-O5'-PA-O2A
3	F	2400	ANP	C5'-O5'-PA-O3A
3	F	2400	ANP	C4'-C5'-O5'-PA
3	F	2400	ANP	C3'-C4'-C5'-O5'
3	F	3400	ANP	PB-N3B-PG-O1G
3	F	3400	ANP	PG-N3B-PB-O1B
3	F	3400	ANP	PG-N3B-PB-O3A
3	F	3400	ANP	C5'-O5'-PA-O3A
3	G	400	ANP	PB-N3B-PG-O1G
3	G	400	ANP	PG-N3B-PB-O1B
3	G	400	ANP	PG-N3B-PB-O3A
3	G	400	ANP	PA-O3A-PB-O2B
3	G	400	ANP	C5'-O5'-PA-O2A
3	G	400	ANP	C5'-O5'-PA-O3A
3	G	400	ANP	C3'-C4'-C5'-O5'
3	G	1400	ANP	PB-N3B-PG-O1G
3	G	1400	ANP	PG-N3B-PB-O1B
3	G	1400	ANP	PG-N3B-PB-O3A
3	G	1400	ANP	PA-O3A-PB-O1B
3	G	1400	ANP	PA-O3A-PB-O2B
3	G	1400	ANP	C5'-O5'-PA-O2A
3	G	1400	ANP	C5'-O5'-PA-O3A
3	G	1400	ANP	C3'-C4'-C5'-O5'
3	G	2400	ANP	PB-N3B-PG-O1G
3	G	2400	ANP	PG-N3B-PB-O1B
3	G	2400	ANP	PG-N3B-PB-O3A
3	G	2400	ANP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
3	G	2400	ANP	C5'-O5'-PA-O2A
3	G	2400	ANP	C5'-O5'-PA-O3A
3	G	2400	ANP	C4'-C5'-O5'-PA
3	G	2400	ANP	C3'-C4'-C5'-O5'
3	G	3400	ANP	PB-N3B-PG-O1G
3	G	3400	ANP	PG-N3B-PB-O1B
3	G	3400	ANP	PG-N3B-PB-O3A
3	G	3400	ANP	C5'-O5'-PA-O3A
3	H	400	ANP	PB-N3B-PG-O1G
3	H	400	ANP	PG-N3B-PB-O1B
3	H	400	ANP	PG-N3B-PB-O3A
3	H	400	ANP	PA-O3A-PB-O2B
3	H	400	ANP	C5'-O5'-PA-O2A
3	H	400	ANP	C5'-O5'-PA-O3A
3	H	400	ANP	C3'-C4'-C5'-O5'
3	H	1400	ANP	PB-N3B-PG-O1G
3	H	1400	ANP	PG-N3B-PB-O1B
3	H	1400	ANP	PG-N3B-PB-O3A
3	H	1400	ANP	PA-O3A-PB-O1B
3	H	1400	ANP	PA-O3A-PB-O2B
3	H	1400	ANP	C5'-O5'-PA-O2A
3	H	1400	ANP	C5'-O5'-PA-O3A
3	H	1400	ANP	C3'-C4'-C5'-O5'
3	H	2400	ANP	PB-N3B-PG-O1G
3	H	2400	ANP	PG-N3B-PB-O1B
3	H	2400	ANP	PG-N3B-PB-O3A
3	H	2400	ANP	PA-O3A-PB-O2B
3	H	2400	ANP	C5'-O5'-PA-O2A
3	H	2400	ANP	C5'-O5'-PA-O3A
3	H	2400	ANP	C4'-C5'-O5'-PA
3	H	2400	ANP	C3'-C4'-C5'-O5'
3	H	3400	ANP	PB-N3B-PG-O1G
3	H	3400	ANP	PG-N3B-PB-O1B
3	H	3400	ANP	PG-N3B-PB-O3A
3	H	3400	ANP	C5'-O5'-PA-O3A
3	A	400	ANP	C4'-C5'-O5'-PA
3	B	400	ANP	C4'-C5'-O5'-PA
3	C	400	ANP	C4'-C5'-O5'-PA
3	D	400	ANP	C4'-C5'-O5'-PA
3	E	400	ANP	C4'-C5'-O5'-PA
3	F	400	ANP	C4'-C5'-O5'-PA
3	G	400	ANP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
3	H	400	ANP	C4'-C5'-O5'-PA
3	B	400	ANP	O4'-C4'-C5'-O5'
3	C	400	ANP	O4'-C4'-C5'-O5'
3	D	400	ANP	O4'-C4'-C5'-O5'
3	F	400	ANP	O4'-C4'-C5'-O5'
3	A	400	ANP	O4'-C4'-C5'-O5'
3	E	400	ANP	O4'-C4'-C5'-O5'
3	G	400	ANP	O4'-C4'-C5'-O5'
3	A	2400	ANP	O4'-C4'-C5'-O5'
3	D	2400	ANP	O4'-C4'-C5'-O5'
3	F	2400	ANP	O4'-C4'-C5'-O5'
3	H	400	ANP	O4'-C4'-C5'-O5'
3	A	1400	ANP	O4'-C4'-C5'-O5'
3	B	1400	ANP	O4'-C4'-C5'-O5'
3	B	2400	ANP	O4'-C4'-C5'-O5'
3	C	1400	ANP	O4'-C4'-C5'-O5'
3	C	2400	ANP	O4'-C4'-C5'-O5'
3	D	1400	ANP	O4'-C4'-C5'-O5'
3	E	1400	ANP	O4'-C4'-C5'-O5'
3	E	2400	ANP	O4'-C4'-C5'-O5'
3	F	1400	ANP	O4'-C4'-C5'-O5'
3	G	1400	ANP	O4'-C4'-C5'-O5'
3	G	2400	ANP	O4'-C4'-C5'-O5'
3	H	1400	ANP	O4'-C4'-C5'-O5'
3	H	2400	ANP	O4'-C4'-C5'-O5'
3	B	1400	ANP	C4'-C5'-O5'-PA
3	F	1400	ANP	C4'-C5'-O5'-PA
3	H	1400	ANP	C4'-C5'-O5'-PA
3	A	1400	ANP	C4'-C5'-O5'-PA
3	C	1400	ANP	C4'-C5'-O5'-PA
3	D	1400	ANP	C4'-C5'-O5'-PA
3	E	1400	ANP	C4'-C5'-O5'-PA
3	G	1400	ANP	C4'-C5'-O5'-PA
3	A	3400	ANP	C5'-O5'-PA-O2A
3	B	3400	ANP	C5'-O5'-PA-O2A
3	C	3400	ANP	C5'-O5'-PA-O2A
3	D	3400	ANP	C5'-O5'-PA-O2A
3	E	3400	ANP	C5'-O5'-PA-O2A
3	F	3400	ANP	C5'-O5'-PA-O2A
3	G	3400	ANP	C5'-O5'-PA-O2A
3	H	3400	ANP	C5'-O5'-PA-O2A
3	E	3400	ANP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
3	H	3400	ANP	C4'-C5'-O5'-PA
3	A	3400	ANP	C4'-C5'-O5'-PA
3	C	3400	ANP	C4'-C5'-O5'-PA
3	D	3400	ANP	C4'-C5'-O5'-PA
3	F	3400	ANP	C4'-C5'-O5'-PA
3	G	3400	ANP	C4'-C5'-O5'-PA
3	B	3400	ANP	C4'-C5'-O5'-PA
3	A	3400	ANP	O4'-C4'-C5'-O5'
3	B	3400	ANP	O4'-C4'-C5'-O5'
3	C	3400	ANP	O4'-C4'-C5'-O5'
3	D	3400	ANP	O4'-C4'-C5'-O5'
3	E	3400	ANP	O4'-C4'-C5'-O5'
3	F	3400	ANP	O4'-C4'-C5'-O5'
3	G	3400	ANP	O4'-C4'-C5'-O5'
3	H	3400	ANP	O4'-C4'-C5'-O5'

There are no ring outliers.

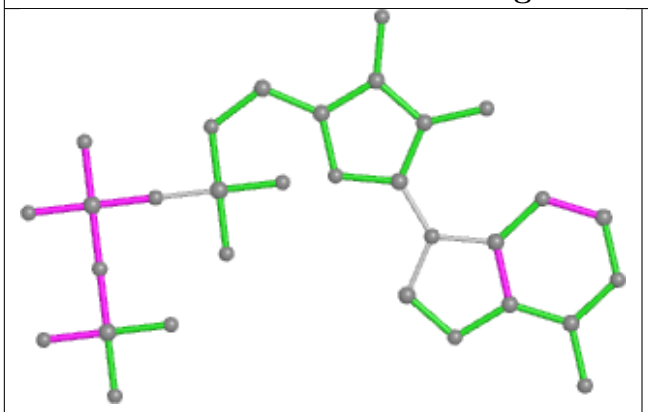
17 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	3400	ANP	1	0
3	F	400	ANP	6	0
3	D	3400	ANP	2	0
3	E	1400	ANP	1	0
3	A	400	ANP	1	0
3	H	3400	ANP	3	0
3	C	3400	ANP	2	0
3	E	400	ANP	1	0
3	G	400	ANP	2	0
3	E	3400	ANP	1	0
3	A	3400	ANP	3	0
3	G	3400	ANP	2	0
3	C	400	ANP	1	0
3	F	3400	ANP	3	0
3	H	400	ANP	1	0
3	A	1400	ANP	3	0
3	B	400	ANP	1	0

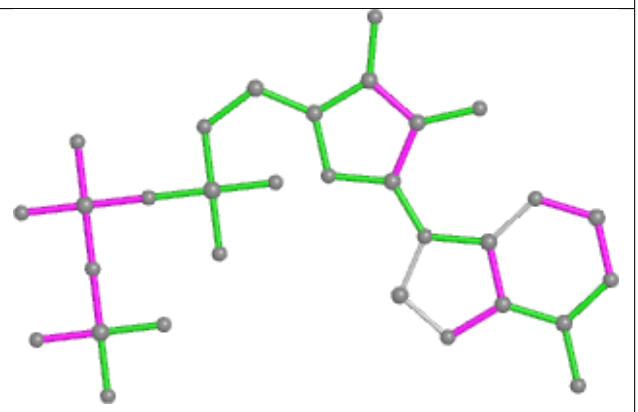
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

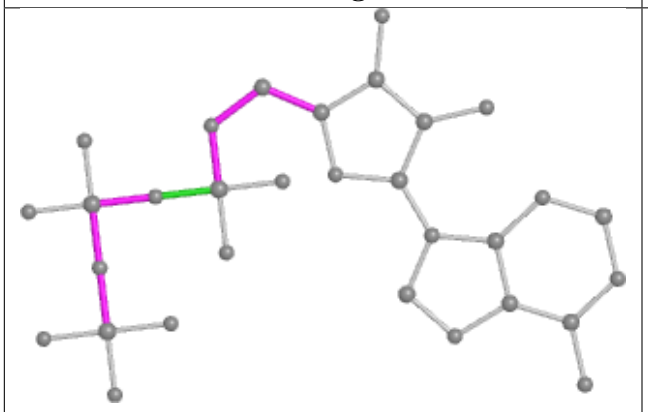
Ligand ANP B 2400



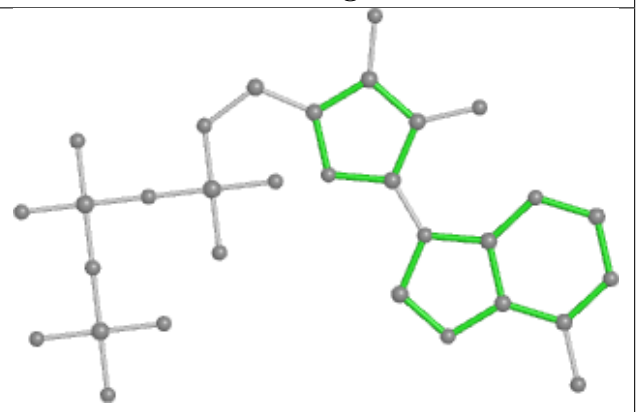
Bond lengths



Bond angles

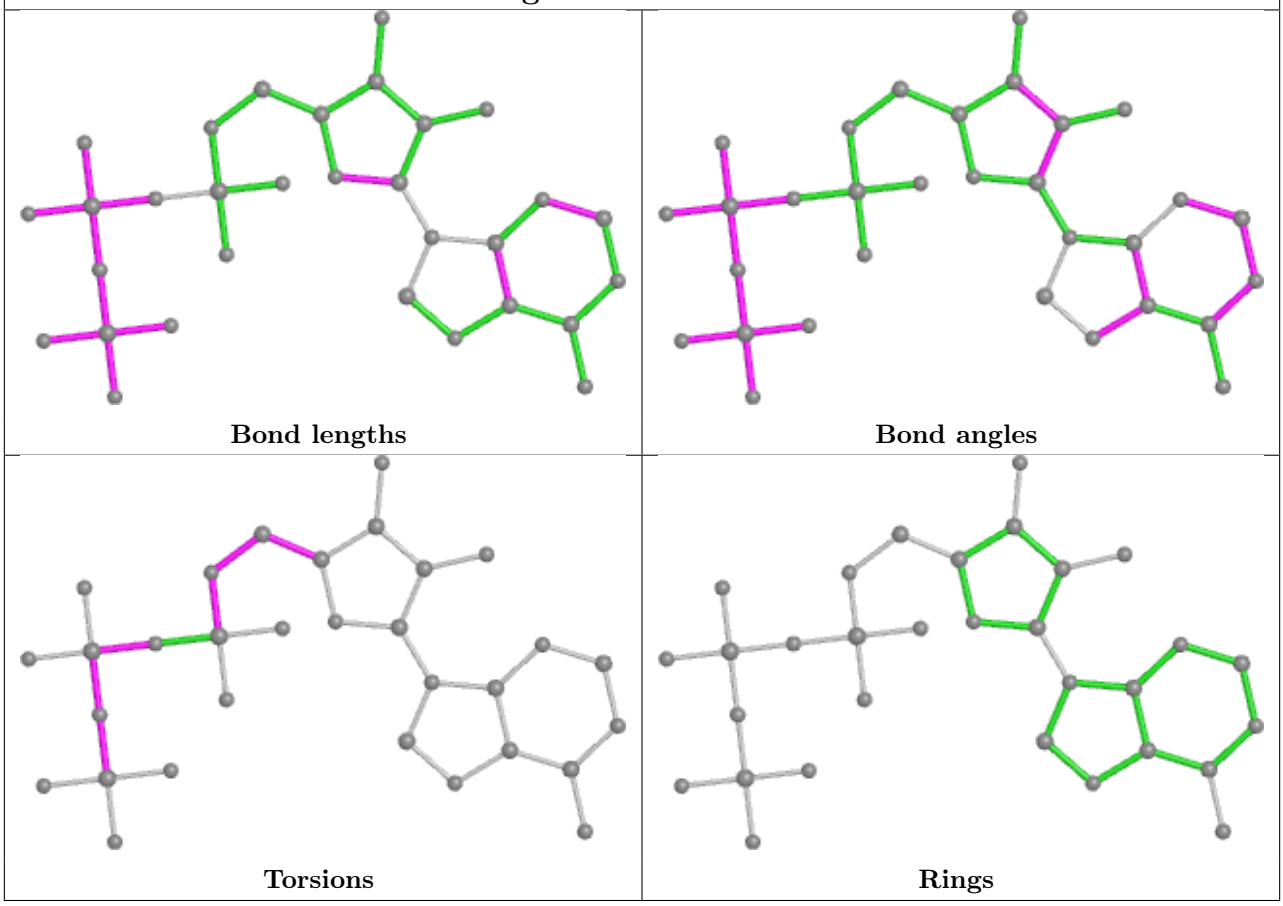


Torsions

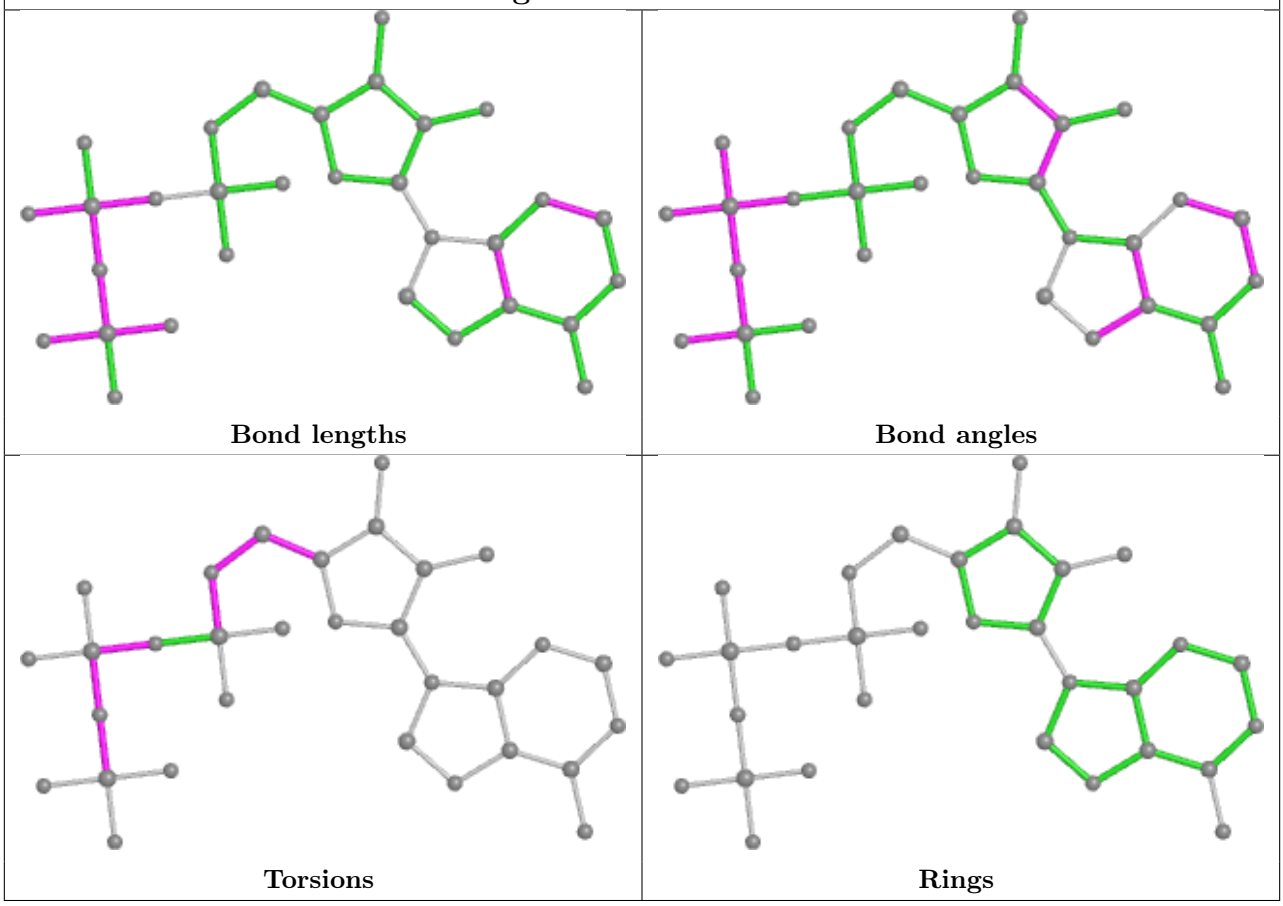


Rings

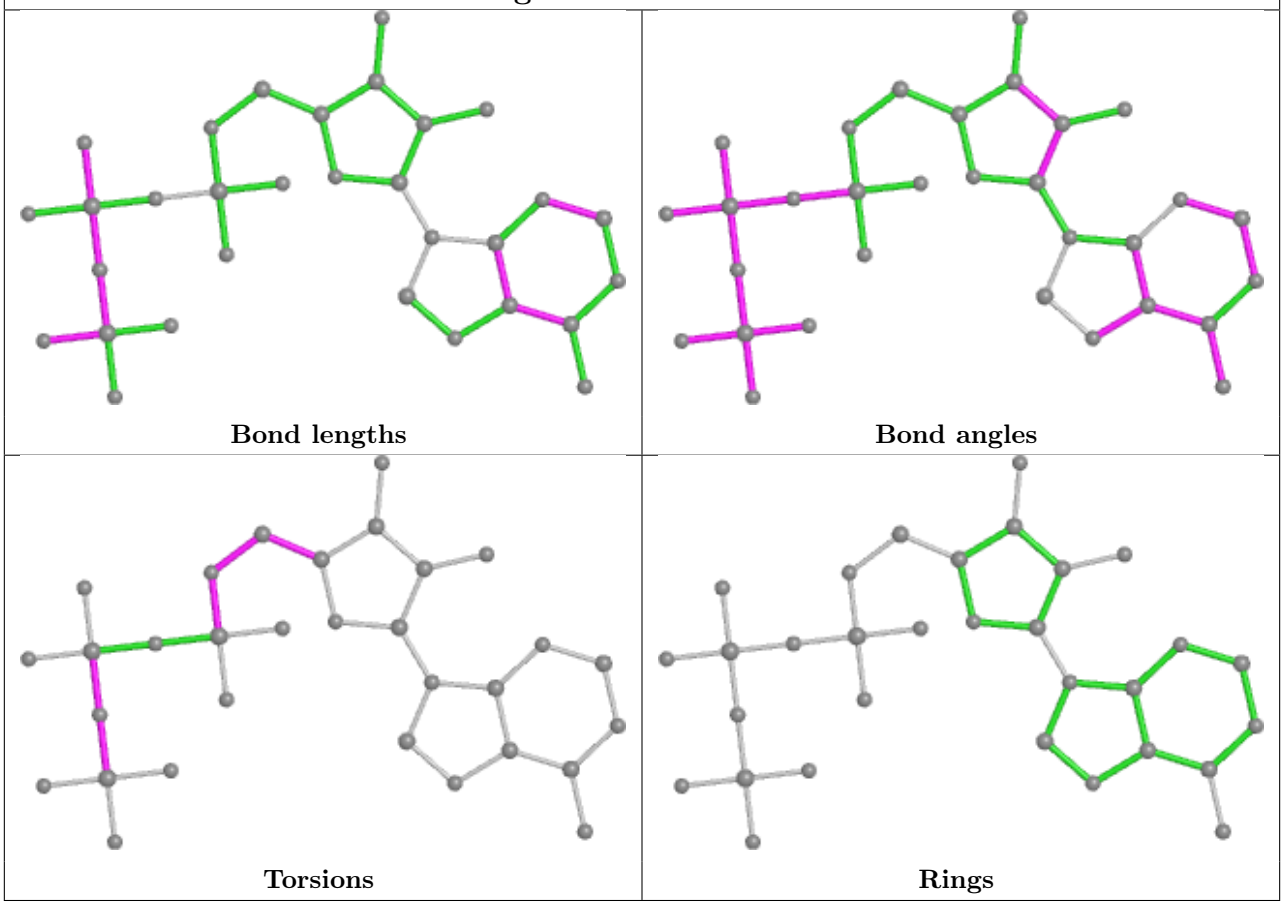
Ligand ANP D 400



Ligand ANP G 2400



Ligand ANP B 3400



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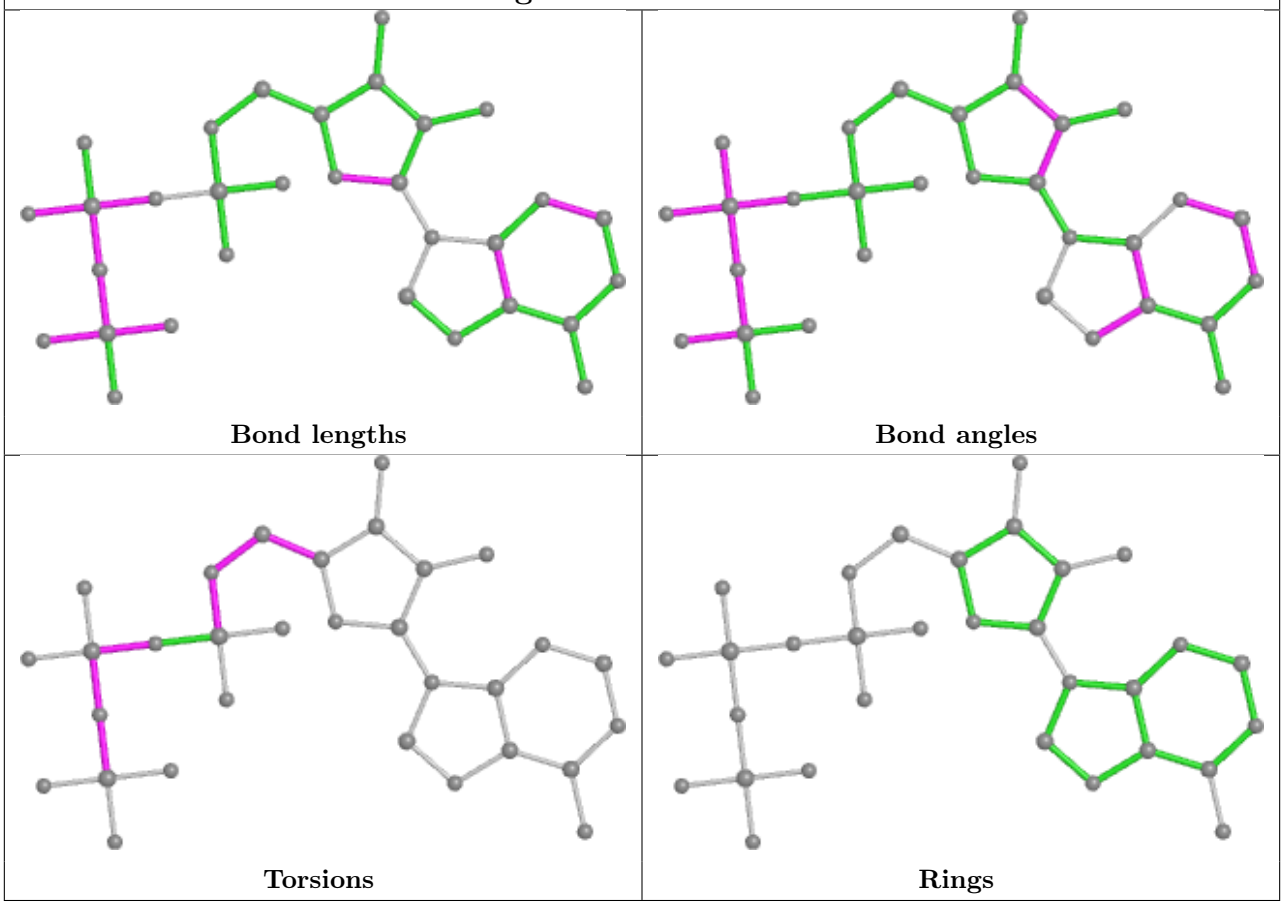

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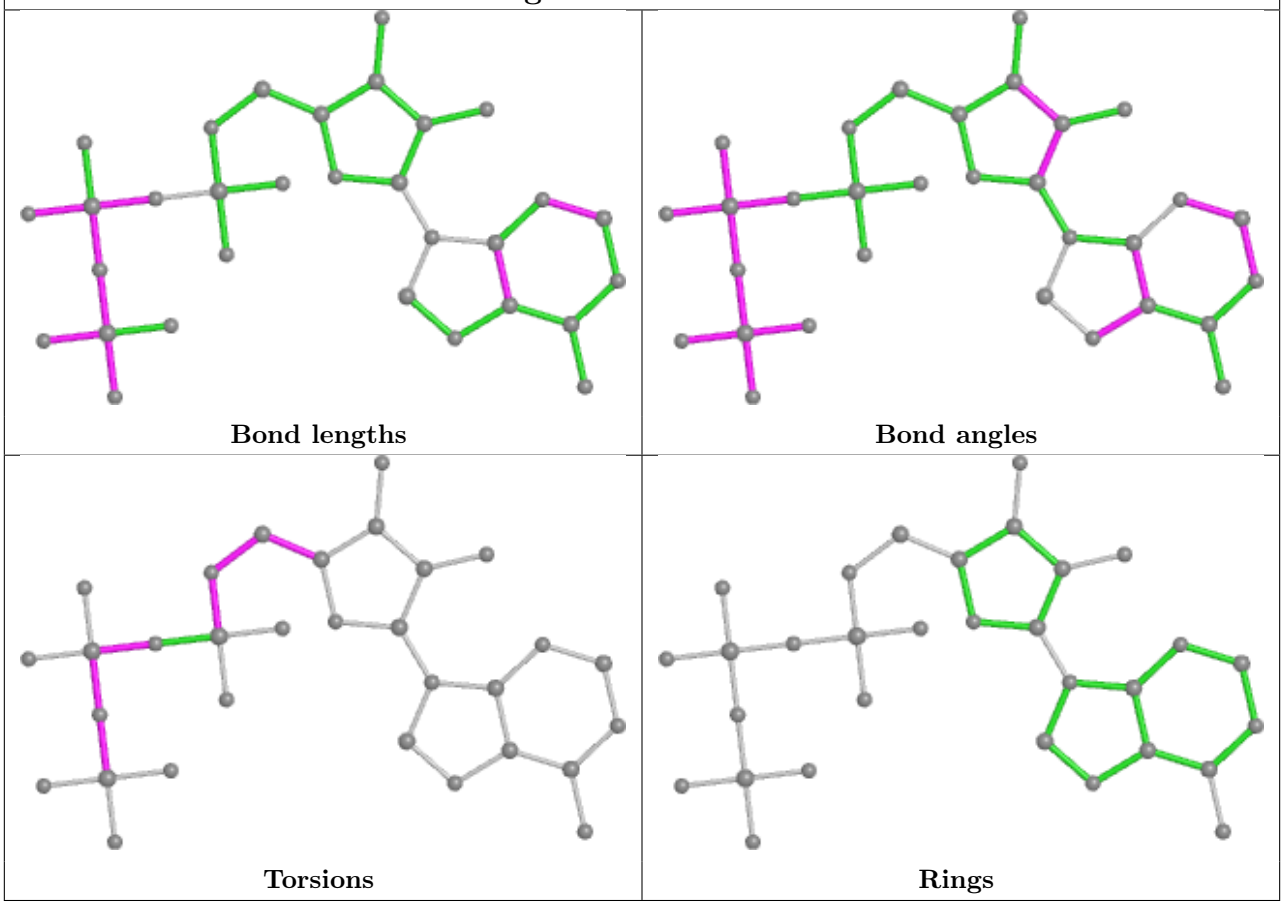
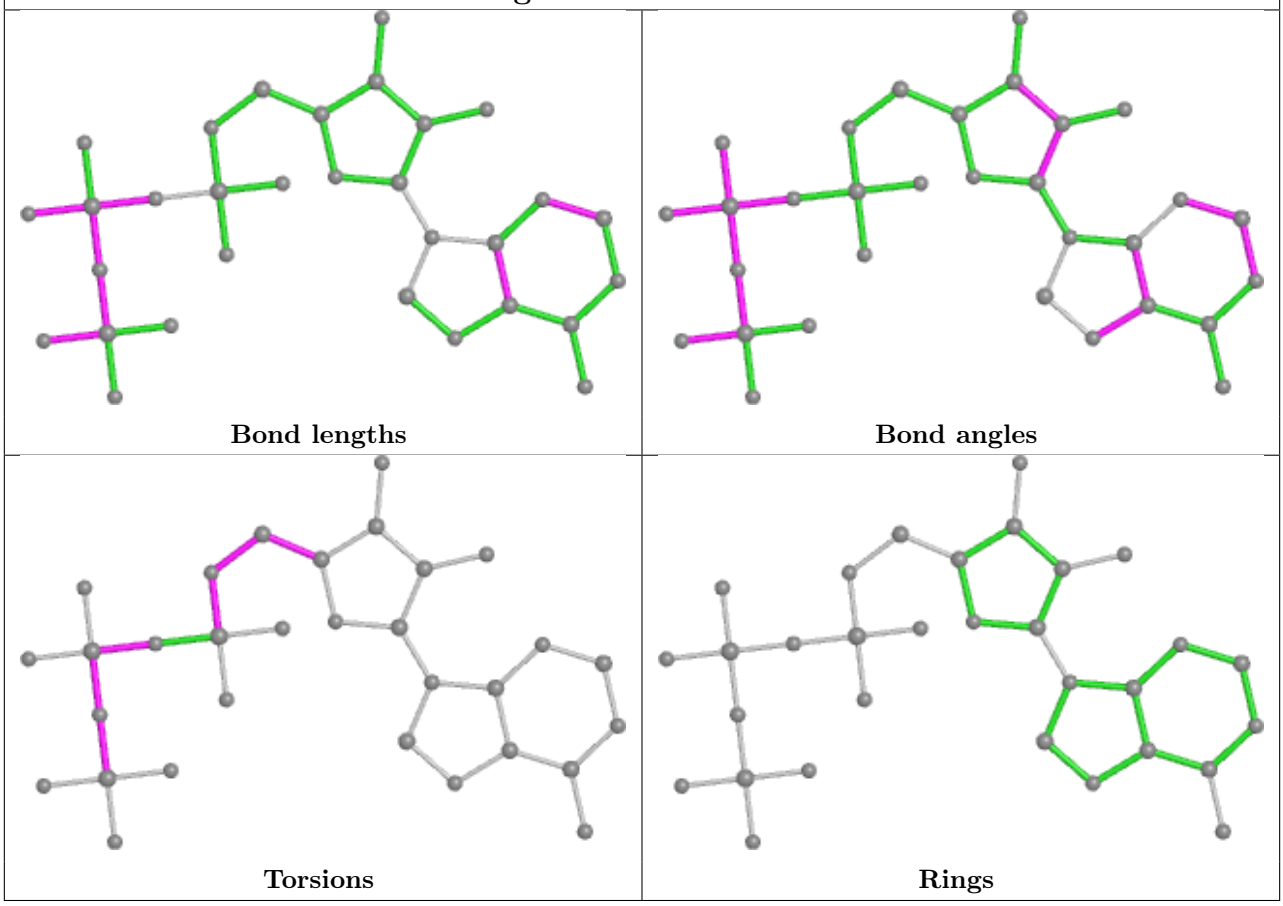


Ligand ANP C 2400



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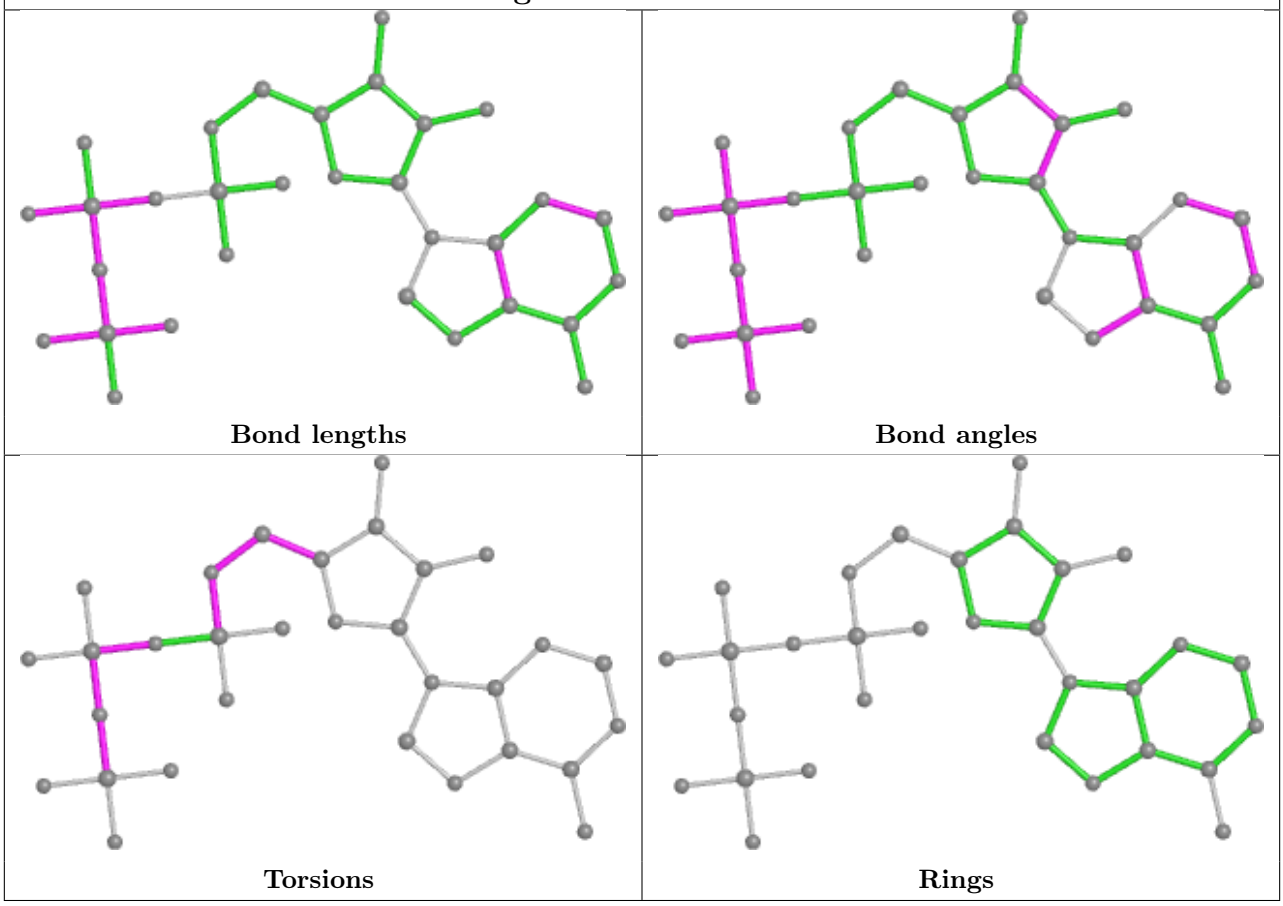

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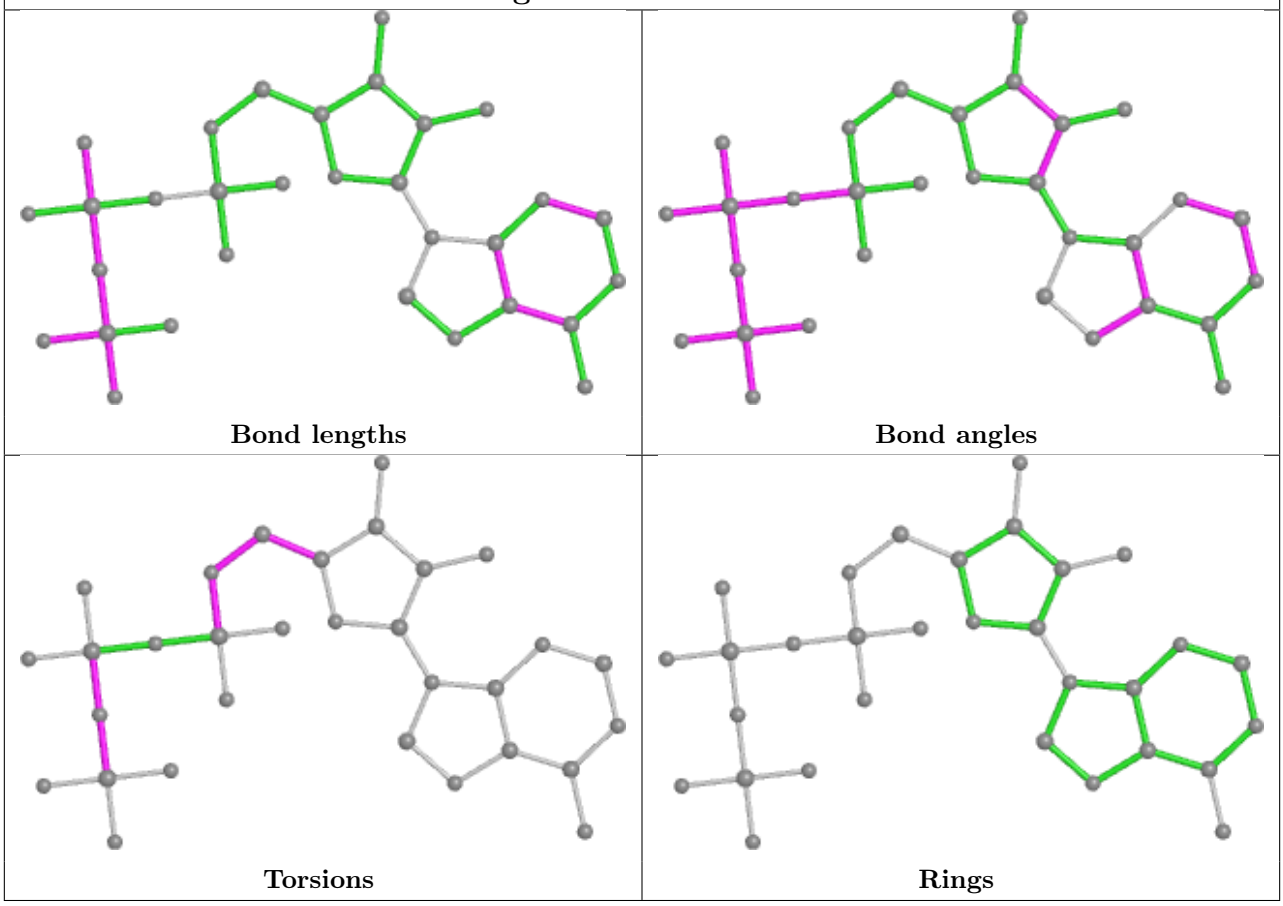

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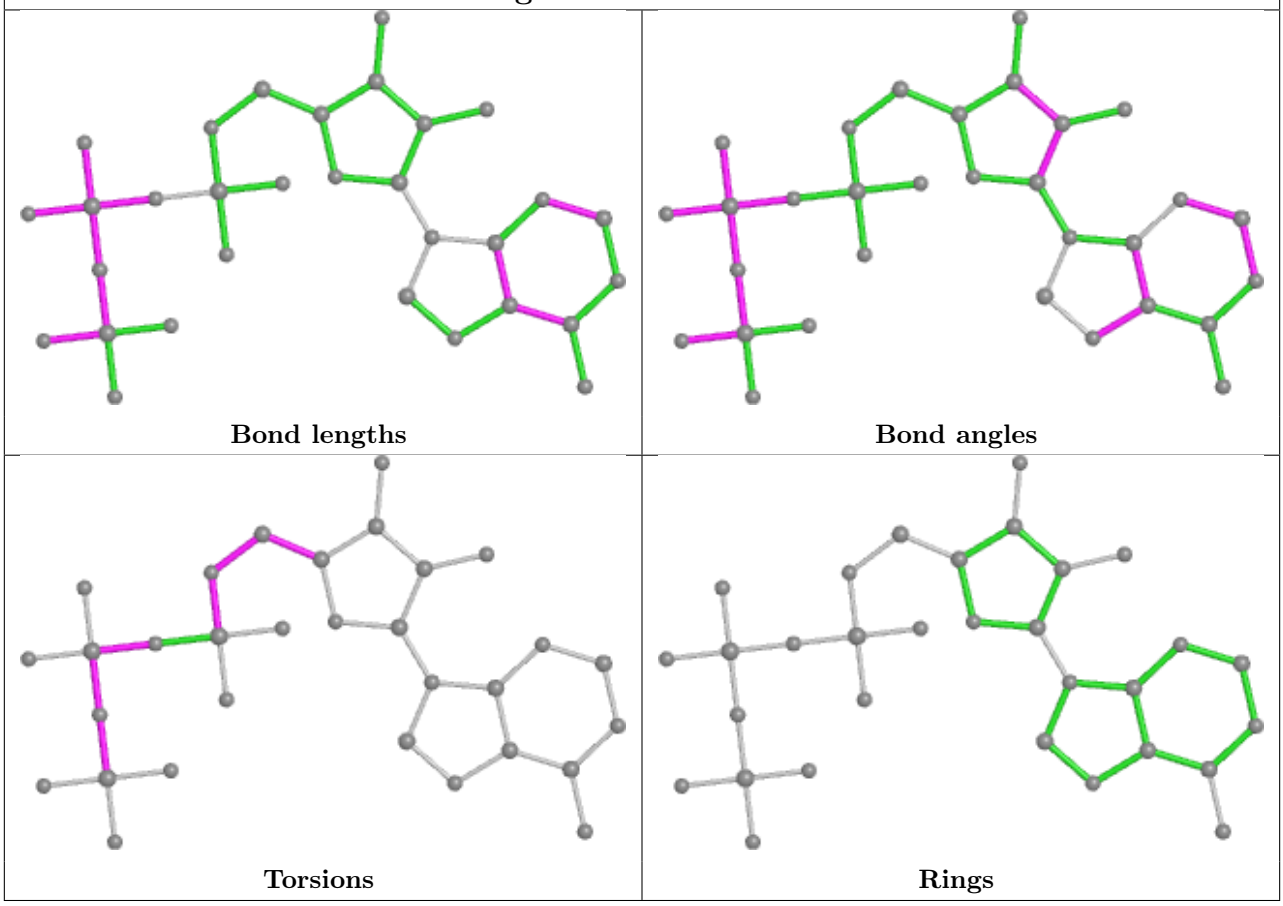

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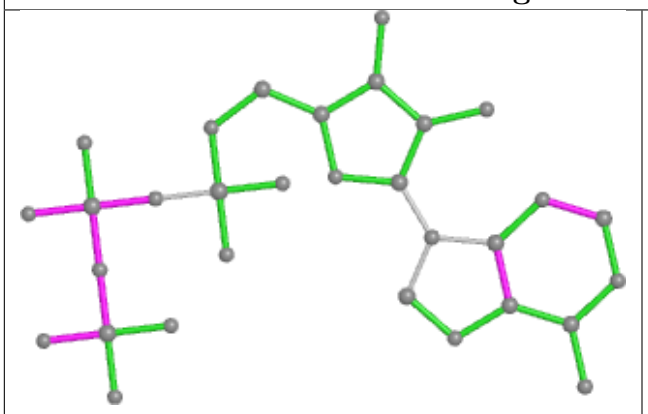
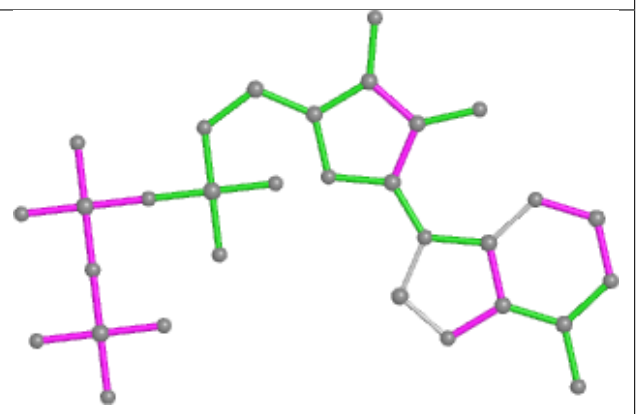
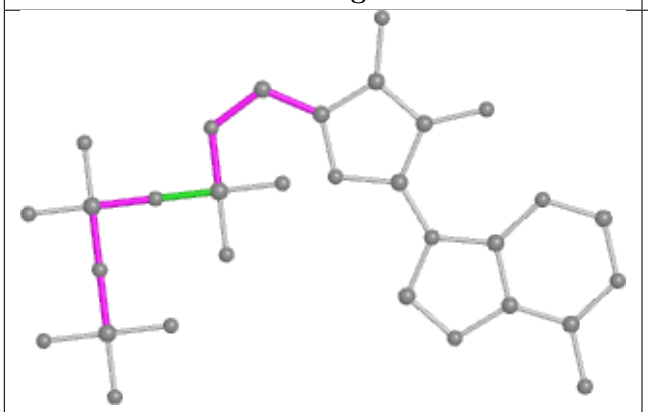


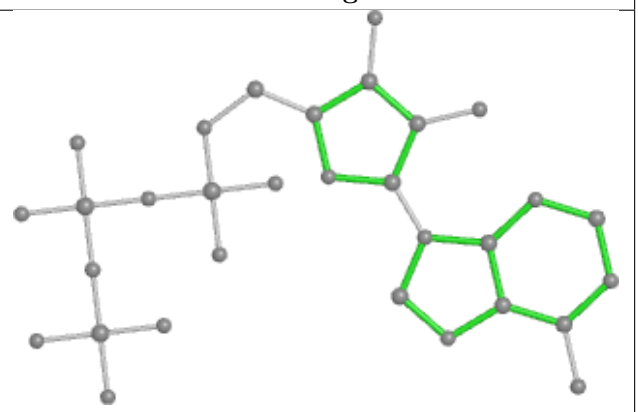
Bond lengths



Bond angles

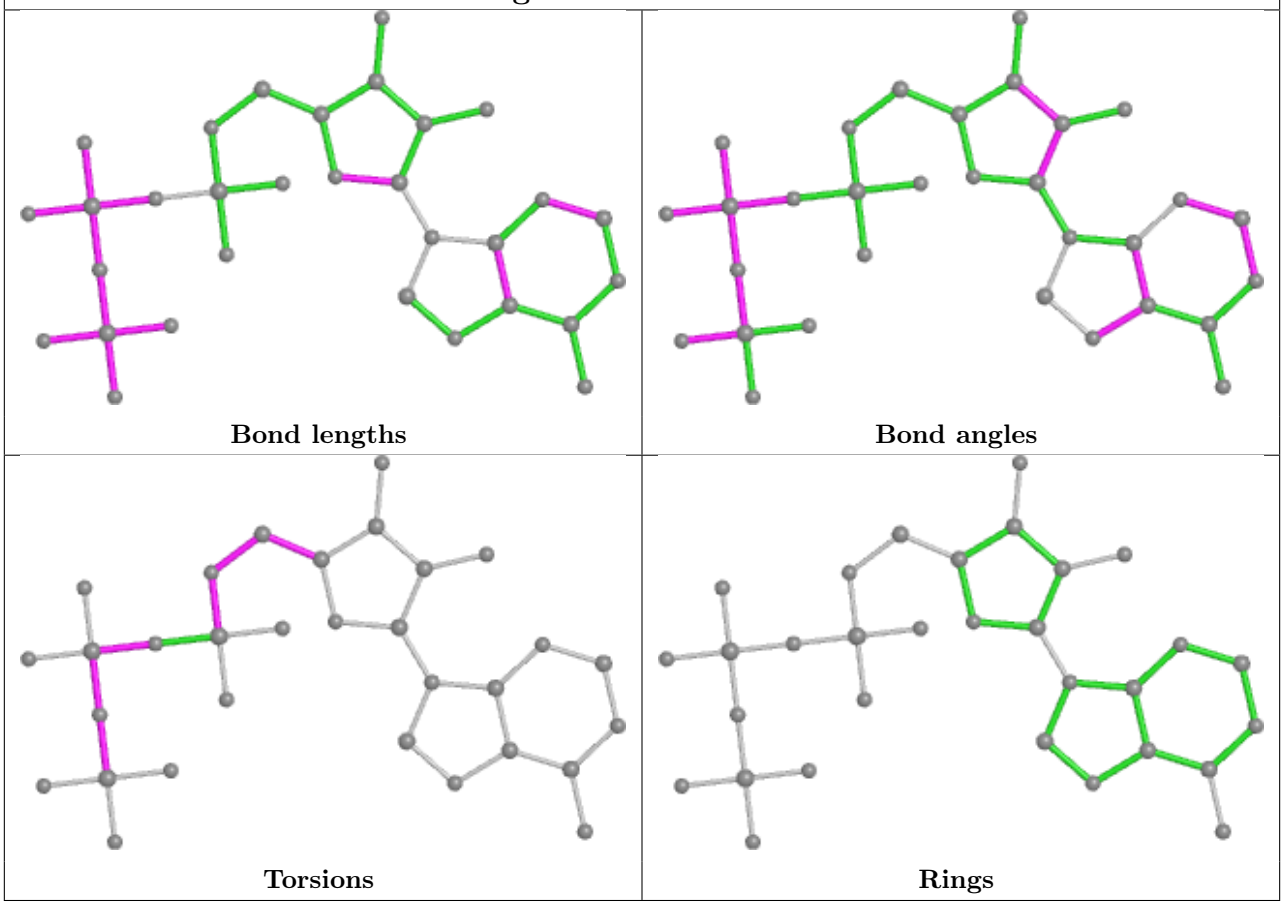


Torsions

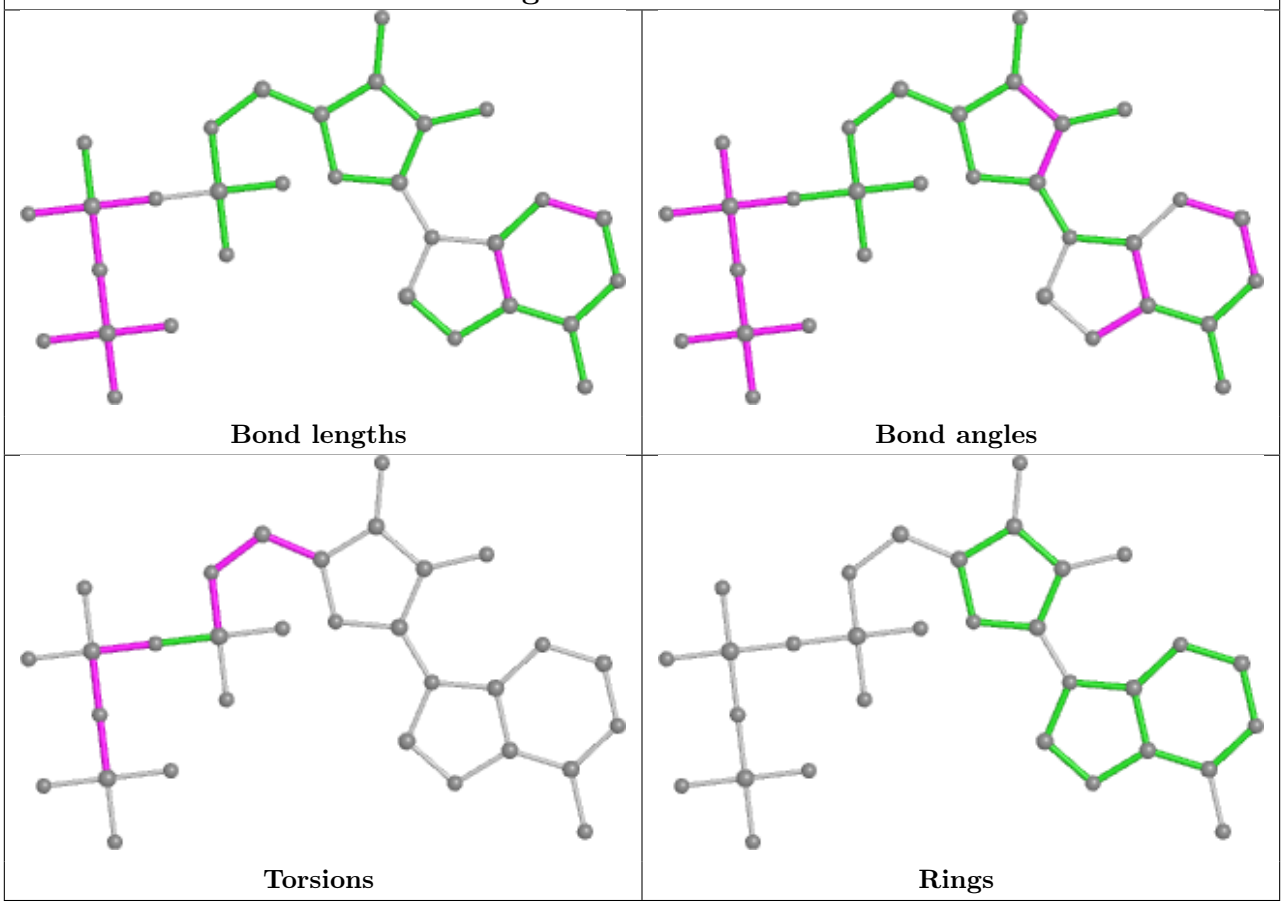


Rings

Ligand ANP H 2400



Ligand ANP A 400



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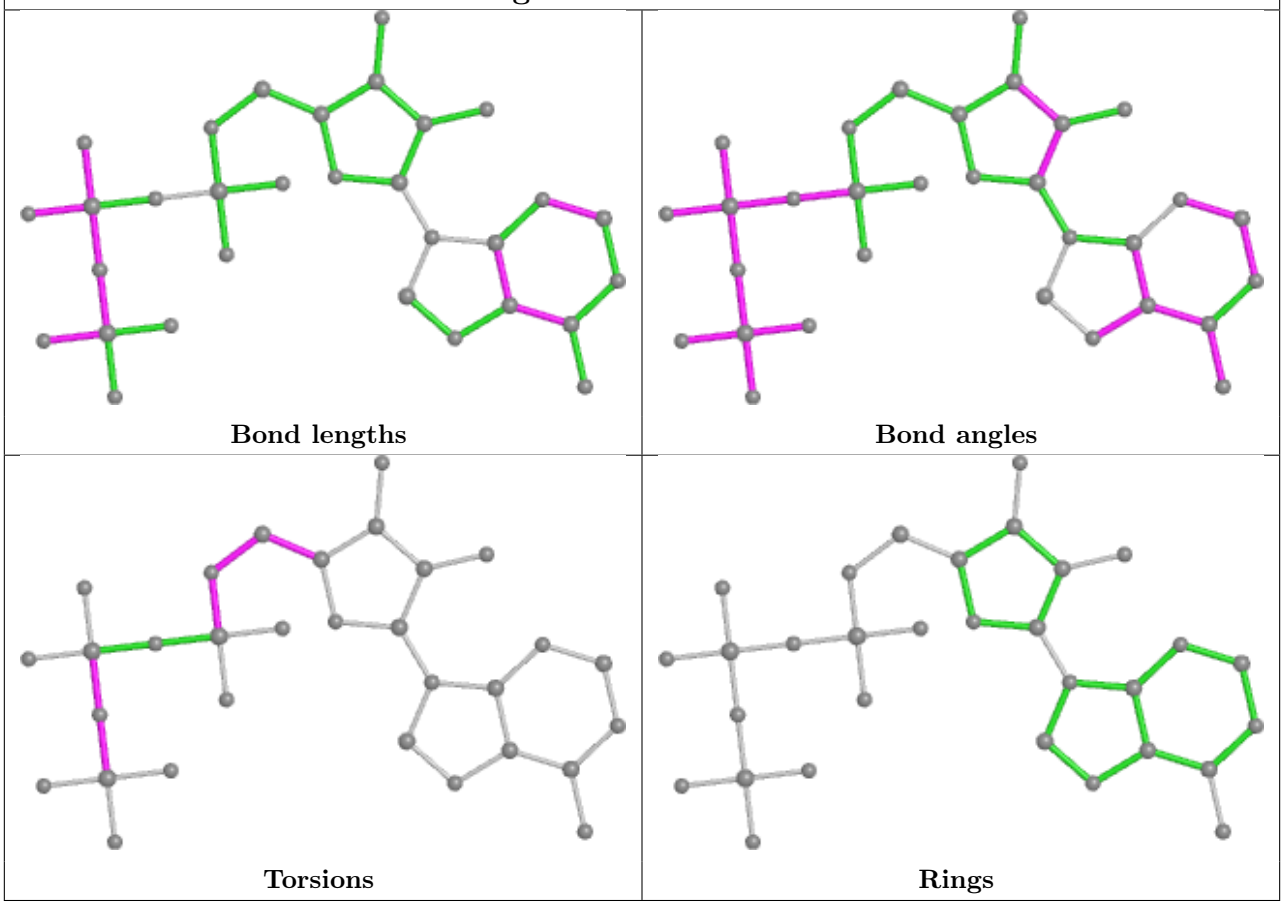

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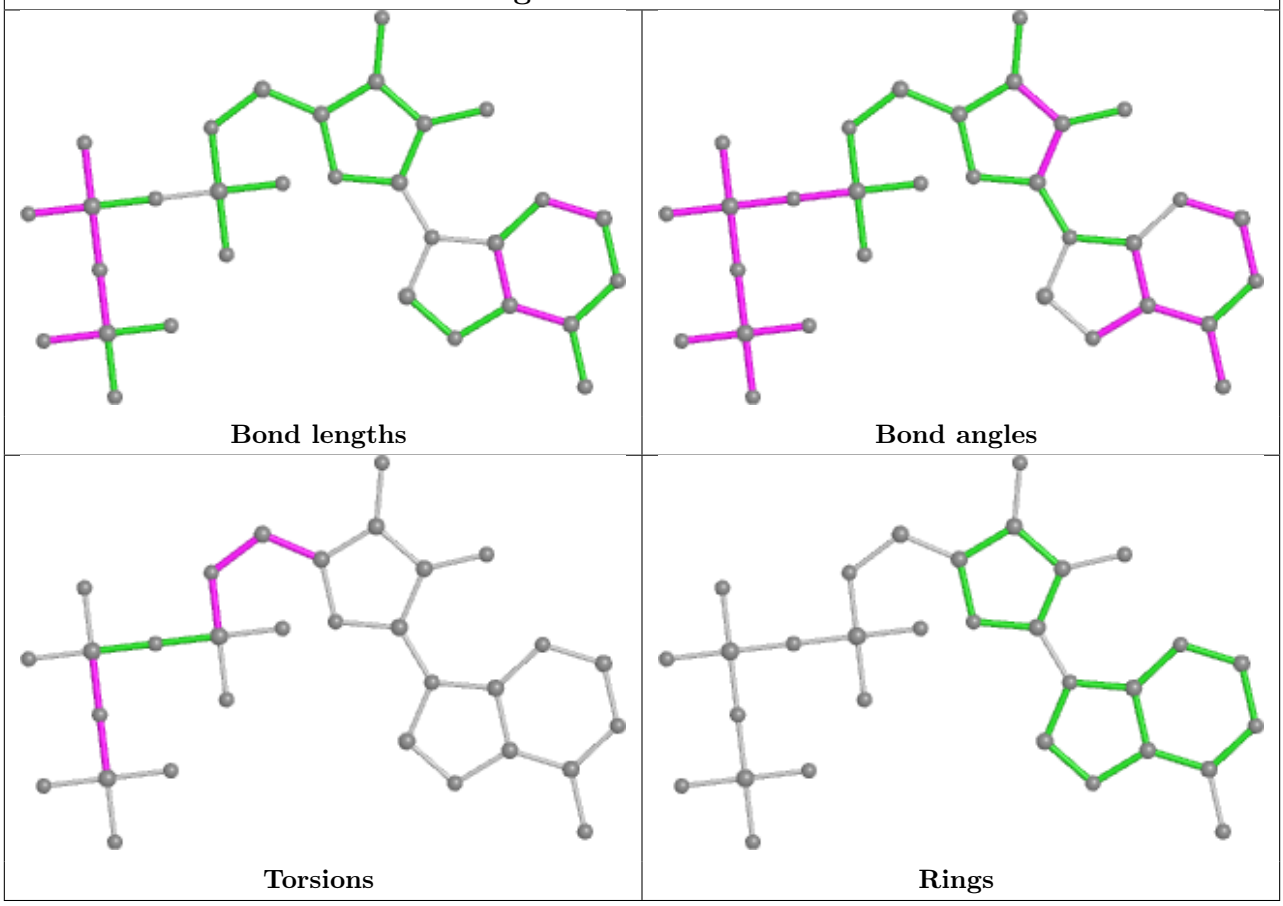

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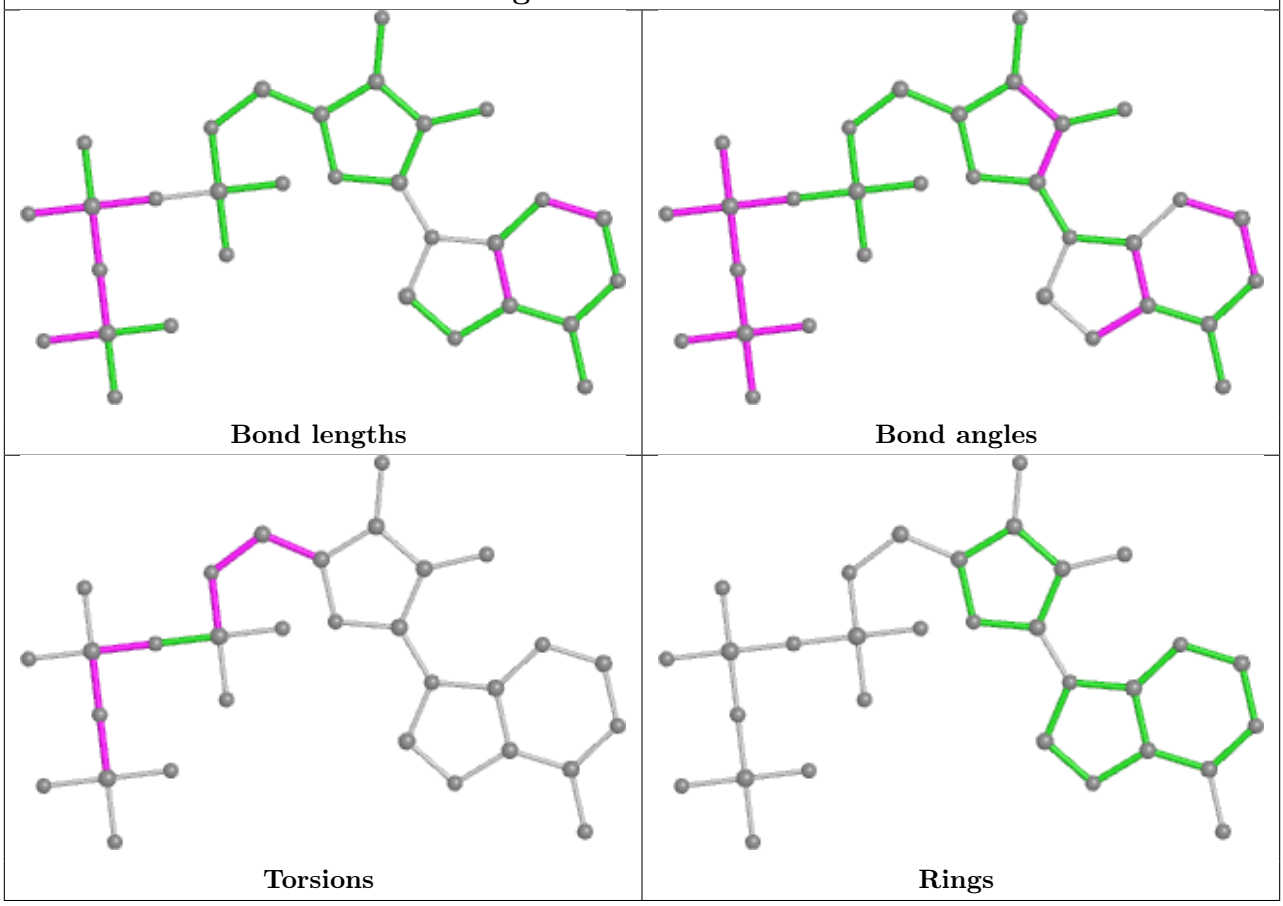

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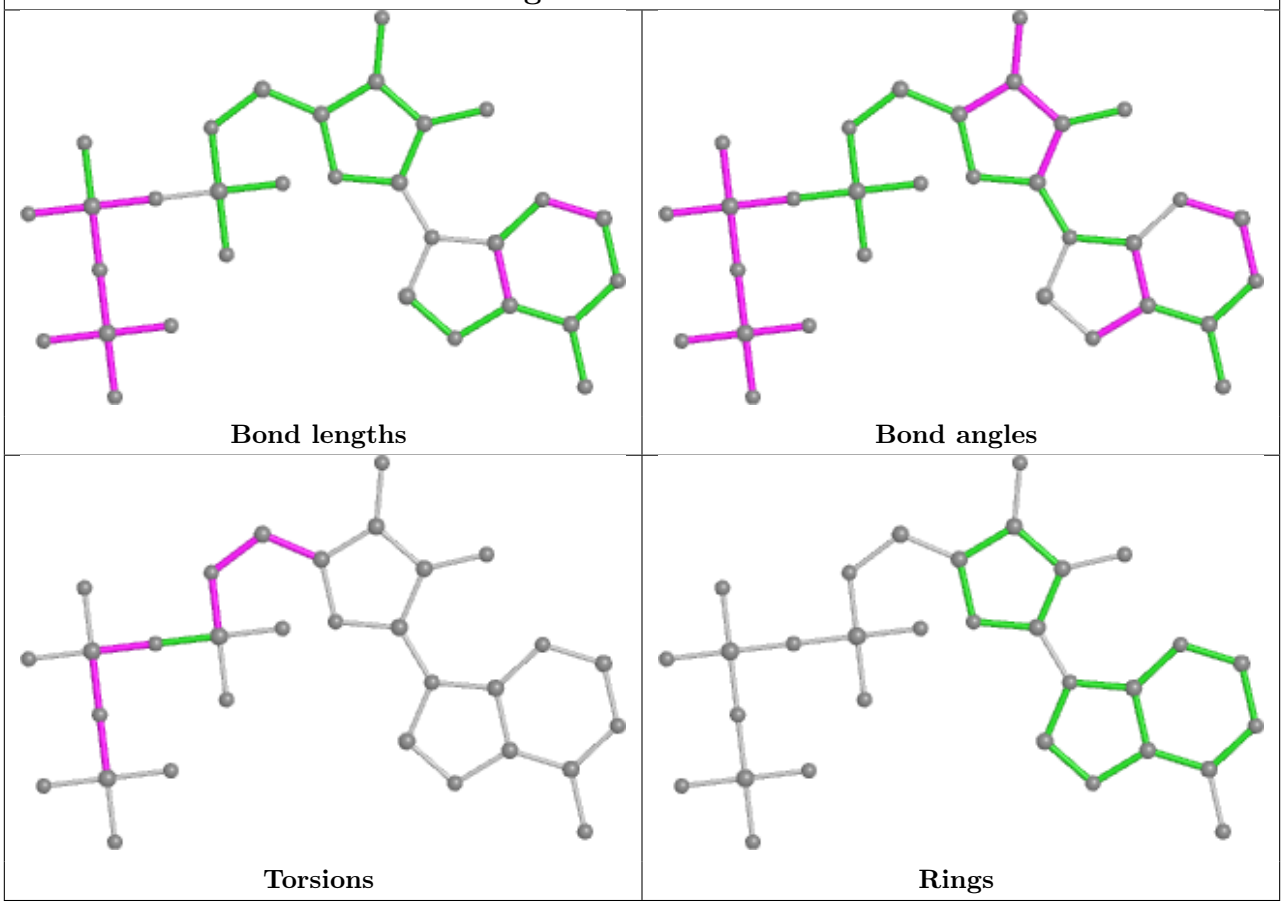

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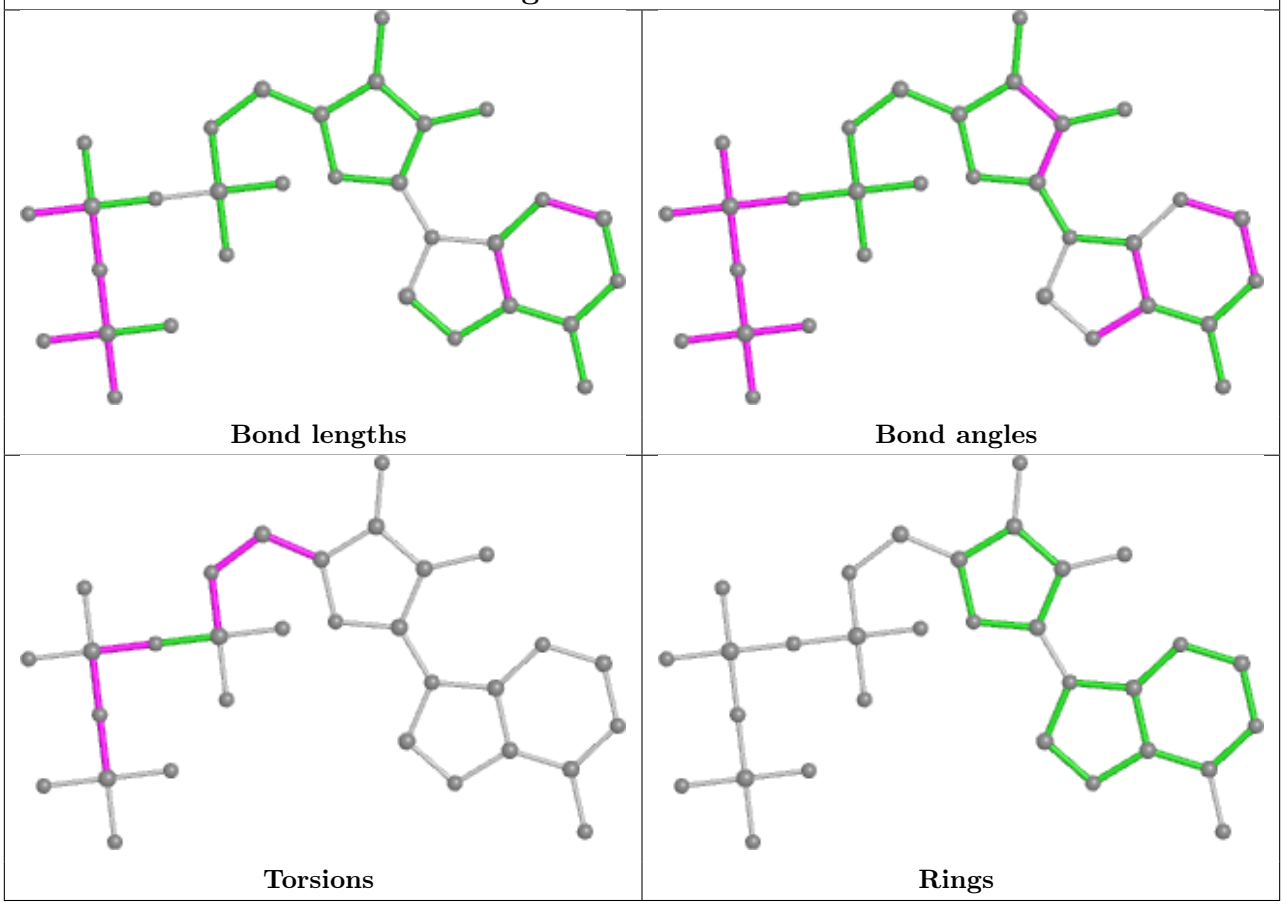

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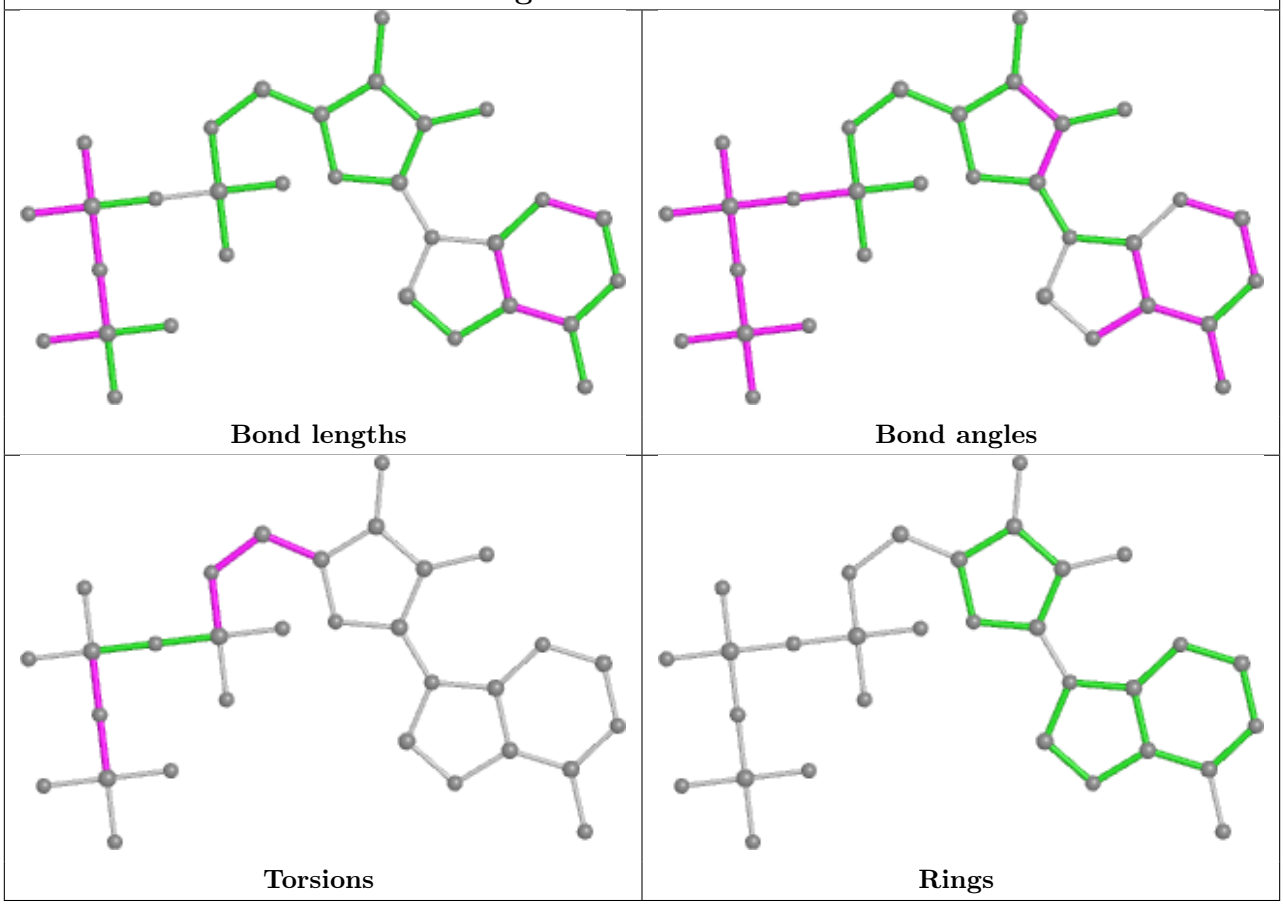
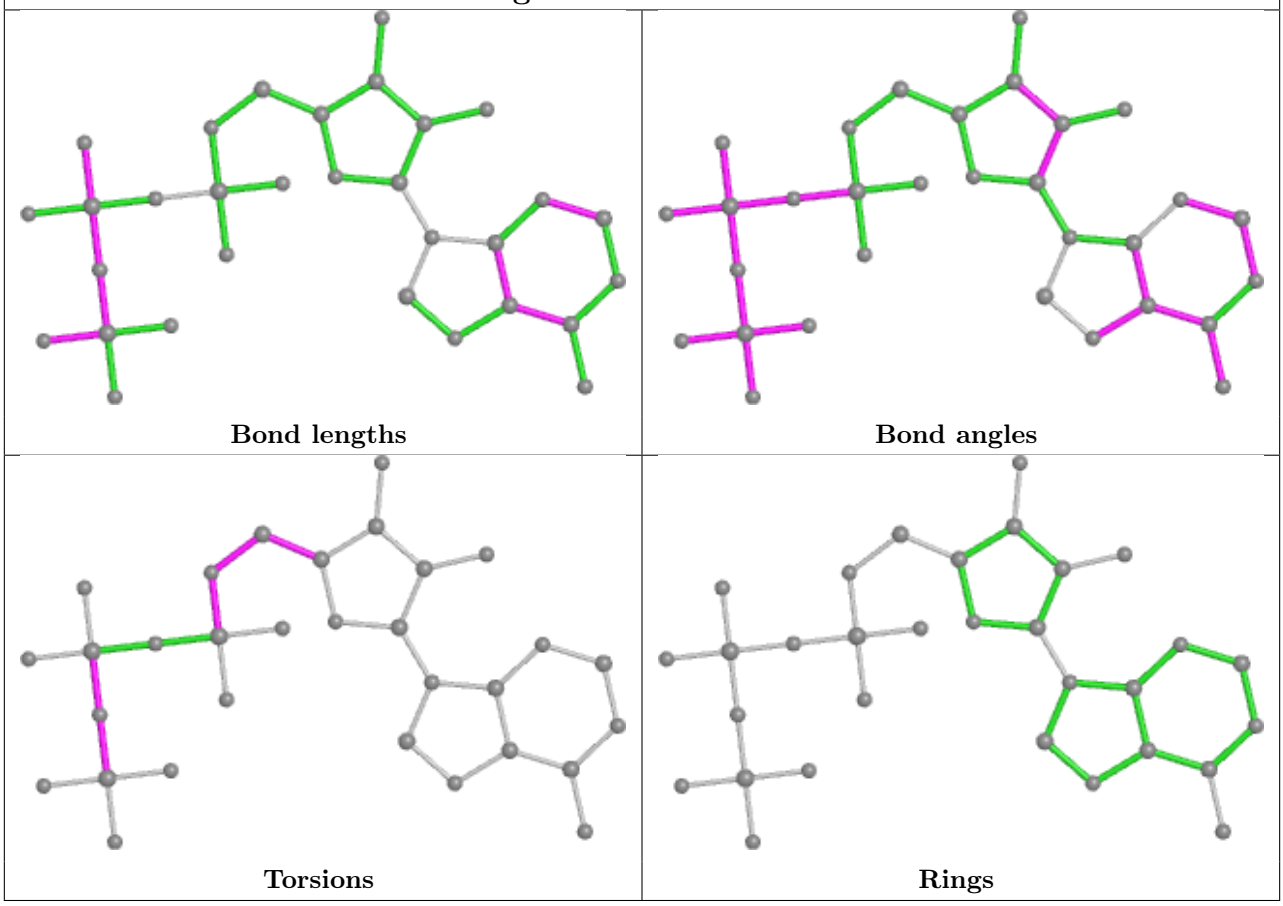
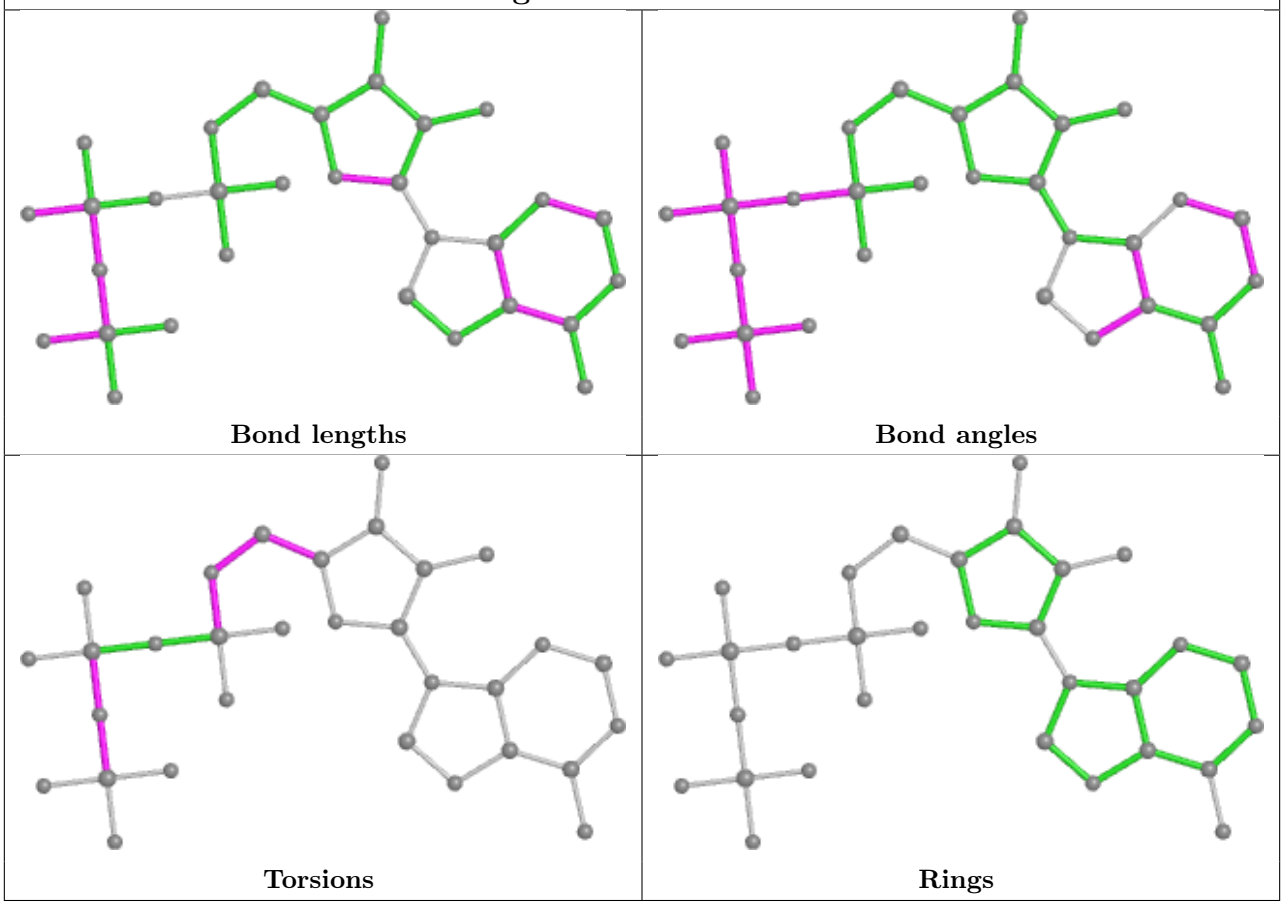


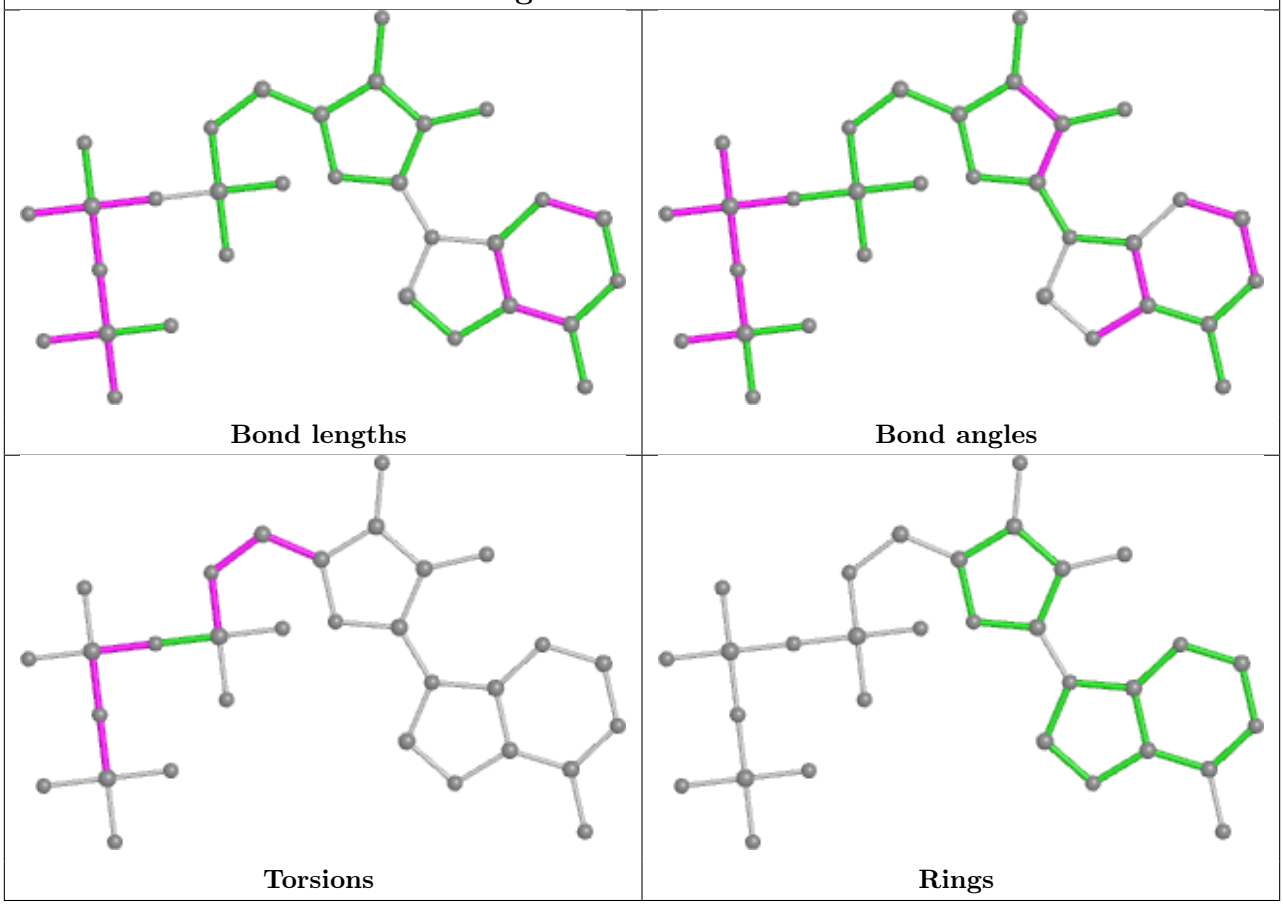
Ligand ANP A 3400



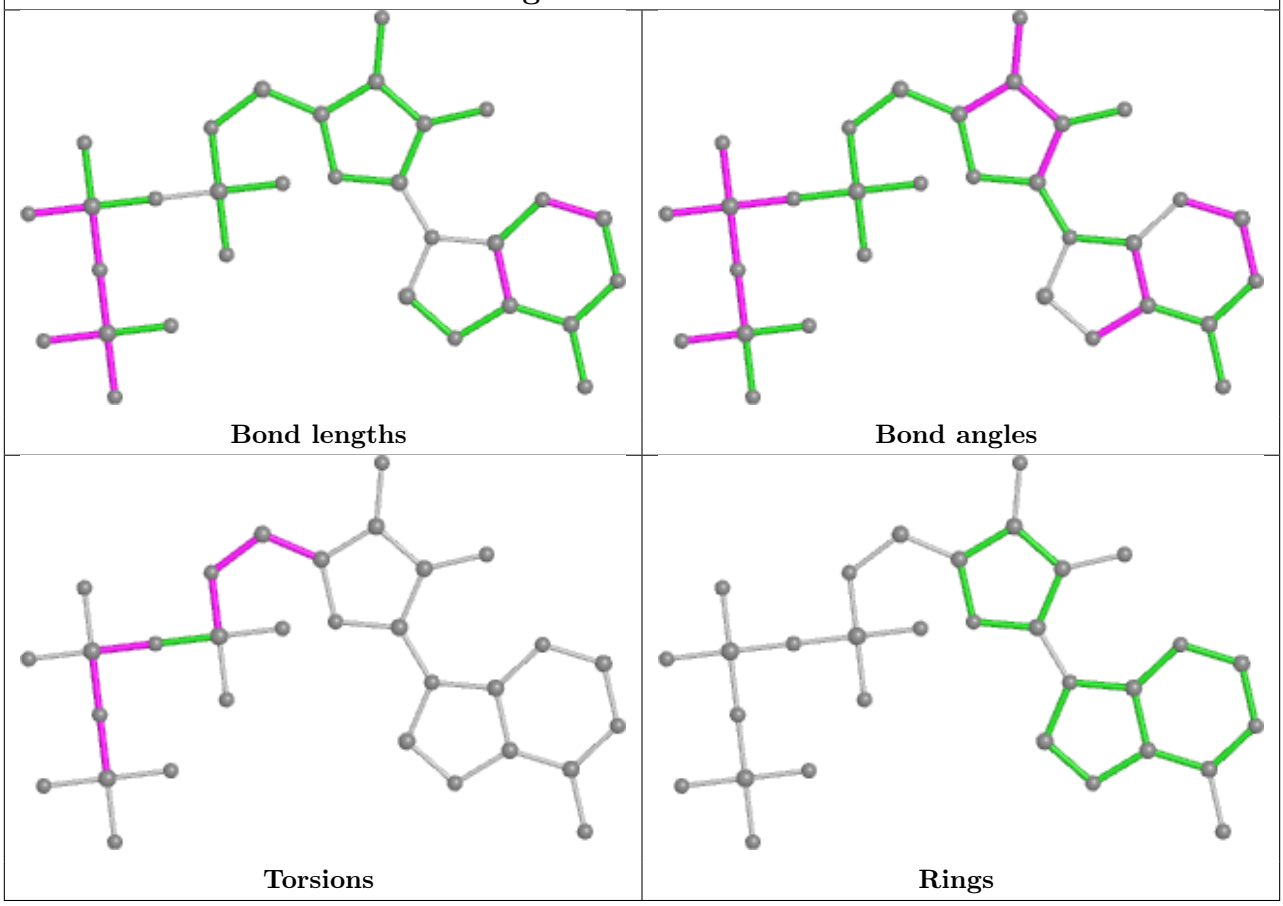
Ligand ANP G 3400



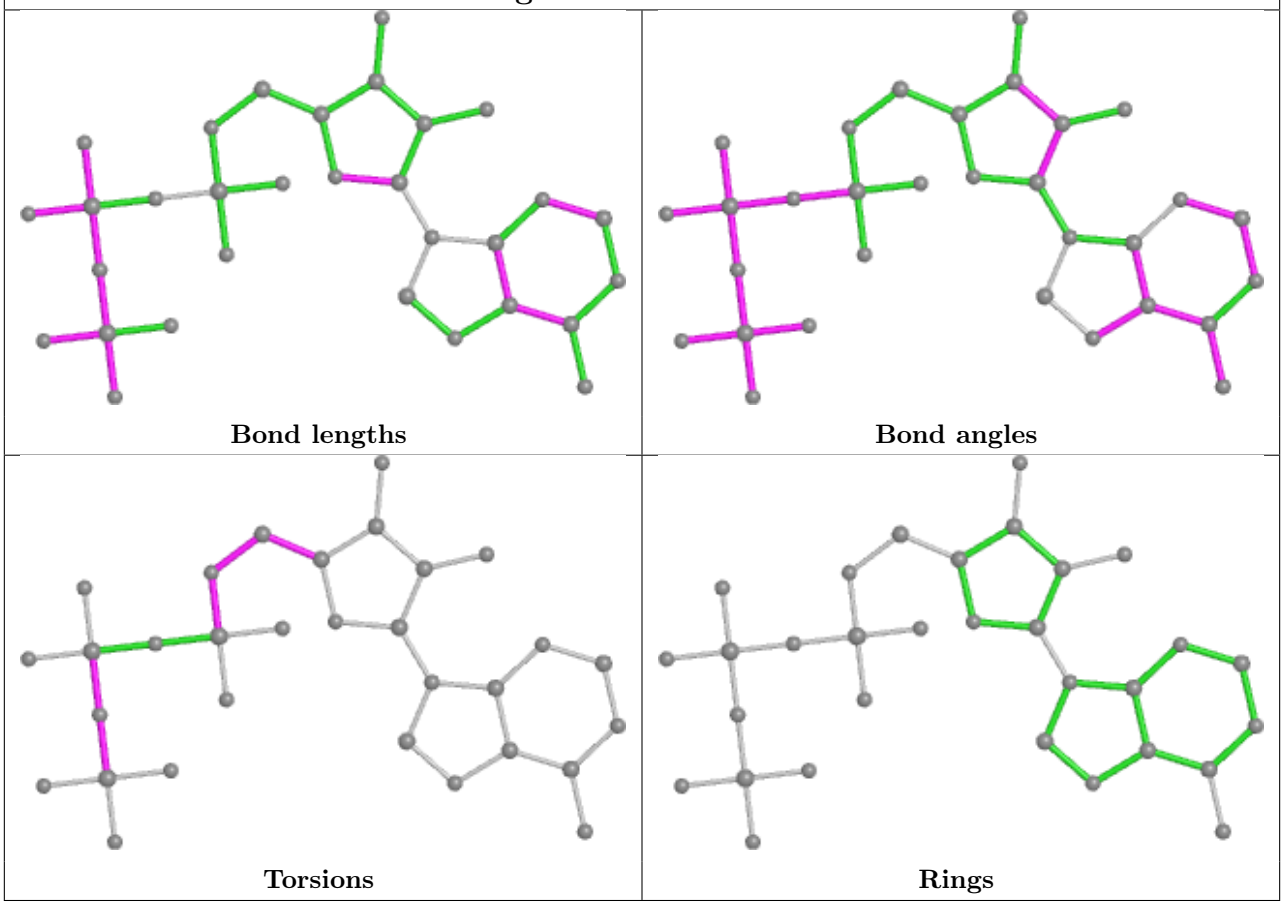
Ligand ANP F 1400



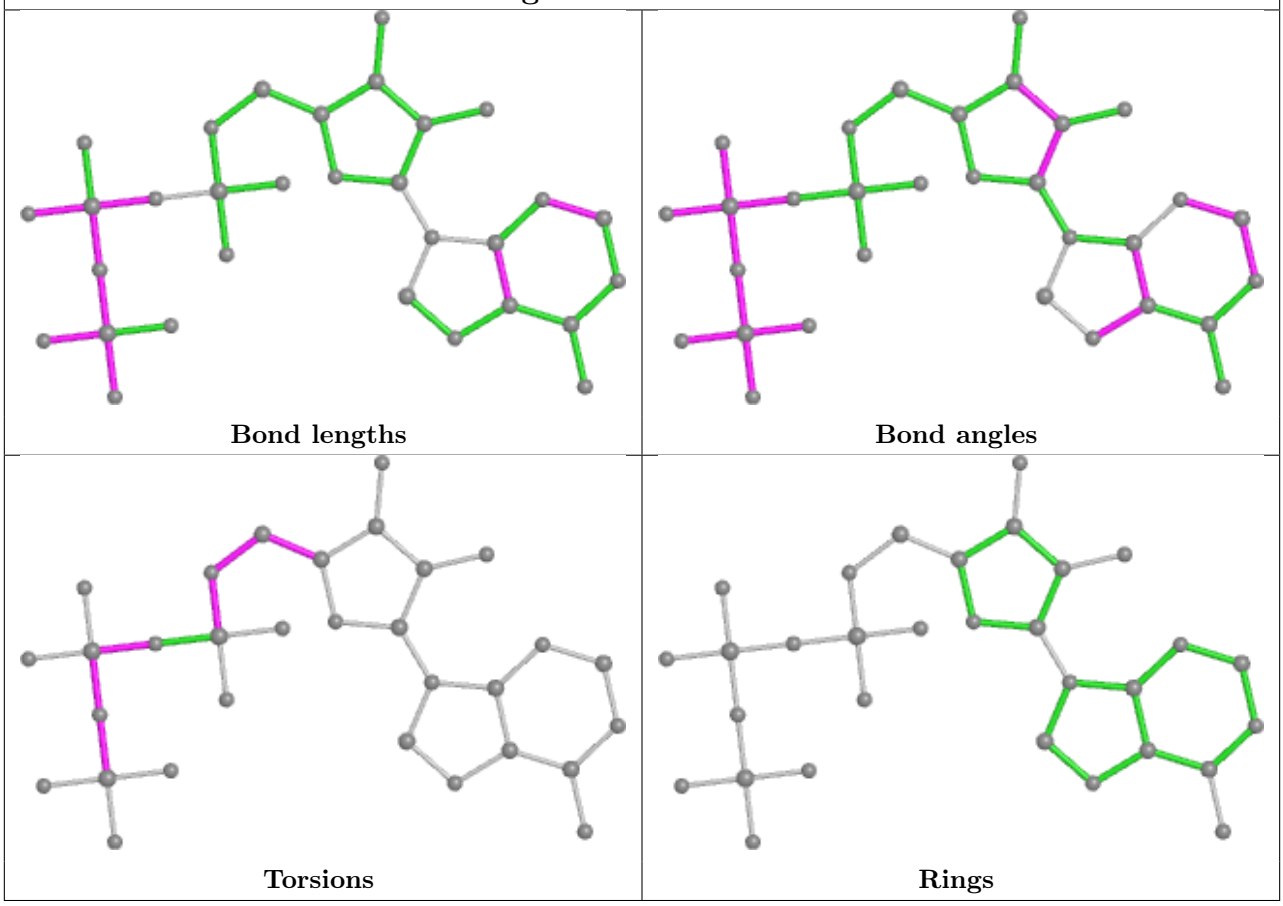
Ligand ANP C 400



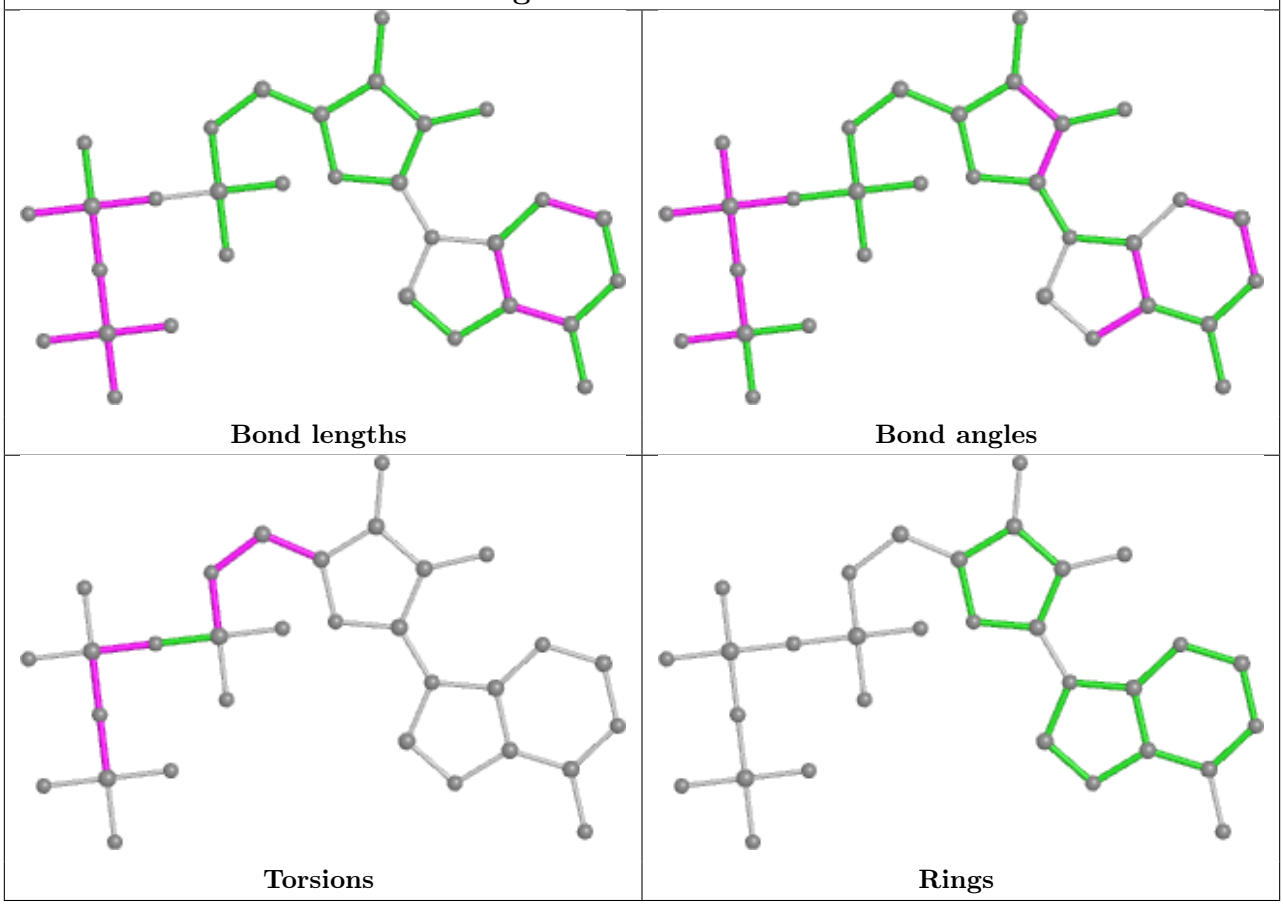
Ligand ANP F 3400



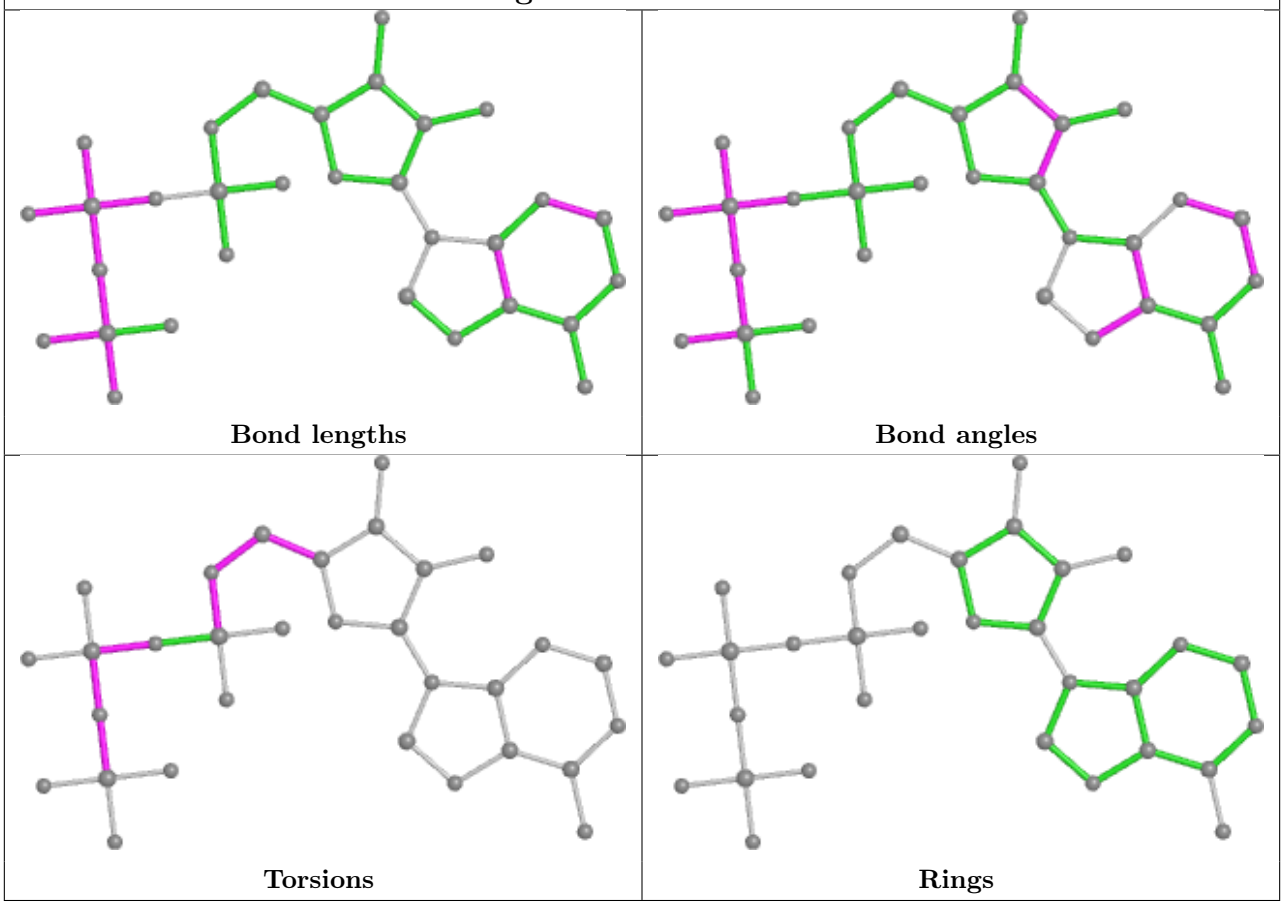
Ligand ANP H 400



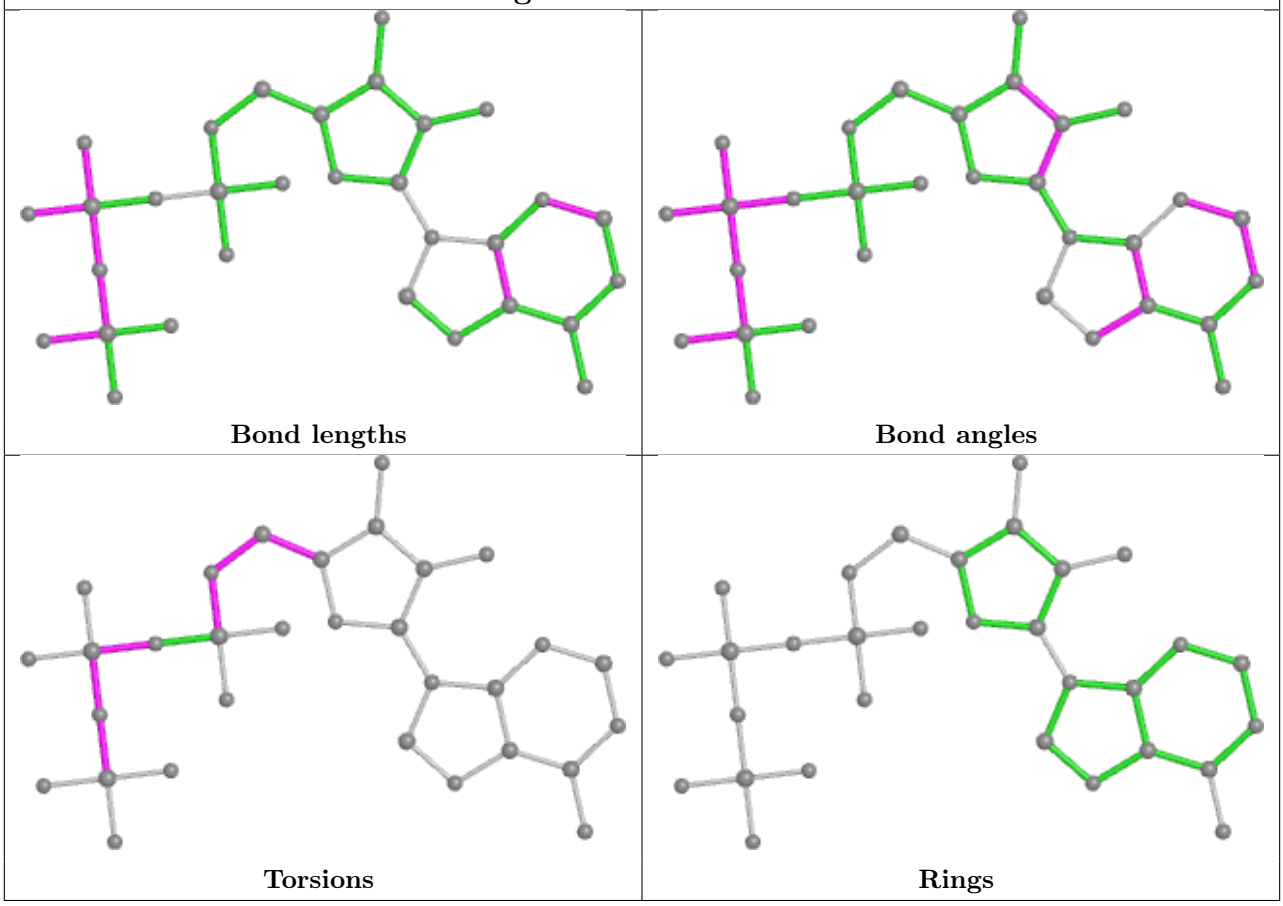
Ligand ANP A 1400



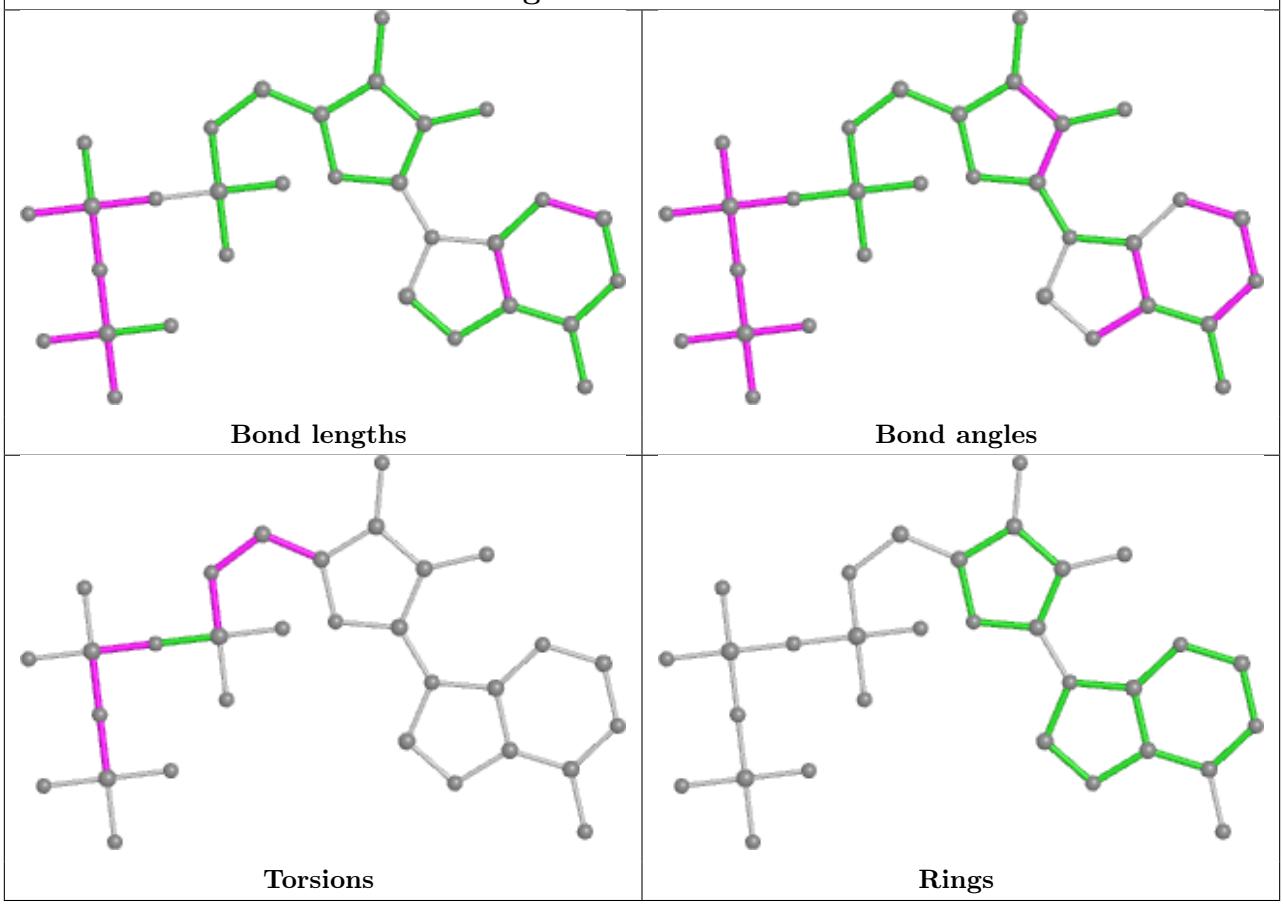
Ligand ANP F 2400



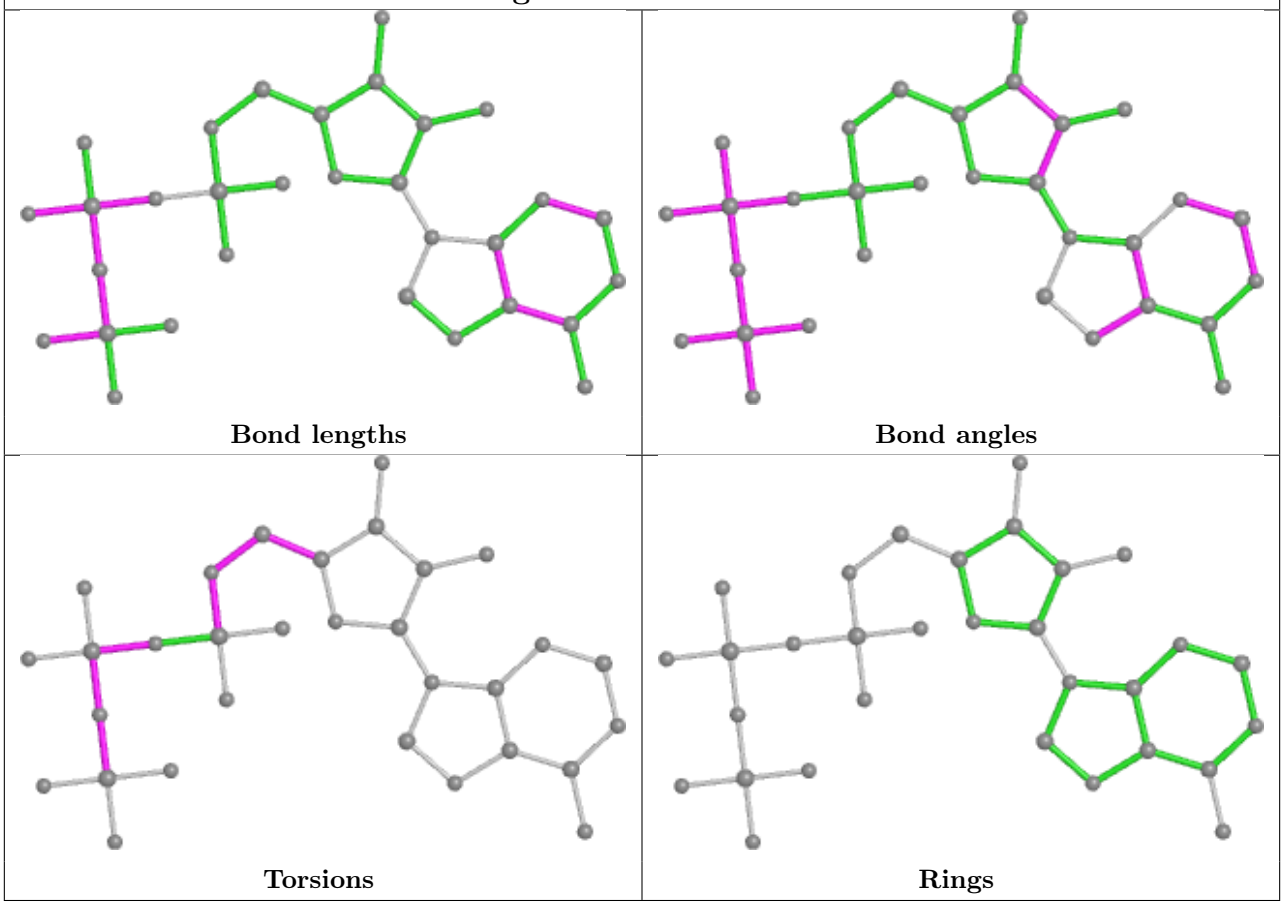
Ligand ANP B 1400



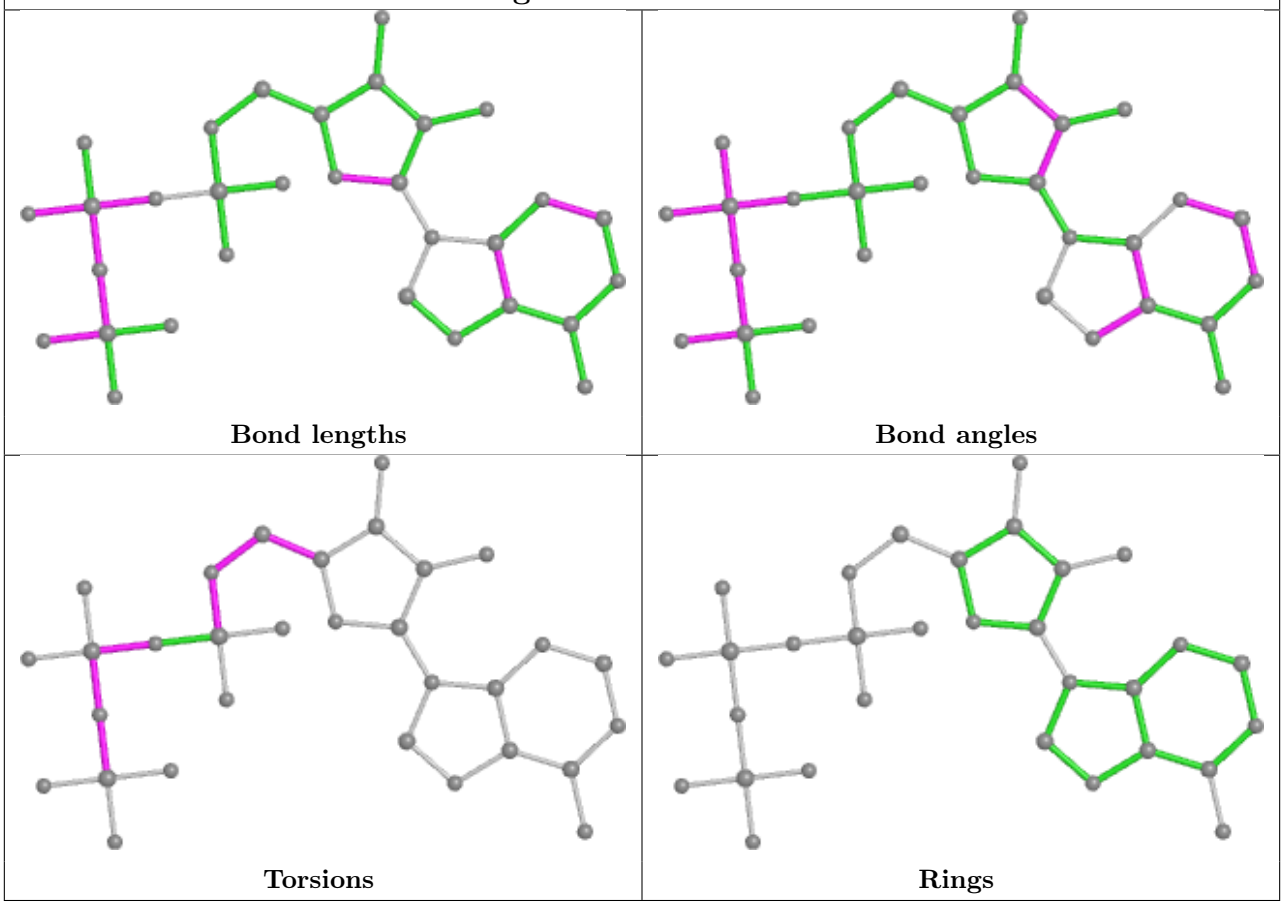
Ligand ANP B 400



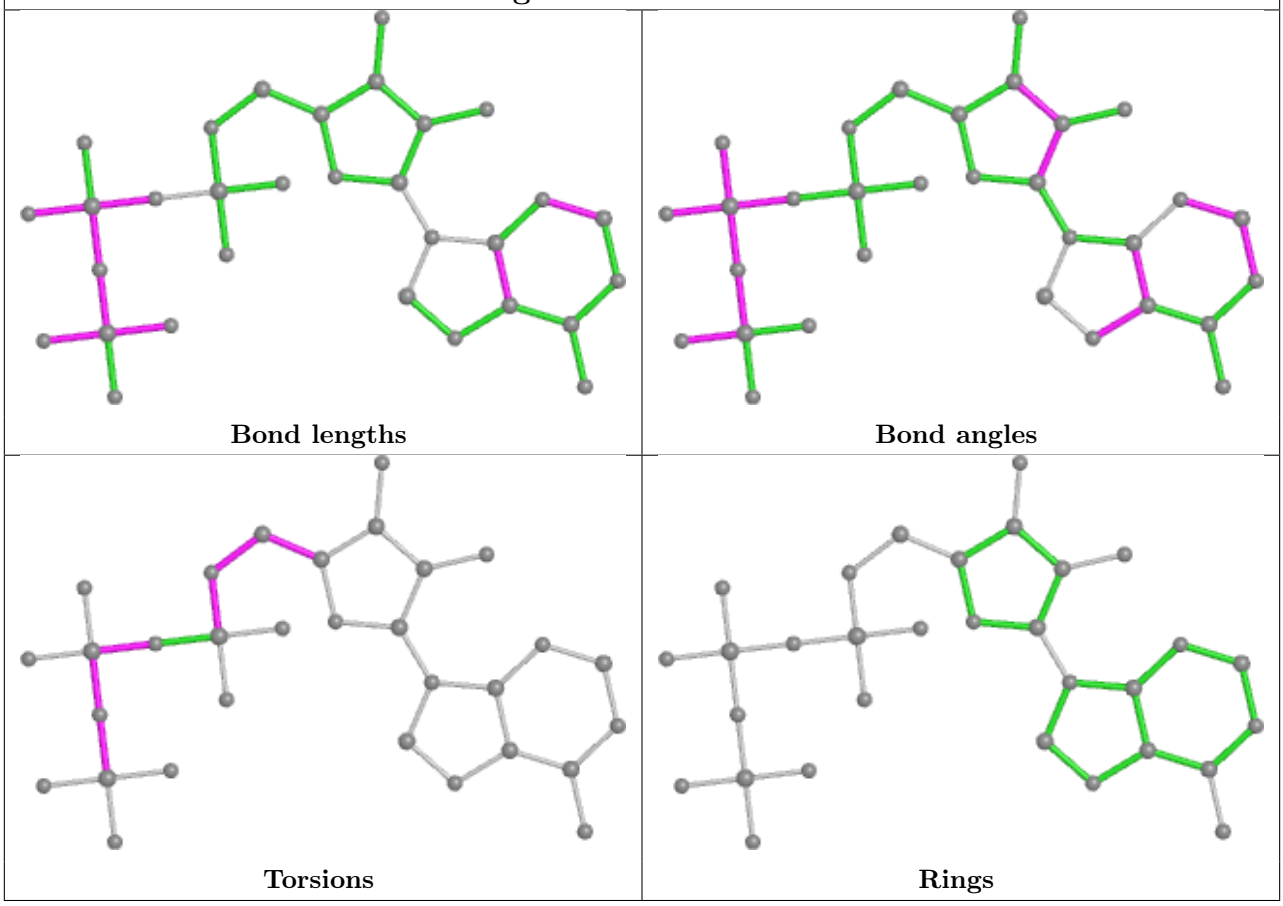
Ligand ANP H 1400



Ligand ANP D 2400



Ligand ANP A 2400



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	1190/1357 (87%)	-0.16	14 (1%)	79	70	181, 217, 253, 285	0
1	B	1163/1357 (85%)	-0.31	10 (0%)	84	77	175, 217, 254, 286	0
1	C	1175/1357 (86%)	-0.23	12 (1%)	82	74	187, 216, 253, 284	0
1	D	1175/1357 (86%)	-0.15	28 (2%)	59	49	181, 218, 256, 286	0
1	E	1165/1357 (85%)	-0.18	16 (1%)	75	66	186, 218, 255, 288	0
1	F	1175/1357 (86%)	-0.19	10 (0%)	84	77	185, 217, 255, 285	0
1	G	1167/1357 (85%)	-0.22	10 (0%)	84	77	185, 216, 254, 291	0
1	H	1173/1357 (86%)	-0.21	23 (1%)	65	56	186, 218, 255, 288	0
All	All	9383/10856 (86%)	-0.21	123 (1%)	77	68	175, 217, 255, 291	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	3151	PRO	6.3
1	A	3151	PRO	5.8
1	C	3151	PRO	4.9
1	E	3151	PRO	4.7
1	G	161	ASP	4.6
1	D	211	GLY	4.5
1	D	38	GLU	4.5
1	C	2137	ALA	4.4
1	D	39	THR	4.2
1	D	3151	PRO	4.2
1	A	3211	GLY	4.1
1	H	1325	GLU	4.1
1	B	3151	PRO	3.8
1	F	3211	GLY	3.8
1	C	211	GLY	3.7
1	A	1053	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	3211	GLY	3.6
1	G	3151	PRO	3.6
1	H	309	LEU	3.5
1	B	2237	VAL	3.5
1	D	212	GLY	3.4
1	B	57	PRO	3.3
1	D	1300	GLN	3.3
1	H	293	TYR	3.3
1	E	120	ASP	3.3
1	C	3211	GLY	3.2
1	E	3136	GLY	3.2
1	D	295	GLY	3.1
1	H	3151	PRO	3.1
1	D	57	PRO	3.1
1	E	37	VAL	3.0
1	E	3135	SER	3.0
1	H	310	LYS	3.0
1	A	1023	LYS	3.0
1	F	294	LYS	3.0
1	H	291	TYR	2.9
1	G	3167	ALA	2.9
1	H	298	ILE	2.9
1	D	137	ALA	2.9
1	D	1299	GLY	2.9
1	A	1197	MET	2.9
1	E	3167	ALA	2.8
1	A	3167	ALA	2.8
1	C	2165	GLY	2.8
1	D	253	ALA	2.8
1	B	1137	ALA	2.8
1	H	308	TRP	2.8
1	F	1150	THR	2.8
1	B	37	VAL	2.7
1	C	3288	GLY	2.7
1	G	60	ARG	2.7
1	D	1211	GLY	2.7
1	D	150	THR	2.6
1	E	2138	VAL	2.6
1	B	60	ARG	2.6
1	F	162	SER	2.5
1	E	137	ALA	2.5
1	F	295	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1163	HIS	2.5
1	G	2054	GLY	2.5
1	F	2298	ILE	2.5
1	H	1237	VAL	2.5
1	D	1298	ILE	2.4
1	D	285	GLU	2.4
1	A	3291	TYR	2.4
1	D	53	ALA	2.4
1	H	305	ALA	2.4
1	H	301	GLY	2.3
1	G	1008	LYS	2.3
1	C	3117	SER	2.3
1	D	172	SER	2.3
1	H	2213	ASN	2.3
1	D	1090	CYS	2.3
1	C	238	VAL	2.3
1	D	55	GLY	2.3
1	H	1137	ALA	2.3
1	H	292	SER	2.3
1	C	240	SER	2.3
1	D	54	GLY	2.2
1	F	3290	TRP	2.2
1	A	53	ALA	2.2
1	D	297	LYS	2.2
1	E	2036	ASP	2.2
1	C	239	GLY	2.2
1	A	3300	GLN	2.2
1	H	162	SER	2.2
1	A	1054	GLY	2.2
1	E	3134	ARG	2.2
1	H	311	ASP	2.2
1	B	38	GLU	2.2
1	G	3176	ARG	2.2
1	A	3297	LYS	2.1
1	D	37	VAL	2.1
1	H	1090	CYS	2.1
1	D	60	ARG	2.1
1	C	3287	ALA	2.1
1	G	1007	GLN	2.1
1	A	284	ILE	2.1
1	D	1291	TYR	2.1
1	E	2281	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	3167	ALA	2.1
1	H	306	THR	2.1
1	D	1325	GLU	2.1
1	H	312	ASN	2.1
1	H	2256	LYS	2.1
1	E	38	GLU	2.1
1	G	315	THR	2.1
1	E	2309	LEU	2.1
1	B	1035	MET	2.1
1	A	1024	GLY	2.1
1	G	2098	ALA	2.1
1	H	2035	MET	2.0
1	B	2238	VAL	2.0
1	D	1297	LYS	2.0
1	E	3211	GLY	2.0
1	H	304	ASN	2.0
1	D	1009	ALA	2.0
1	F	3287	ALA	2.0
1	E	295	GLY	2.0
1	D	1012	ALA	2.0
1	F	302	LYS	2.0
1	A	3299	GLY	2.0
1	E	2316	ALA	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	G	701	1/1	0.54	0.94	215,215,215,215	0
2	MG	E	701	1/1	0.57	1.16	204,204,204,204	0
2	MG	C	701	1/1	0.59	0.60	177,177,177,177	0
2	MG	D	2701	1/1	0.69	0.40	237,237,237,237	0
2	MG	B	2701	1/1	0.70	0.25	238,238,238,238	0
3	ANP	F	2400	31/31	0.72	0.43	286,303,310,310	0
3	ANP	G	2400	31/31	0.72	0.41	303,308,315,315	0
3	ANP	H	2400	31/31	0.72	0.38	298,312,316,316	0
2	MG	B	1701	1/1	0.74	0.41	214,214,214,214	0
3	ANP	D	1400	31/31	0.75	0.38	287,290,294,294	0
2	MG	D	1701	1/1	0.75	1.14	212,212,212,212	0
3	ANP	A	1400	31/31	0.76	0.36	267,280,283,283	0
2	MG	D	701	1/1	0.77	0.62	261,261,261,261	0
3	ANP	E	1400	31/31	0.79	0.31	287,293,296,296	0
3	ANP	B	2400	31/31	0.79	0.34	306,312,314,314	0
2	MG	F	2701	1/1	0.80	0.37	232,232,232,232	0
3	ANP	B	400	31/31	0.80	0.33	242,255,259,260	0
3	ANP	G	1400	31/31	0.81	0.25	279,285,289,290	0
2	MG	H	2701	1/1	0.82	0.35	271,271,271,271	0
2	MG	E	1701	1/1	0.83	0.48	190,190,190,190	0
3	ANP	F	1400	31/31	0.83	0.34	271,280,286,286	0
3	ANP	H	1400	31/31	0.83	0.31	296,299,304,304	0
2	MG	C	3701	1/1	0.83	0.14	140,140,140,140	0
3	ANP	C	1400	31/31	0.84	0.25	288,291,293,294	0
3	ANP	G	400	31/31	0.84	0.28	253,262,264,265	0
3	ANP	D	400	31/31	0.84	0.29	263,273,274,274	0
2	MG	B	701	1/1	0.84	1.12	184,184,184,184	0
3	ANP	H	400	31/31	0.84	0.42	254,263,265,265	0
2	MG	H	1701	1/1	0.84	0.67	188,188,188,188	0
3	ANP	C	400	31/31	0.84	0.29	226,245,250,250	0
2	MG	A	701	1/1	0.86	0.65	143,143,143,143	0
3	ANP	D	2400	31/31	0.86	0.30	305,310,315,315	0
3	ANP	A	2400	31/31	0.86	0.34	308,311,315,315	0
3	ANP	F	400	31/31	0.86	0.33	243,257,263,263	0
2	MG	A	1701	1/1	0.86	0.84	181,181,181,181	0
3	ANP	B	1400	31/31	0.86	0.30	275,286,290,290	0
2	MG	E	3701	1/1	0.87	0.20	131,131,131,131	0
2	MG	F	1701	1/1	0.87	0.57	175,175,175,175	0
3	ANP	A	400	31/31	0.88	0.27	246,250,255,256	0
2	MG	A	2701	1/1	0.88	0.16	247,247,247,247	0

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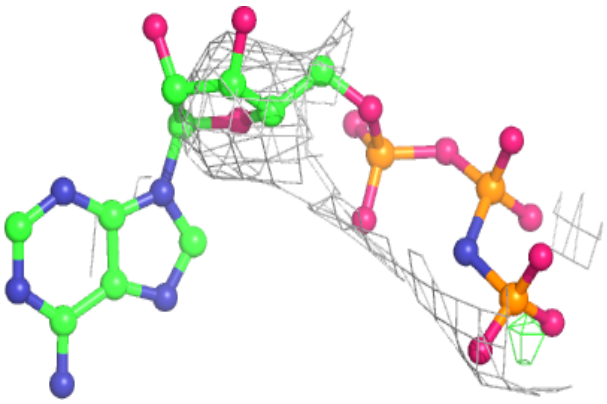
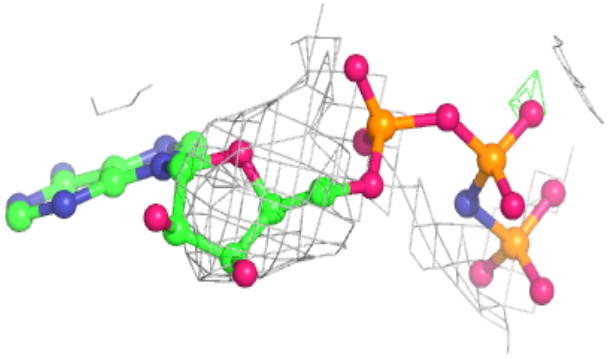
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	E	2701	1/1	0.88	0.34	228,228,228,228	0
2	MG	G	1701	1/1	0.89	0.56	191,191,191,191	0
3	ANP	E	400	31/31	0.89	0.26	256,261,264,265	0
3	ANP	C	2400	31/31	0.89	0.28	296,309,314,315	0
3	ANP	E	2400	31/31	0.90	0.25	307,317,320,320	0
3	ANP	H	3400	31/31	0.90	0.18	180,187,196,197	0
3	ANP	G	3400	31/31	0.91	0.19	153,176,191,192	0
2	MG	G	2701	1/1	0.92	0.45	192,192,192,192	0
2	MG	H	701	1/1	0.92	0.18	200,200,200,200	0
3	ANP	D	3400	31/31	0.92	0.16	149,170,188,189	0
3	ANP	F	3400	31/31	0.92	0.20	148,171,183,183	0
2	MG	C	2701	1/1	0.93	0.26	211,211,211,211	0
3	ANP	C	3400	31/31	0.93	0.14	176,190,200,200	0
3	ANP	B	3400	31/31	0.93	0.17	143,159,176,178	0
3	ANP	A	3400	31/31	0.94	0.17	152,165,180,181	0
2	MG	F	701	1/1	0.94	0.56	189,189,189,189	0
3	ANP	E	3400	31/31	0.94	0.19	163,180,187,187	0
2	MG	D	3701	1/1	0.95	0.14	108,108,108,108	0
2	MG	H	3701	1/1	0.95	0.15	121,121,121,121	0
2	MG	B	3701	1/1	0.96	0.17	69,69,69,69	0
2	MG	C	1701	1/1	0.96	0.18	132,132,132,132	0
2	MG	A	3701	1/1	0.97	0.09	116,116,116,116	0
2	MG	G	3701	1/1	0.97	0.10	100,100,100,100	0
2	MG	F	3701	1/1	0.98	0.09	77,77,77,77	0

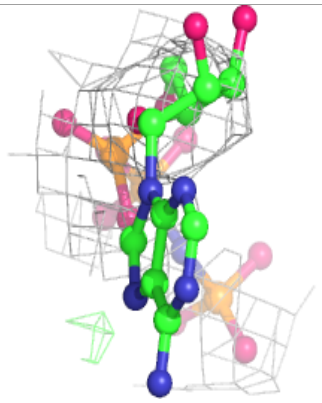
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP F 2400:

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

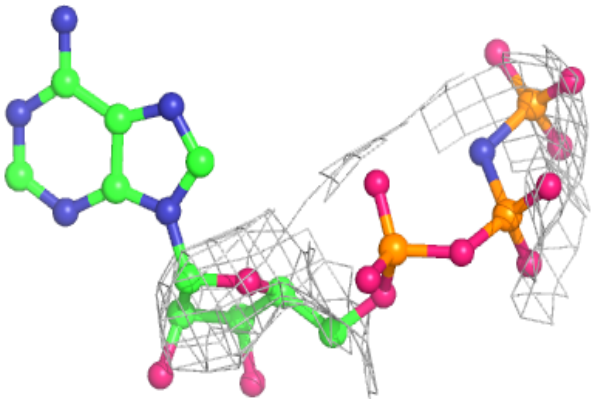


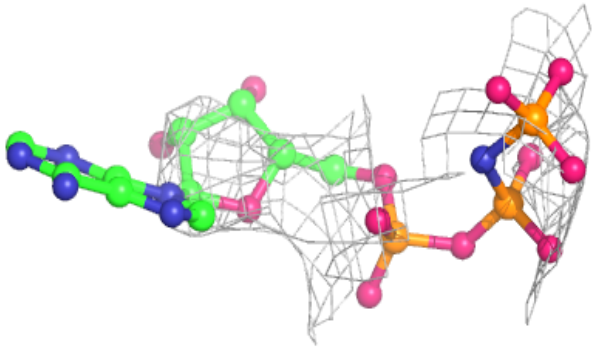


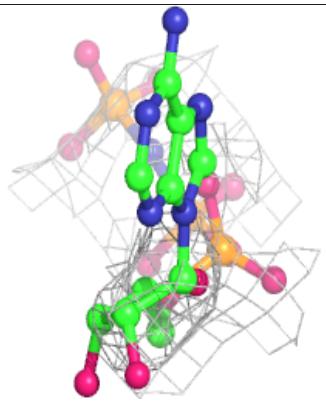


Electron density around ANP G 2400:

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

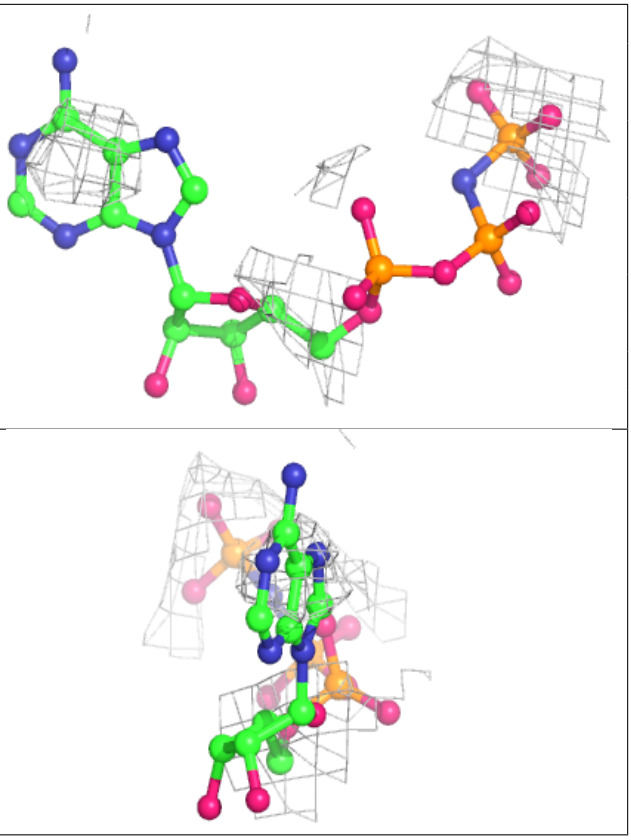






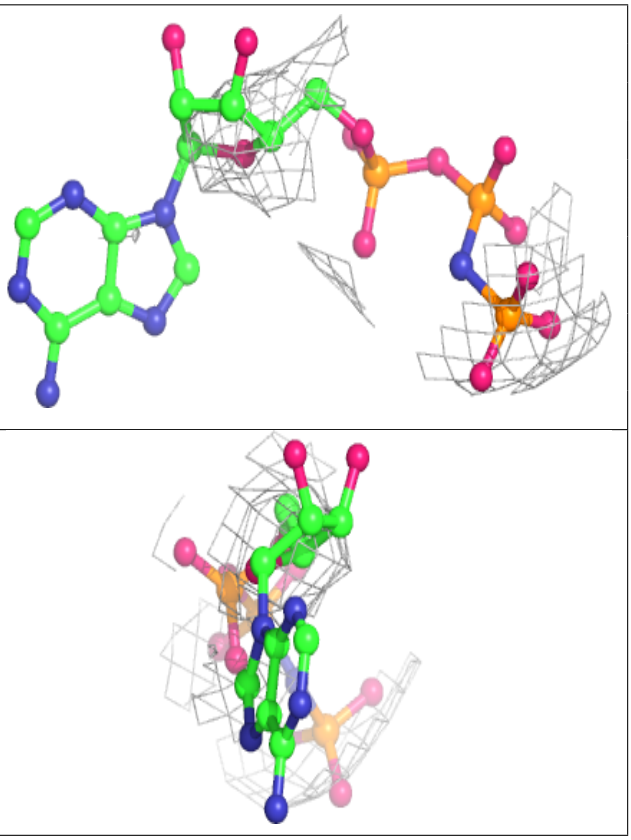
Electron density around ANP H 2400:

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



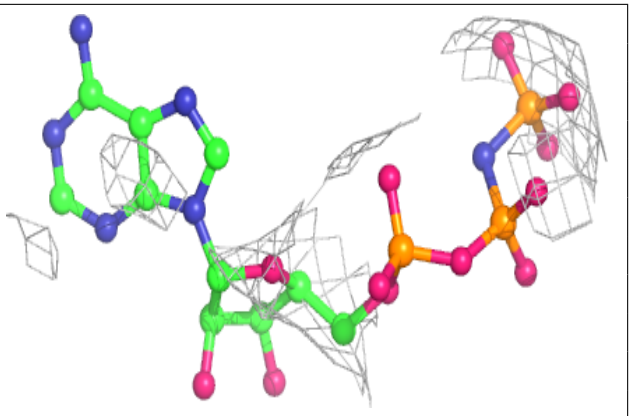
Electron density around ANP D 1400:

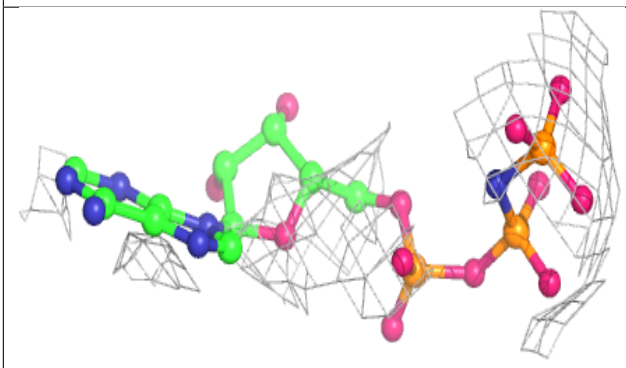
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

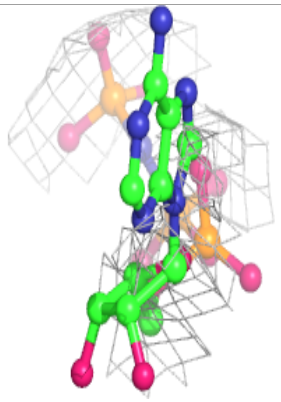


Electron density around ANP A 1400:

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

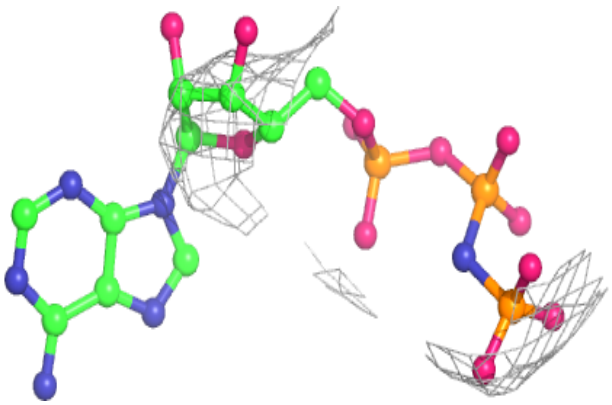


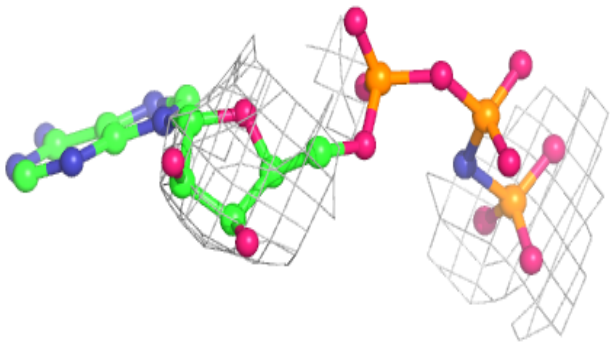


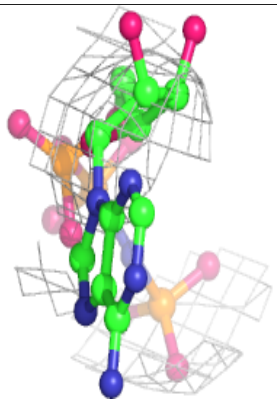


Electron density around ANP E 1400:

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

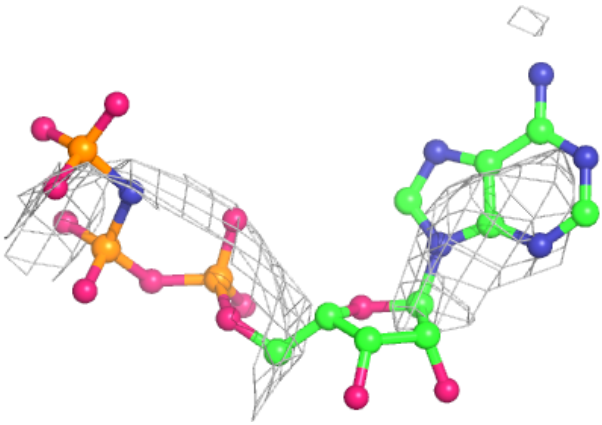


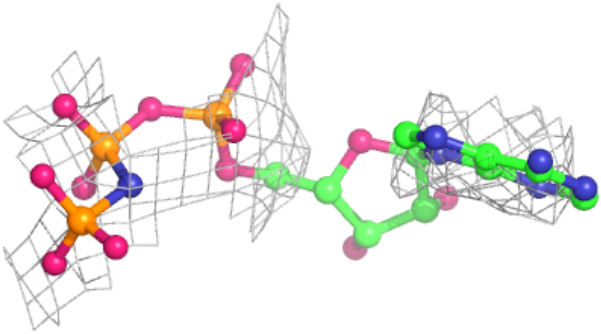


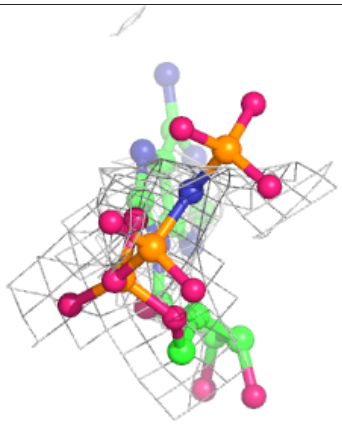


Electron density around ANP B 2400:

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

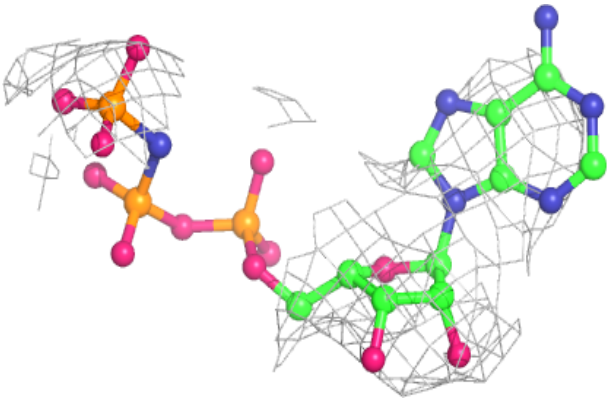


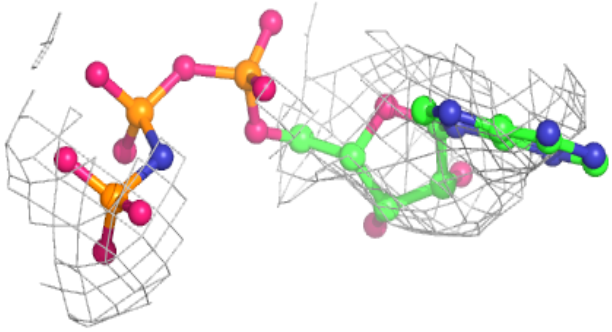


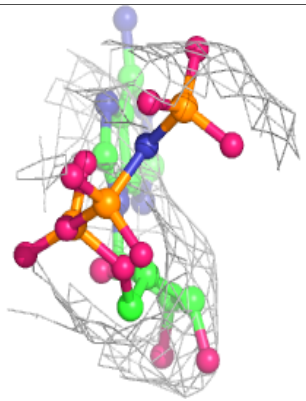


Electron density around ANP B 400:

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

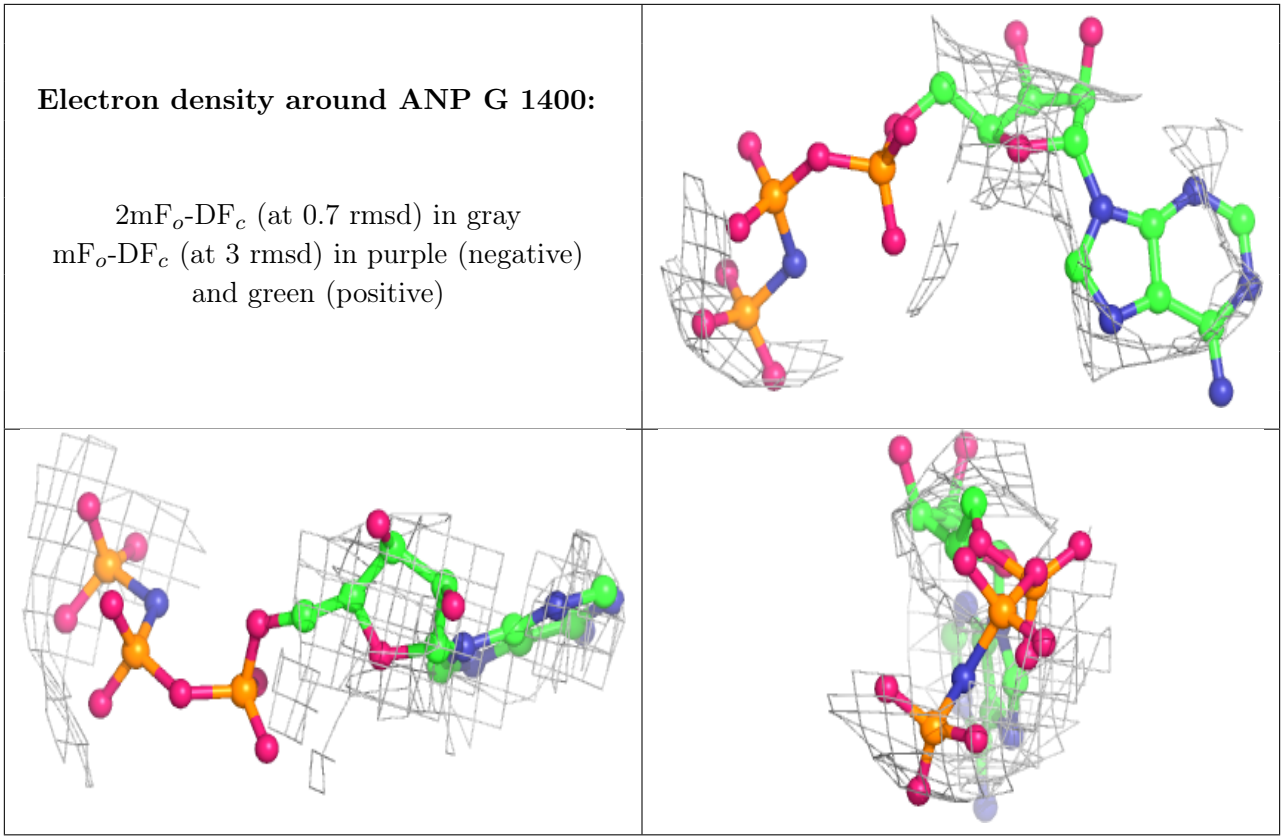






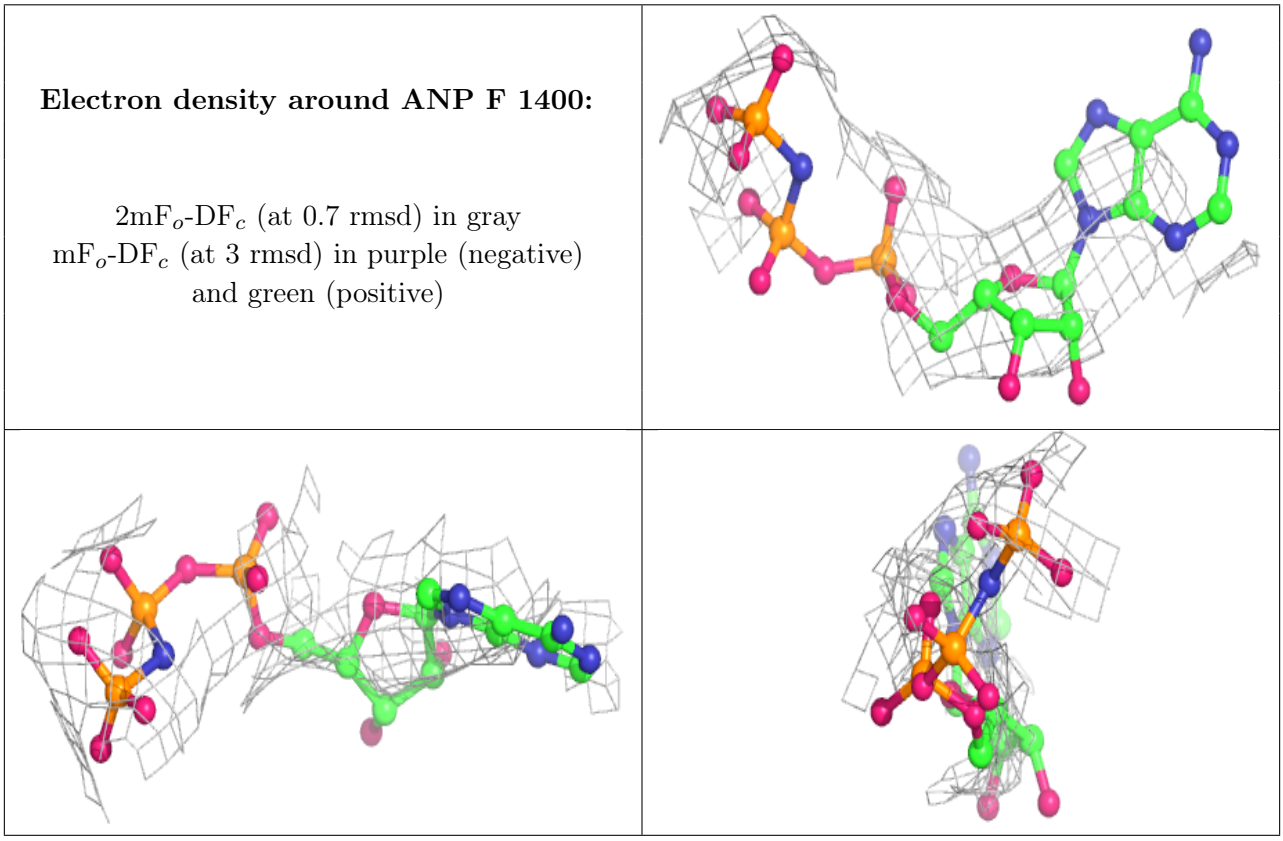
Electron density around ANP G 1400:

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



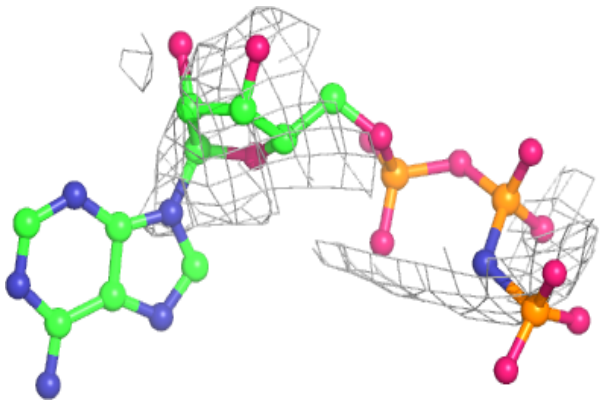
Electron density around ANP F 1400:

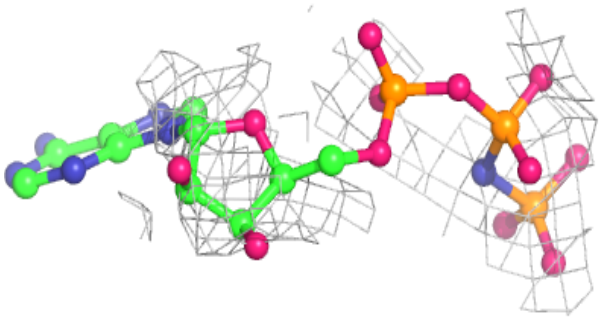
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

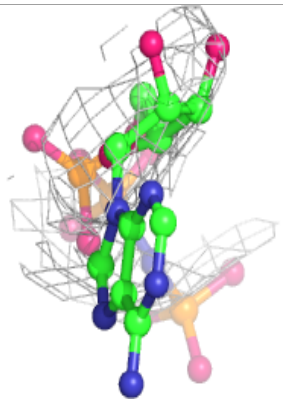


Electron density around ANP H 1400:

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

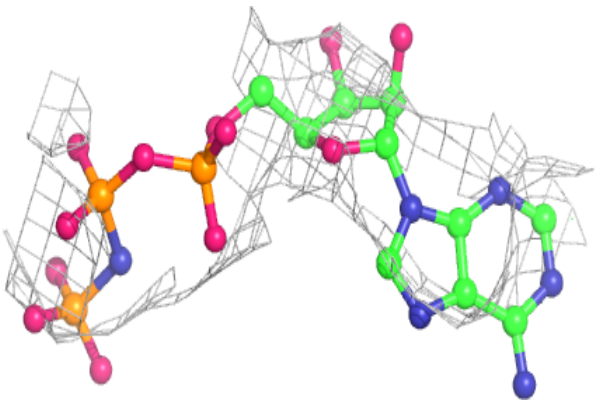


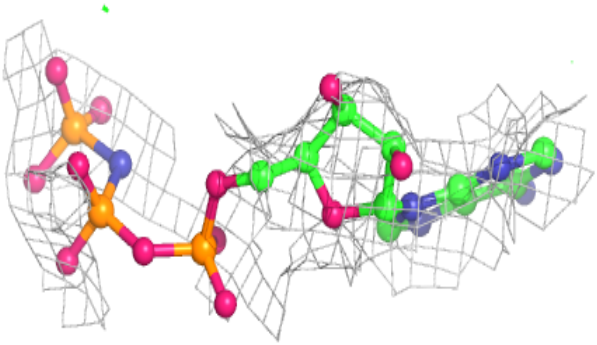


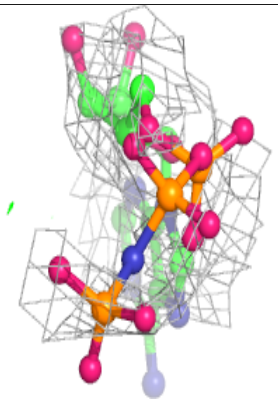


Electron density around ANP C 1400:

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

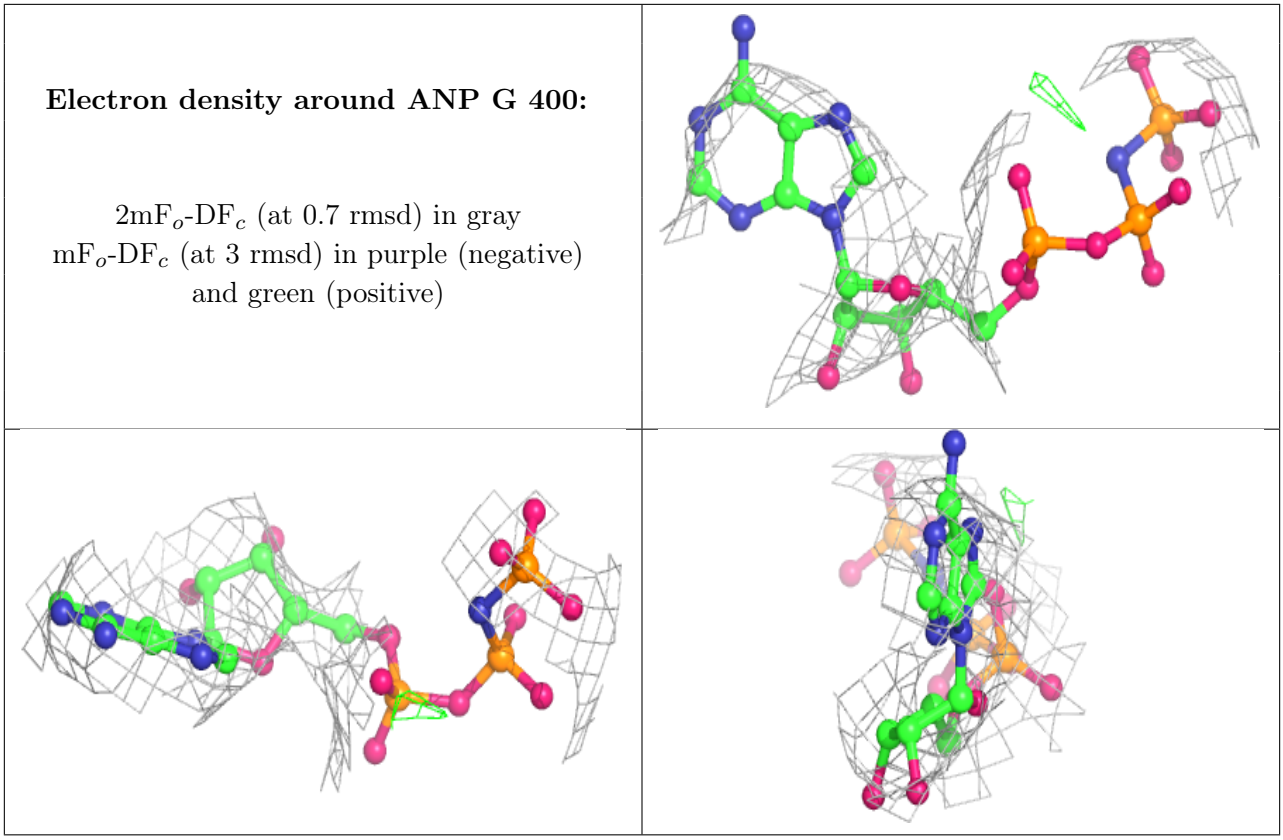






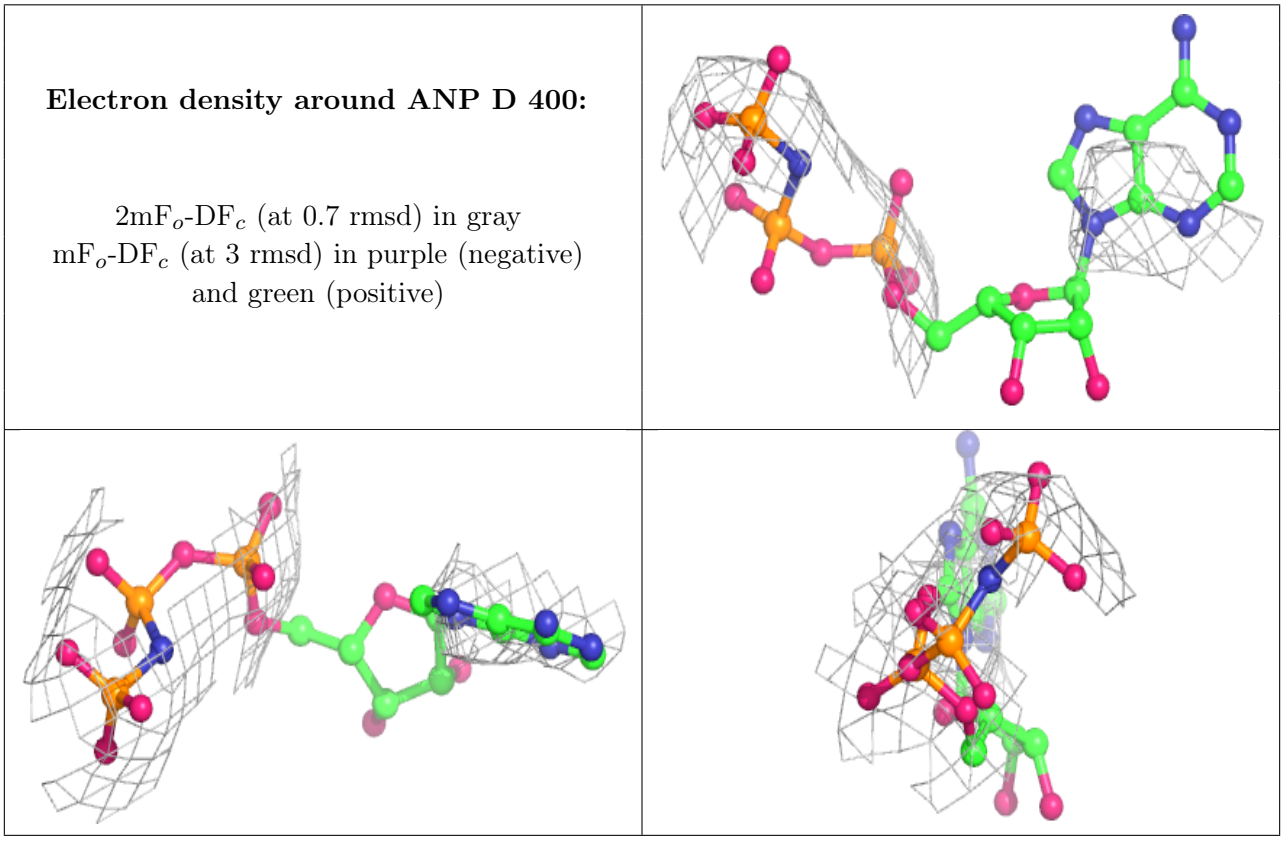
Electron density around ANP G 400:

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



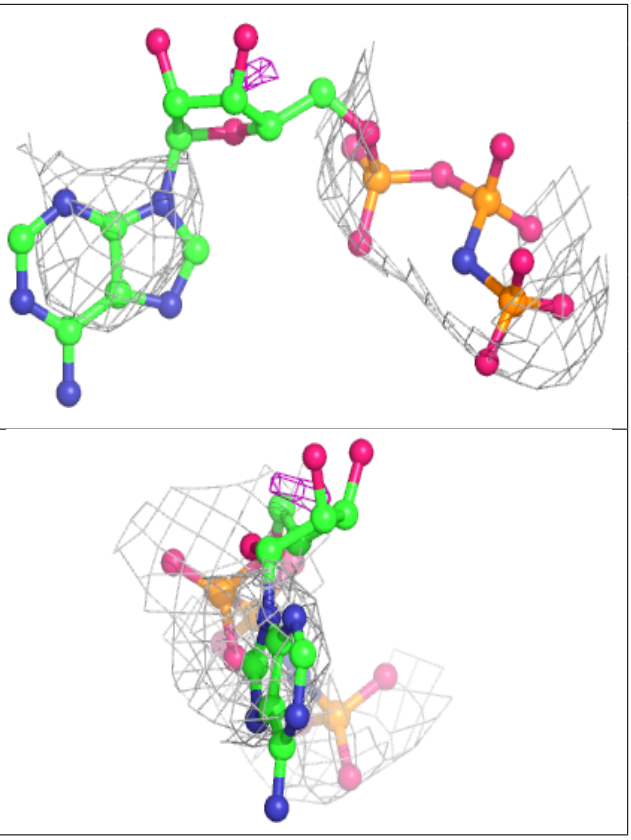
Electron density around ANP D 400:

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



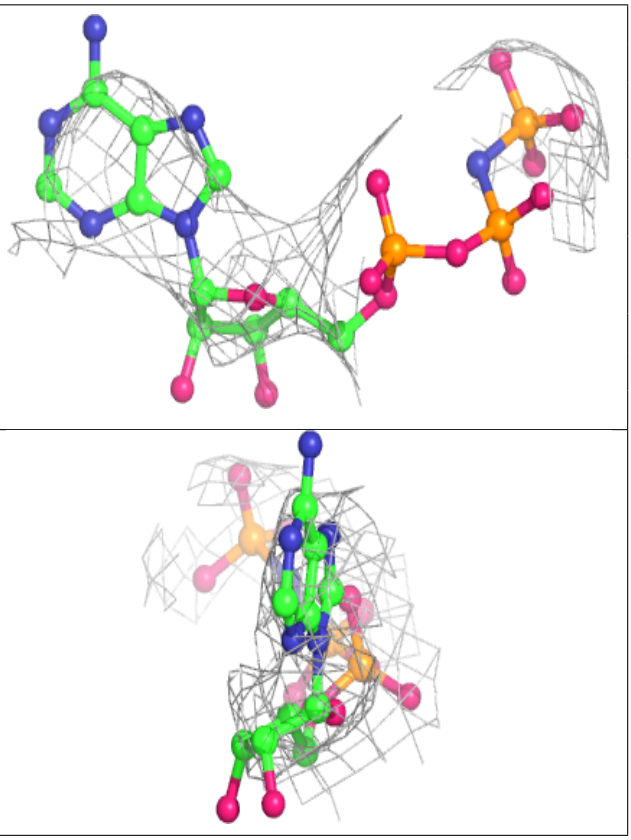
Electron density around ANP H 400:

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



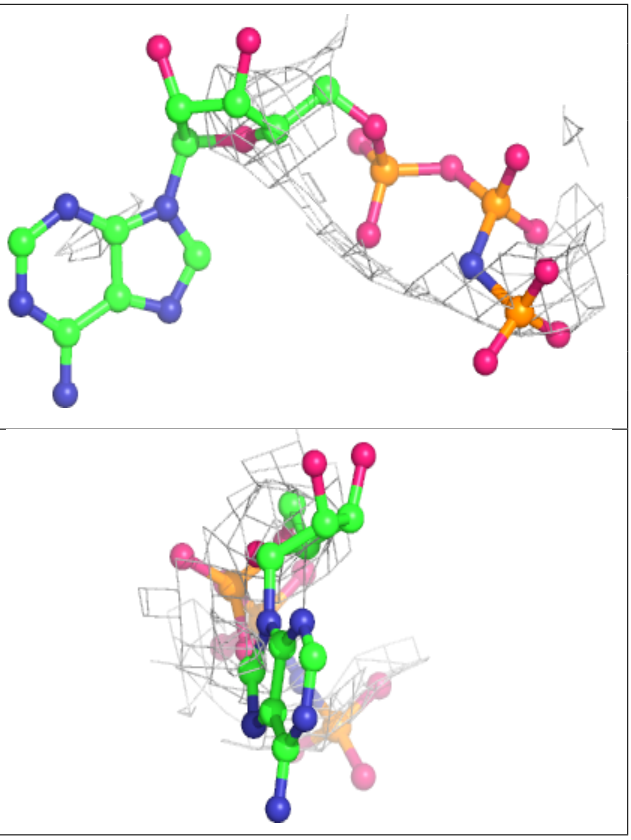
Electron density around ANP C 400:

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



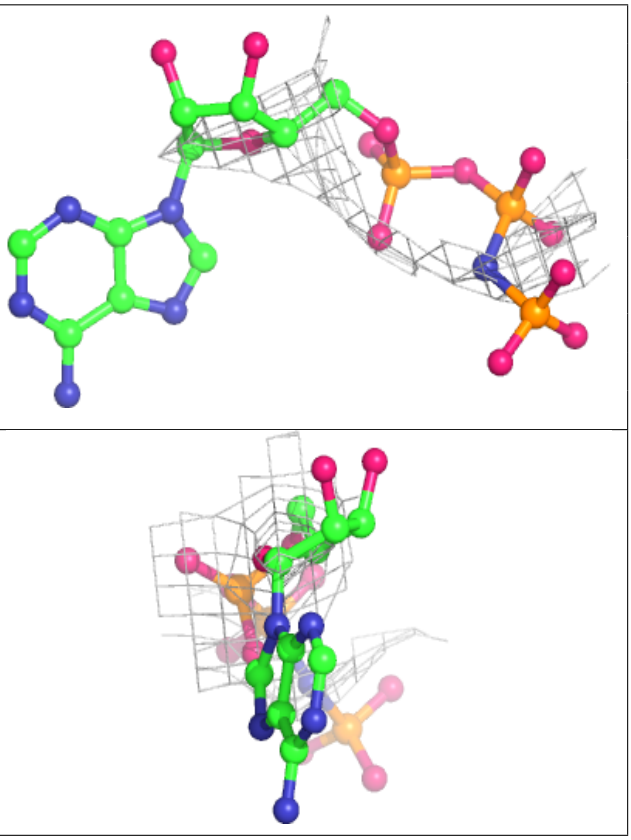
Electron density around ANP D 2400:

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



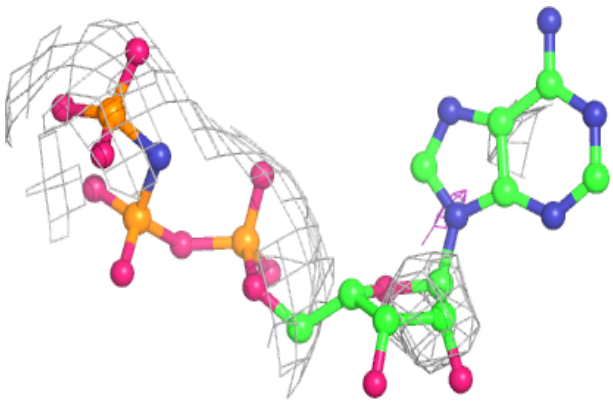
Electron density around ANP A 2400:

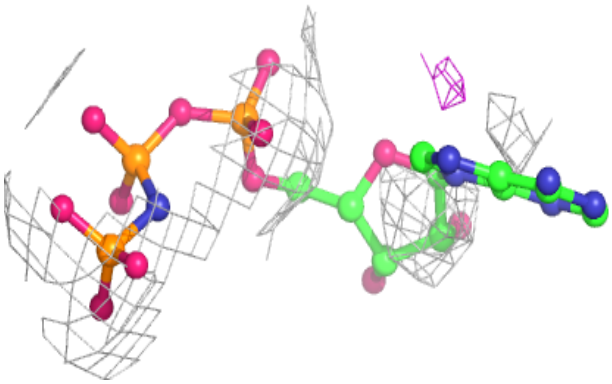
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ANP F 400:

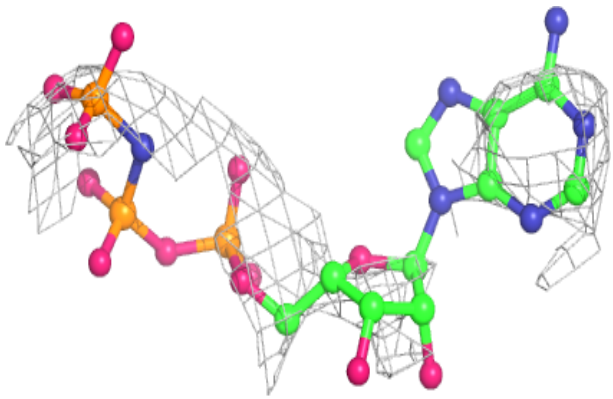
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

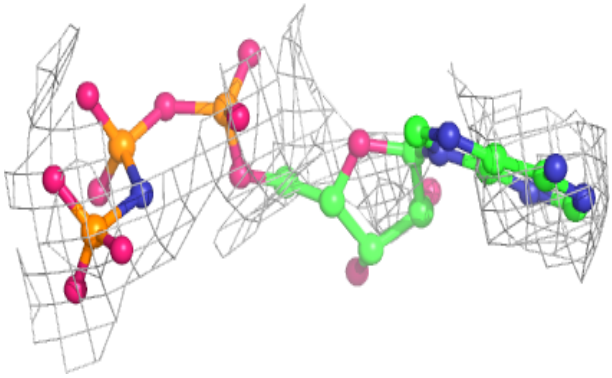




Electron density around ANP B 1400:

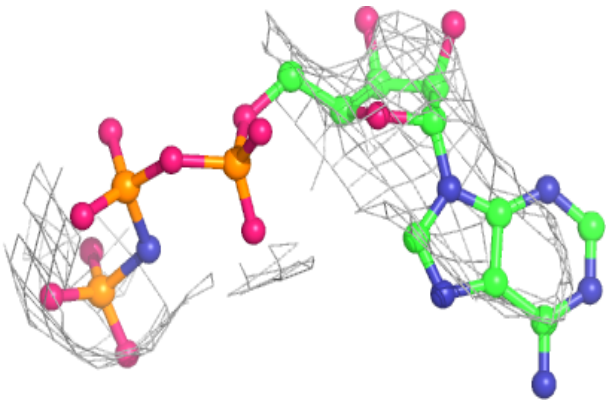
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

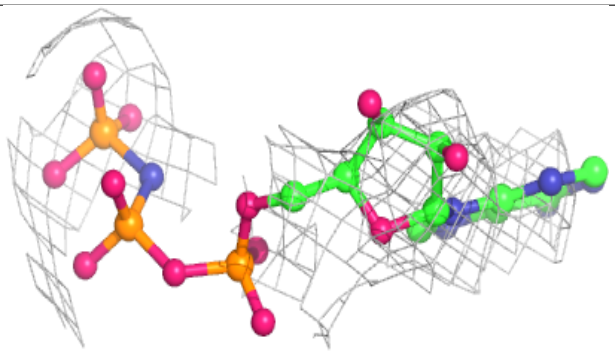




Electron density around ANP A 400:

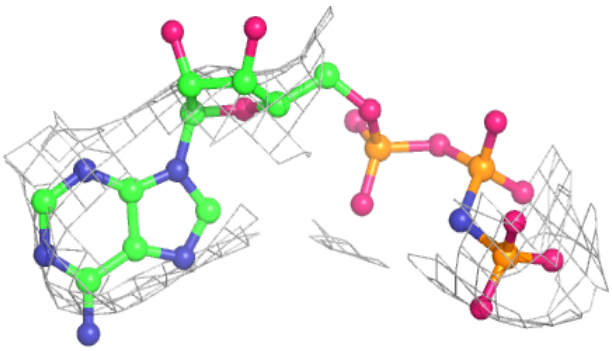
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

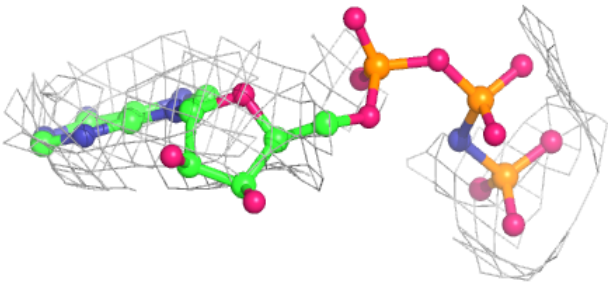


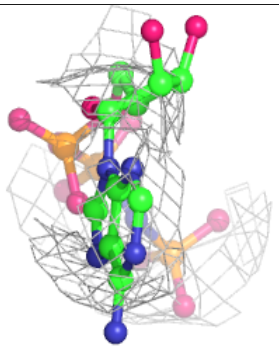


Electron density around ANP E 400:

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

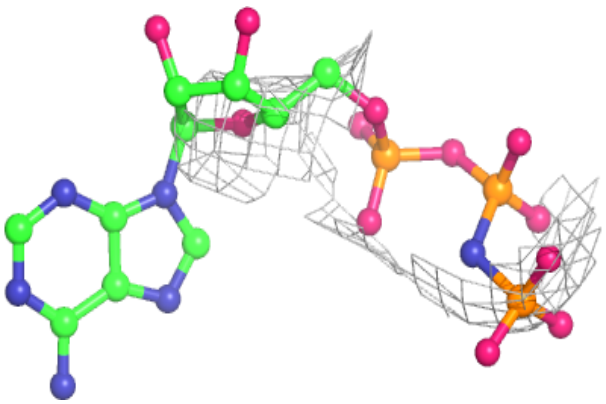


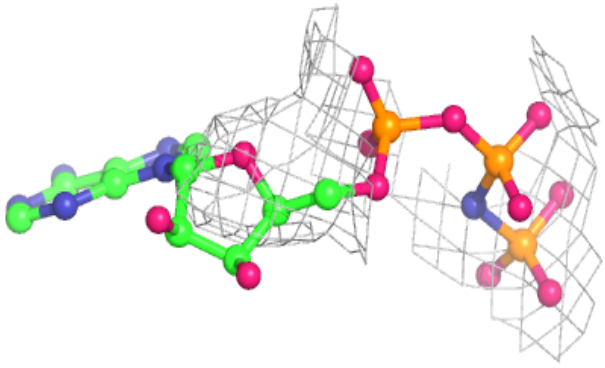


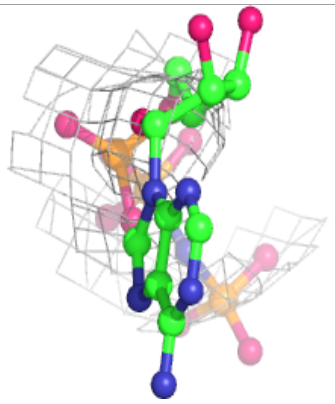


Electron density around ANP C 2400:

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

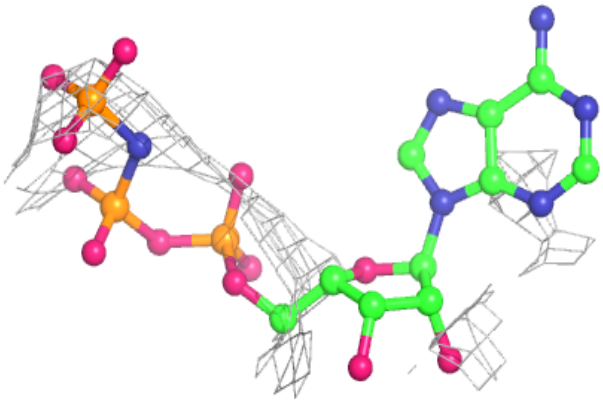


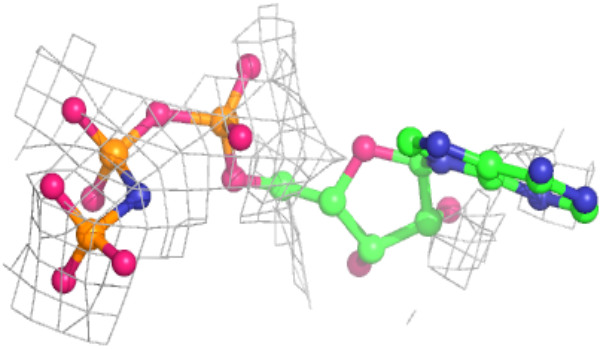




Electron density around ANP E 2400:

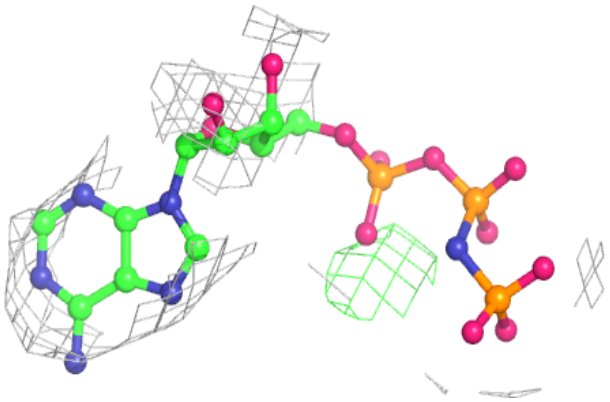
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

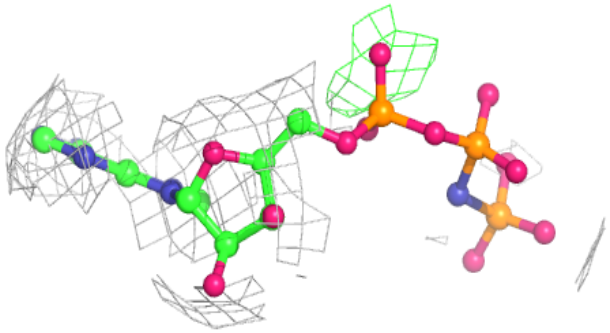


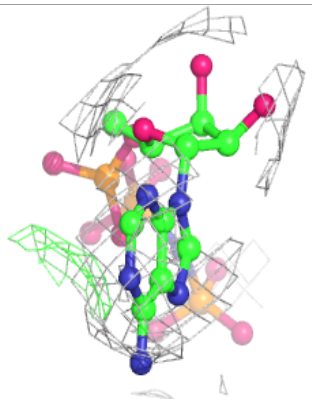


Electron density around ANP H 3400:

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

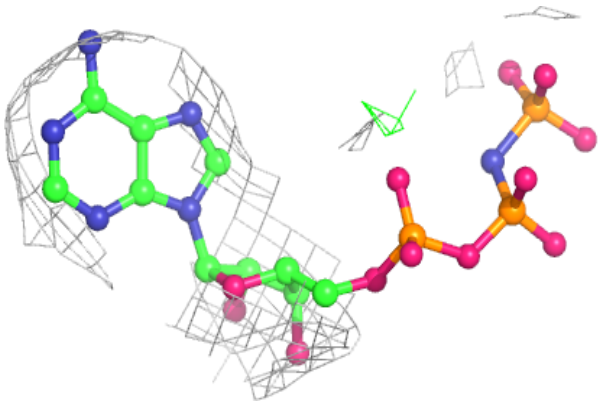


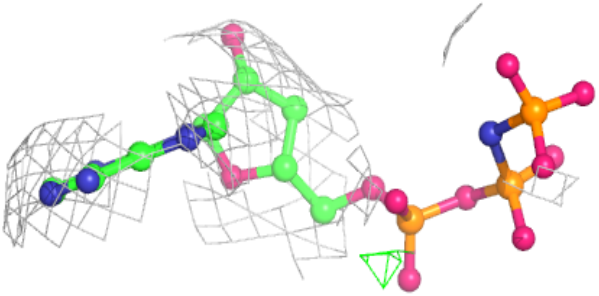


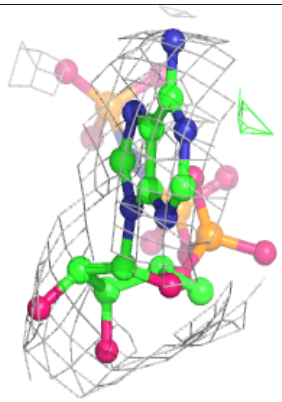


Electron density around ANP G 3400:

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

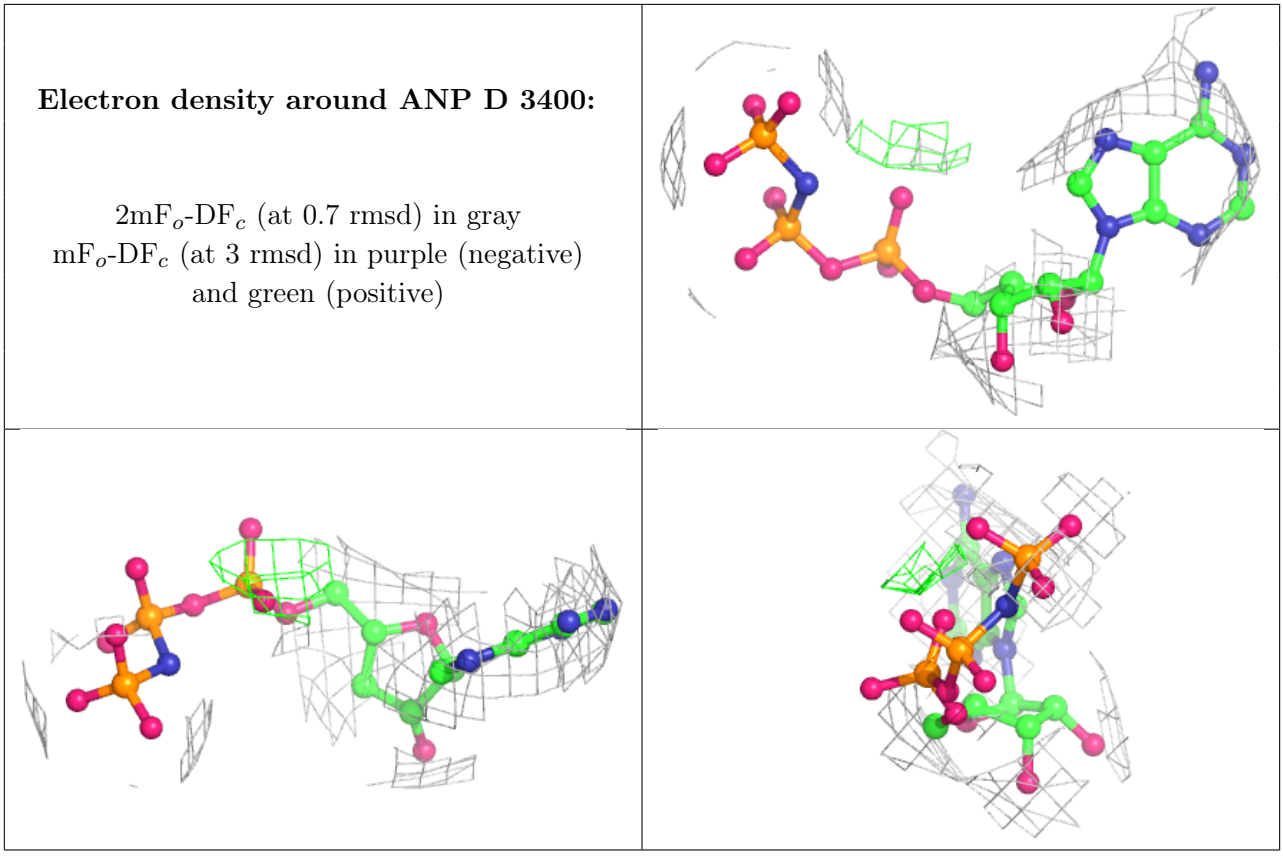






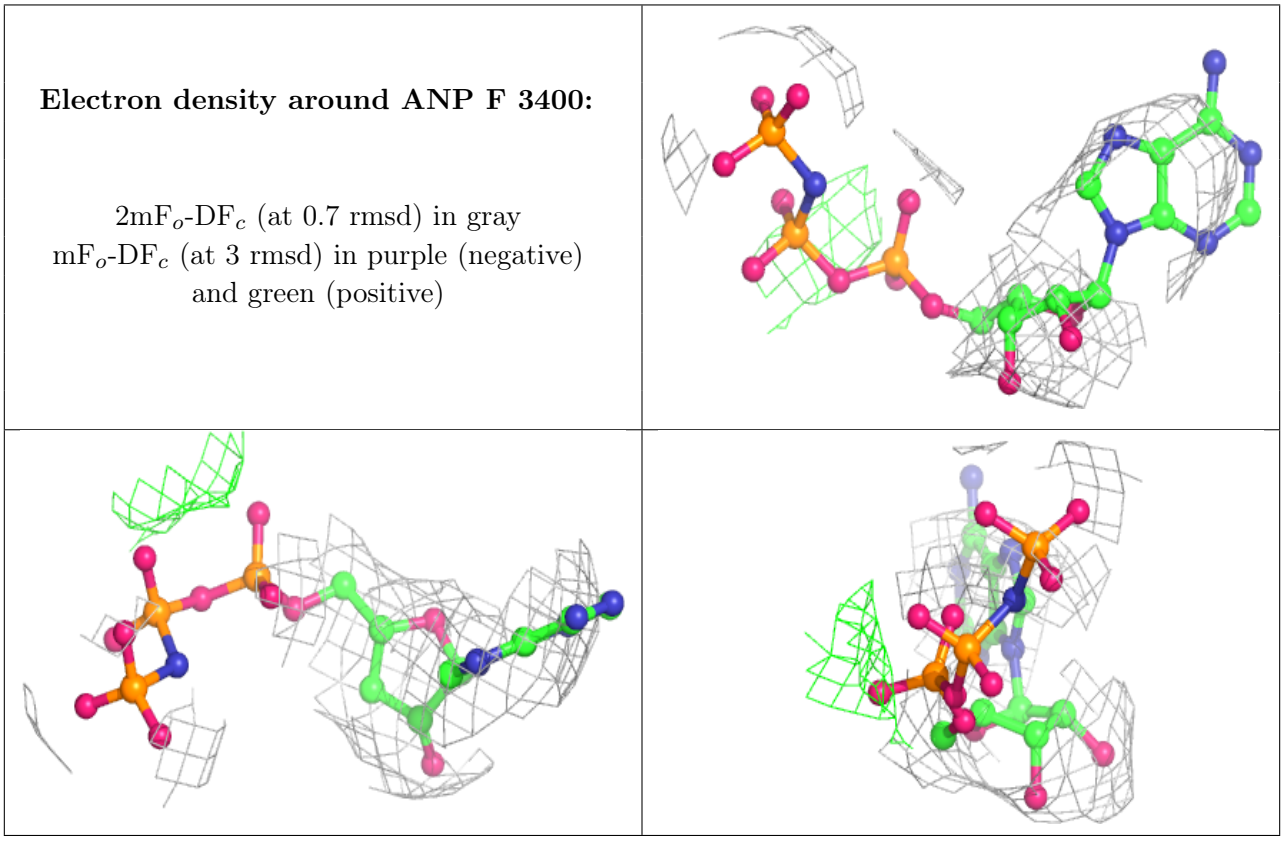
Electron density around ANP D 3400:

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



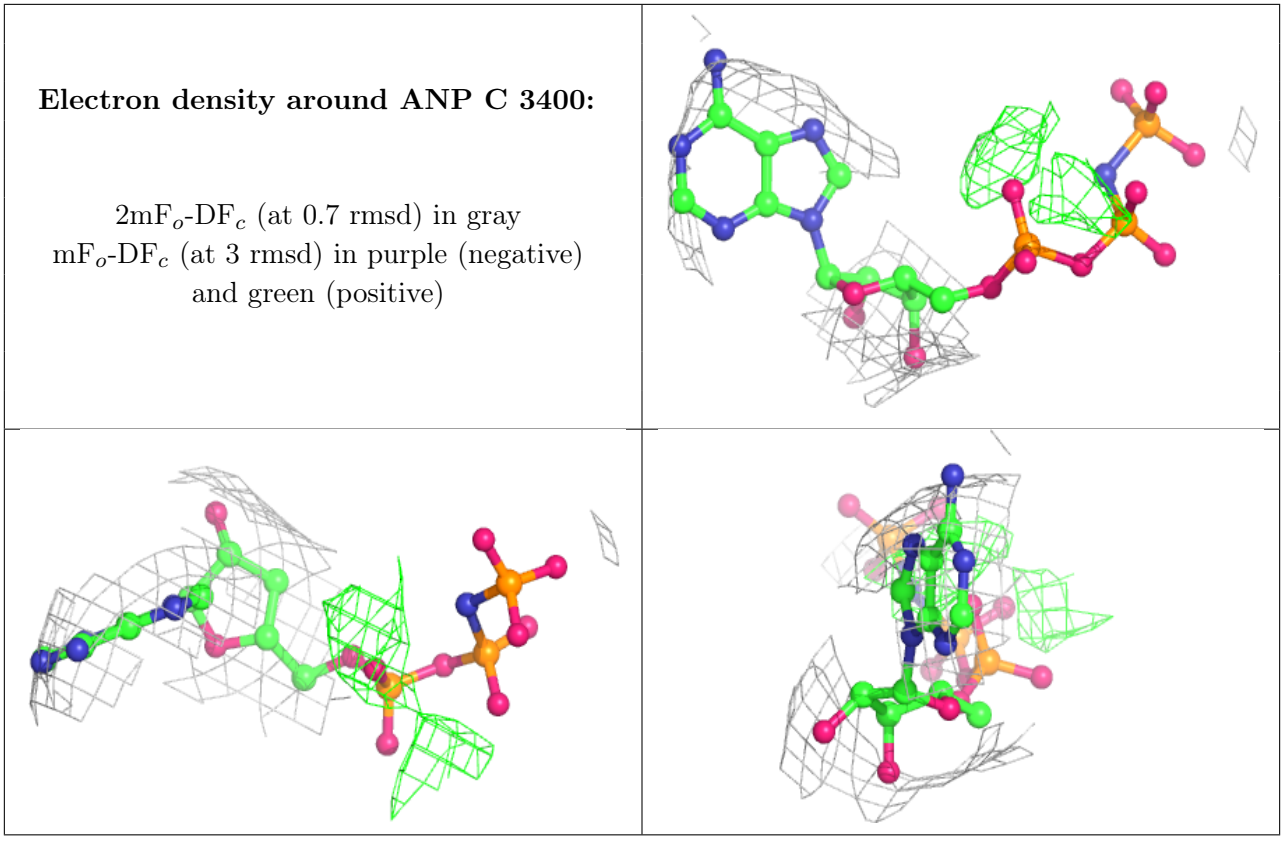
Electron density around ANP F 3400:

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



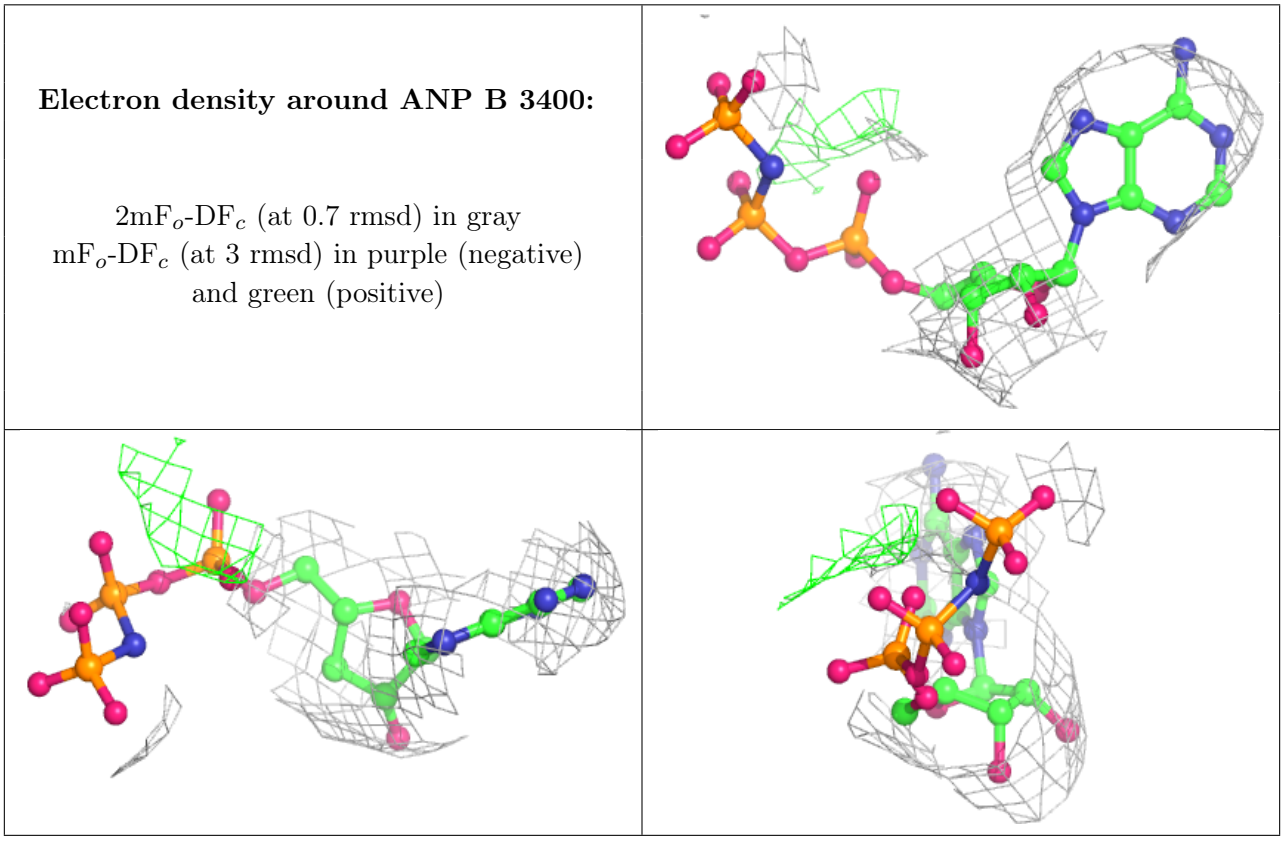
Electron density around ANP C 3400:

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



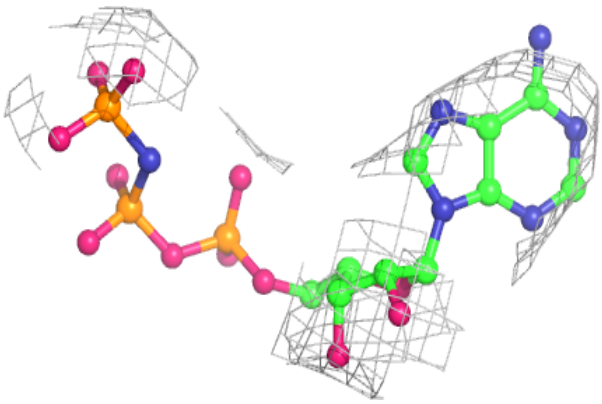
Electron density around ANP B 3400:

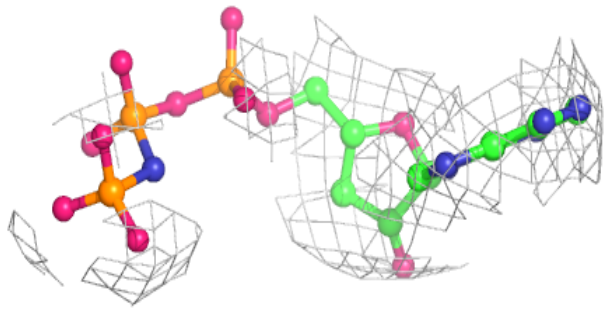
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

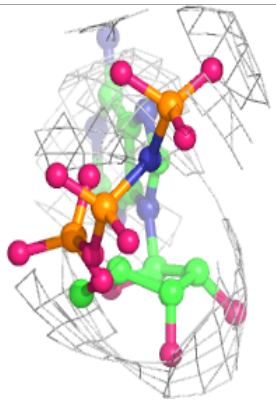


Electron density around ANP A 3400:

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

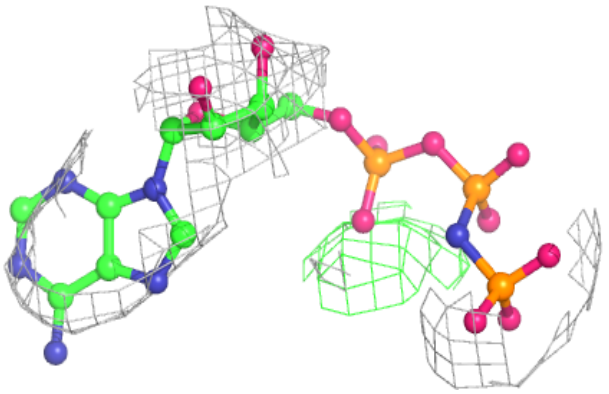


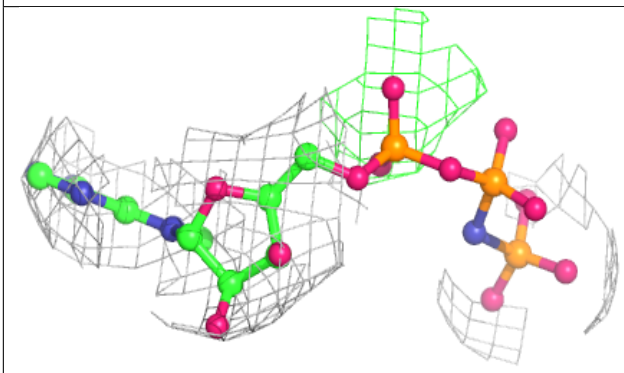


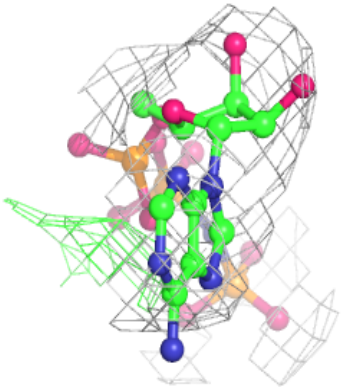


Electron density around ANP E 3400:

$2mF_o$-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.