



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:00 AM UTC

PDB ID : 3CMV / pdb_00003cmv
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

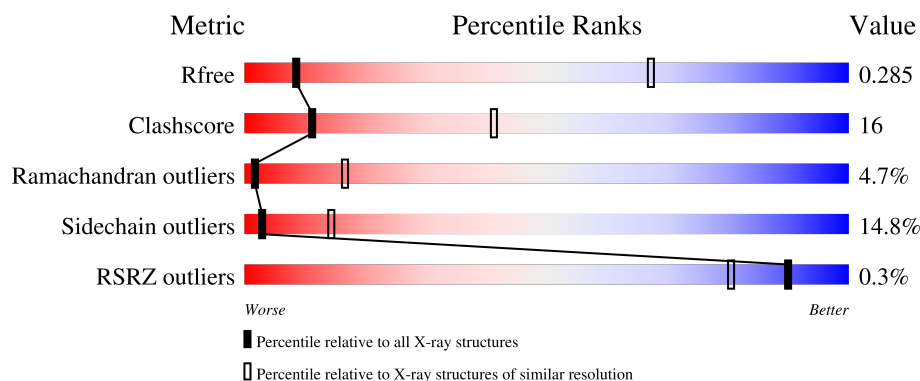
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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

Mol	Chain	Length	Quality of chain
1	A	1357	
1	B	1357	
1	C	1357	
1	D	1357	
1	E	1357	

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Mol	Chain	Length	Quality of chain
1	F	1357	
1	G	1357	
1	H	1357	

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
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	-	-	-
3	ANP	F	3400	X	-	-	-
3	ANP	F	400	X	-	-	-
3	ANP	G	1400	X	-	-	-
3	ANP	G	2400	X	-	-	-
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

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

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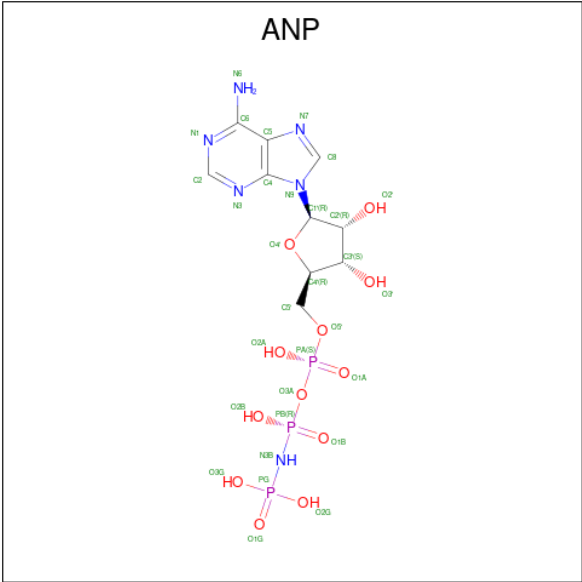
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Chain	Residue	Modelled	Actual	Comment	Reference
H	2992	SER	-	linker	UNP P0A7G6
H	2993	GLY	-	linker	UNP P0A7G6
H	2994	SER	-	linker	UNP P0A7G6
H	2995	SER	-	linker	UNP P0A7G6
H	2996	THR	-	linker	UNP P0A7G6
H	2997	GLY	-	linker	UNP P0A7G6
H	2998	SER	-	linker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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

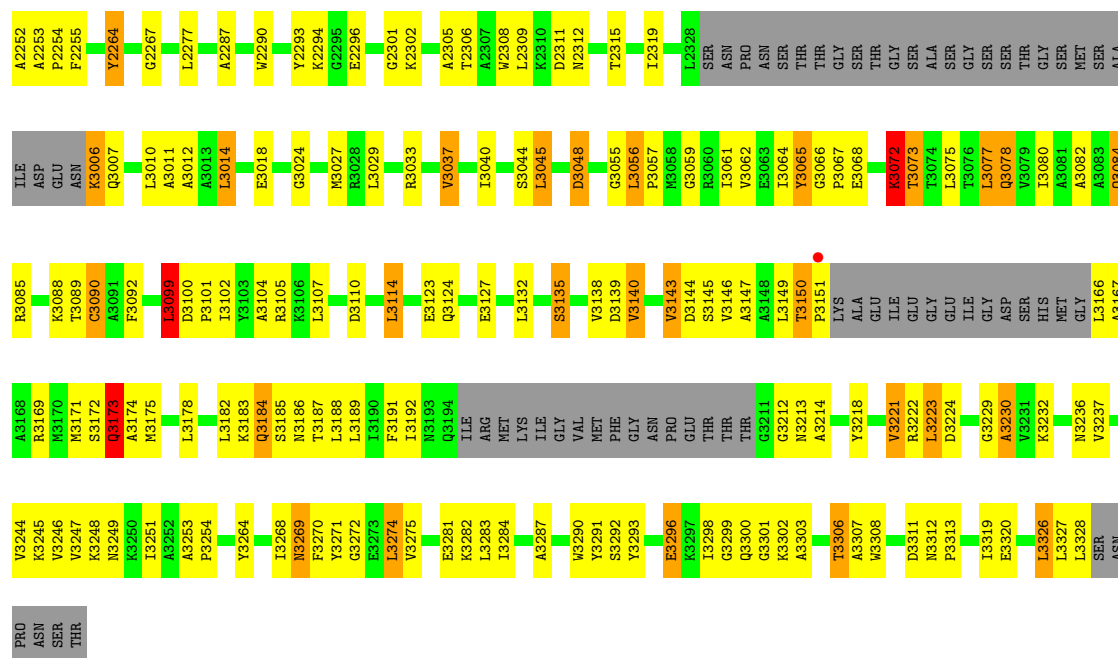
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Mg 4 4	0	0
2	B	4	Total Mg 4 4	0	0
2	C	4	Total Mg 4 4	0	0
2	D	4	Total Mg 4 4	0	0
2	E	4	Total Mg 4 4	0	0
2	F	4	Total Mg 4 4	0	0
2	G	4	Total Mg 4 4	0	0
2	H	4	Total Mg 4 4	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

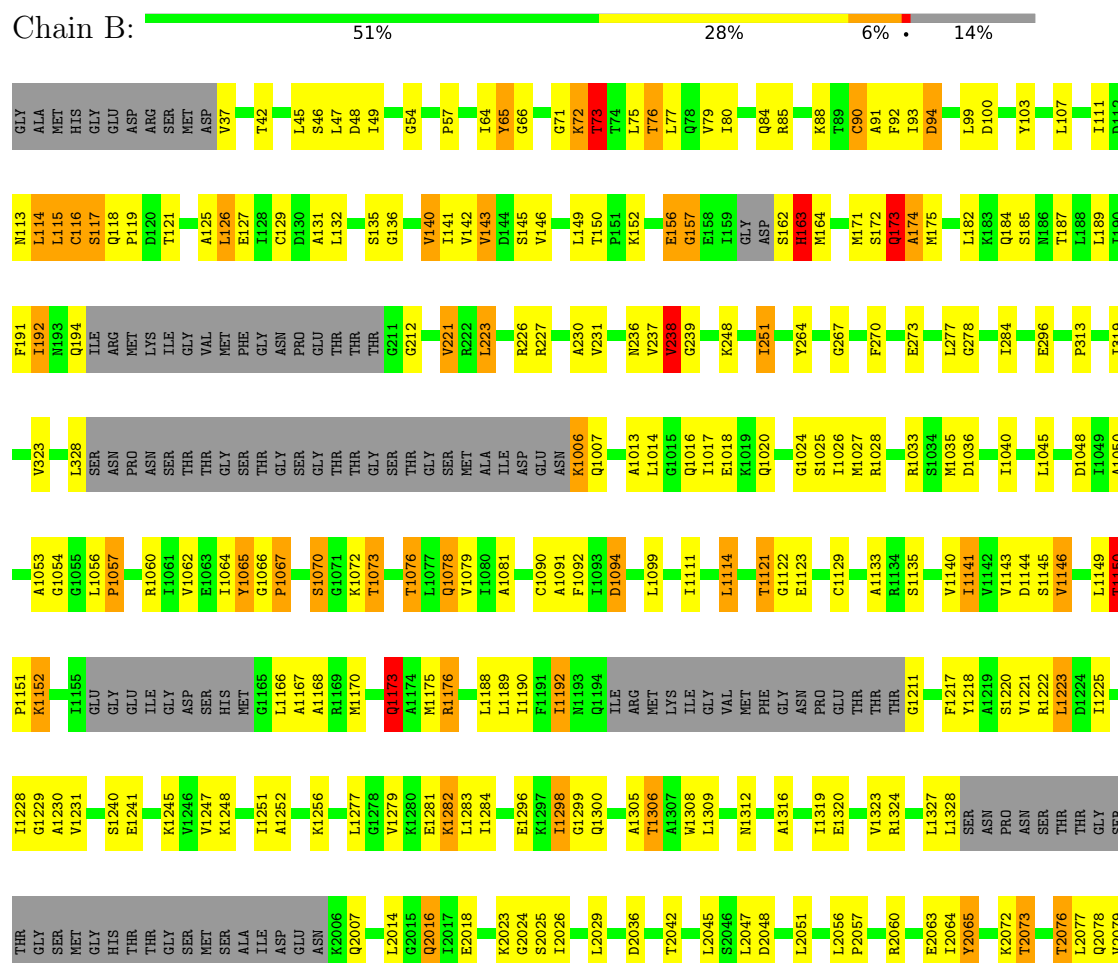


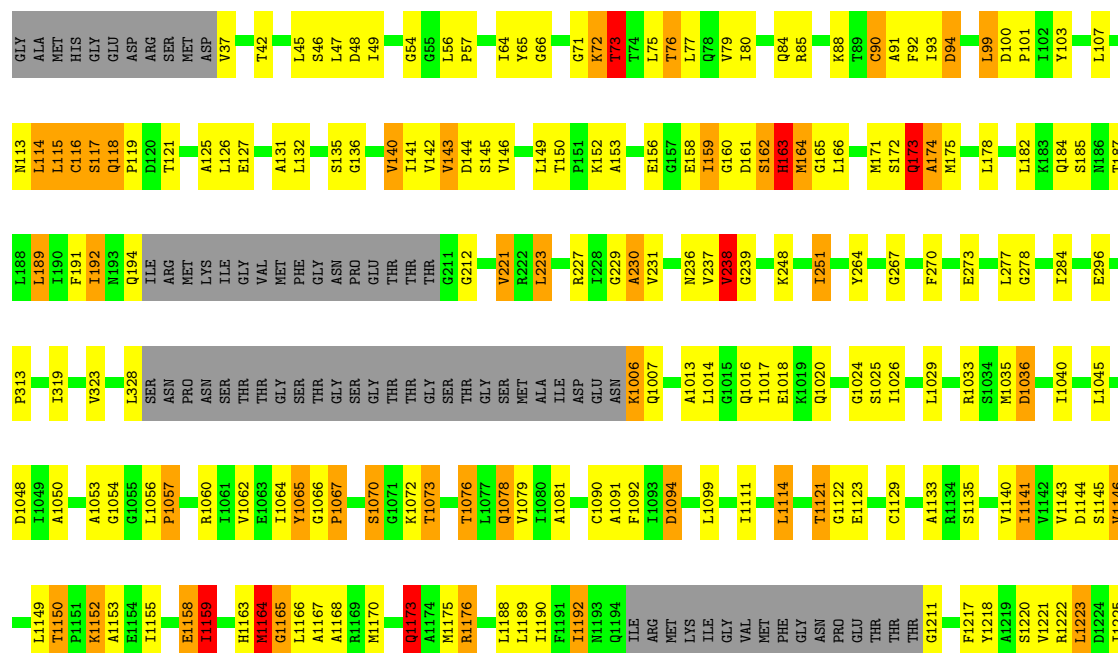
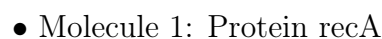
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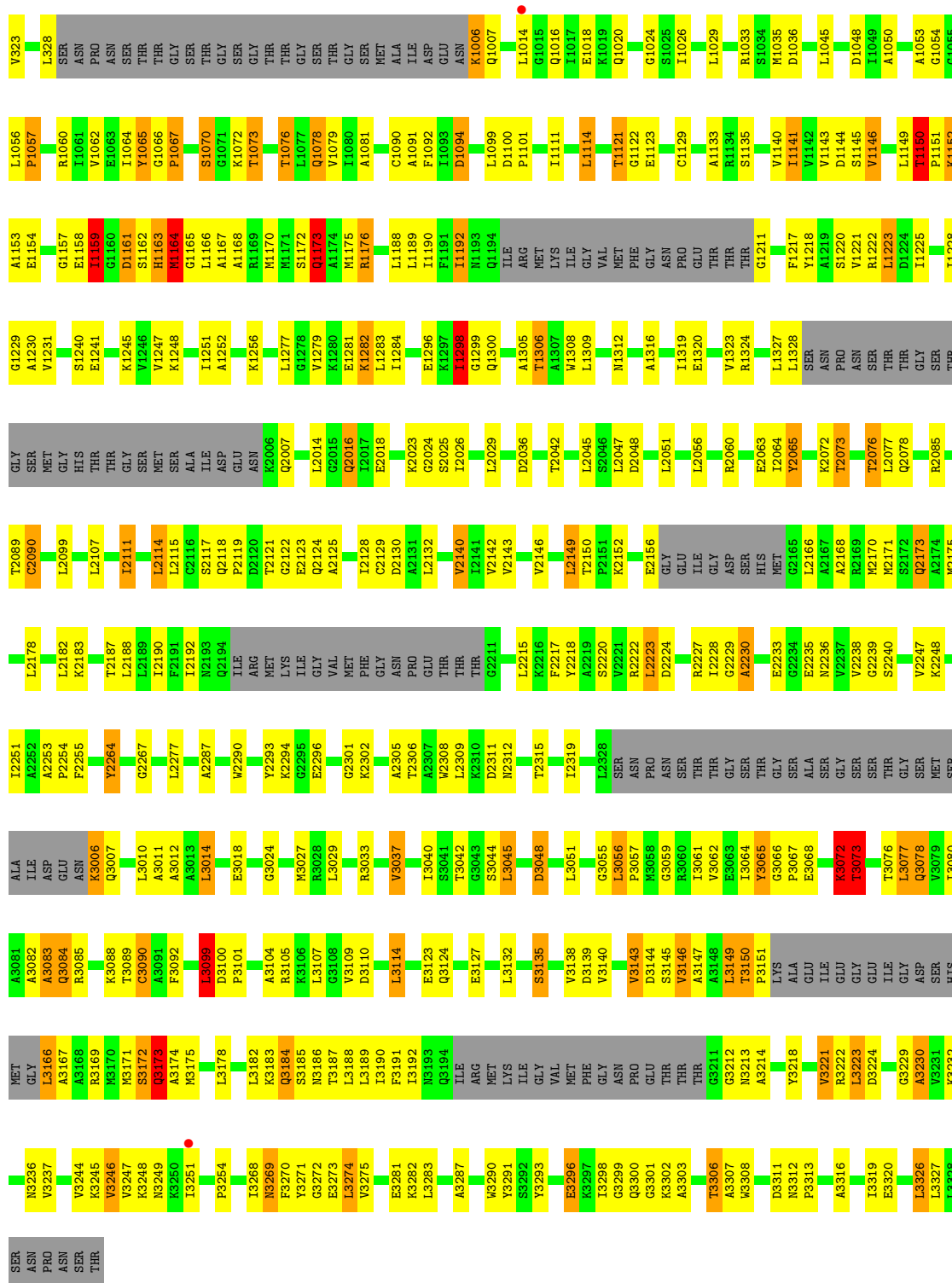
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F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



- Molecule 1: Protein recA

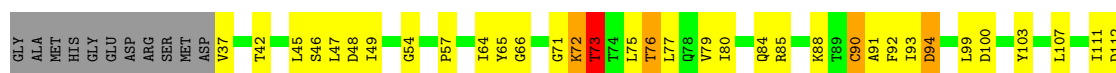


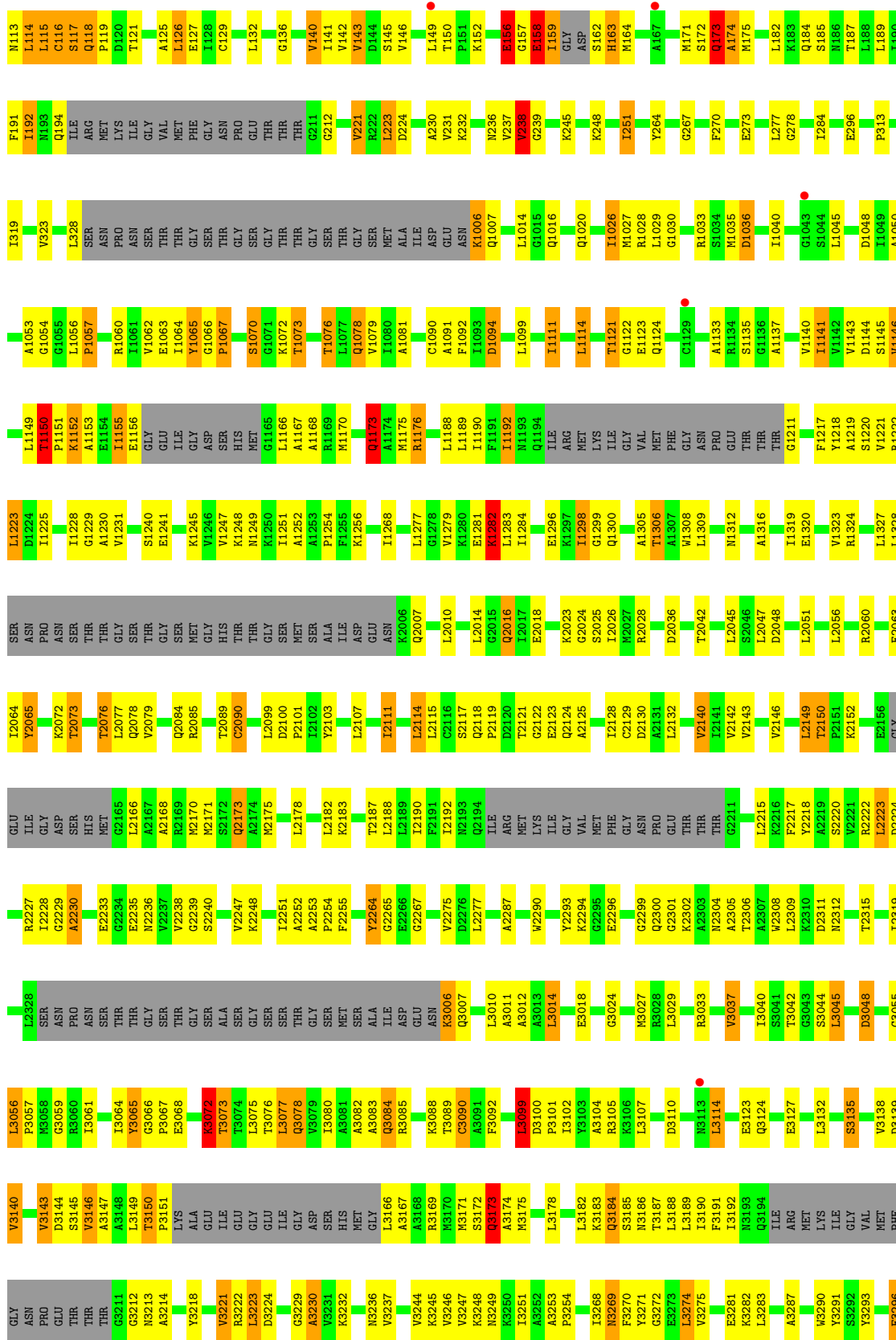




• Molecule 1: Protein recA

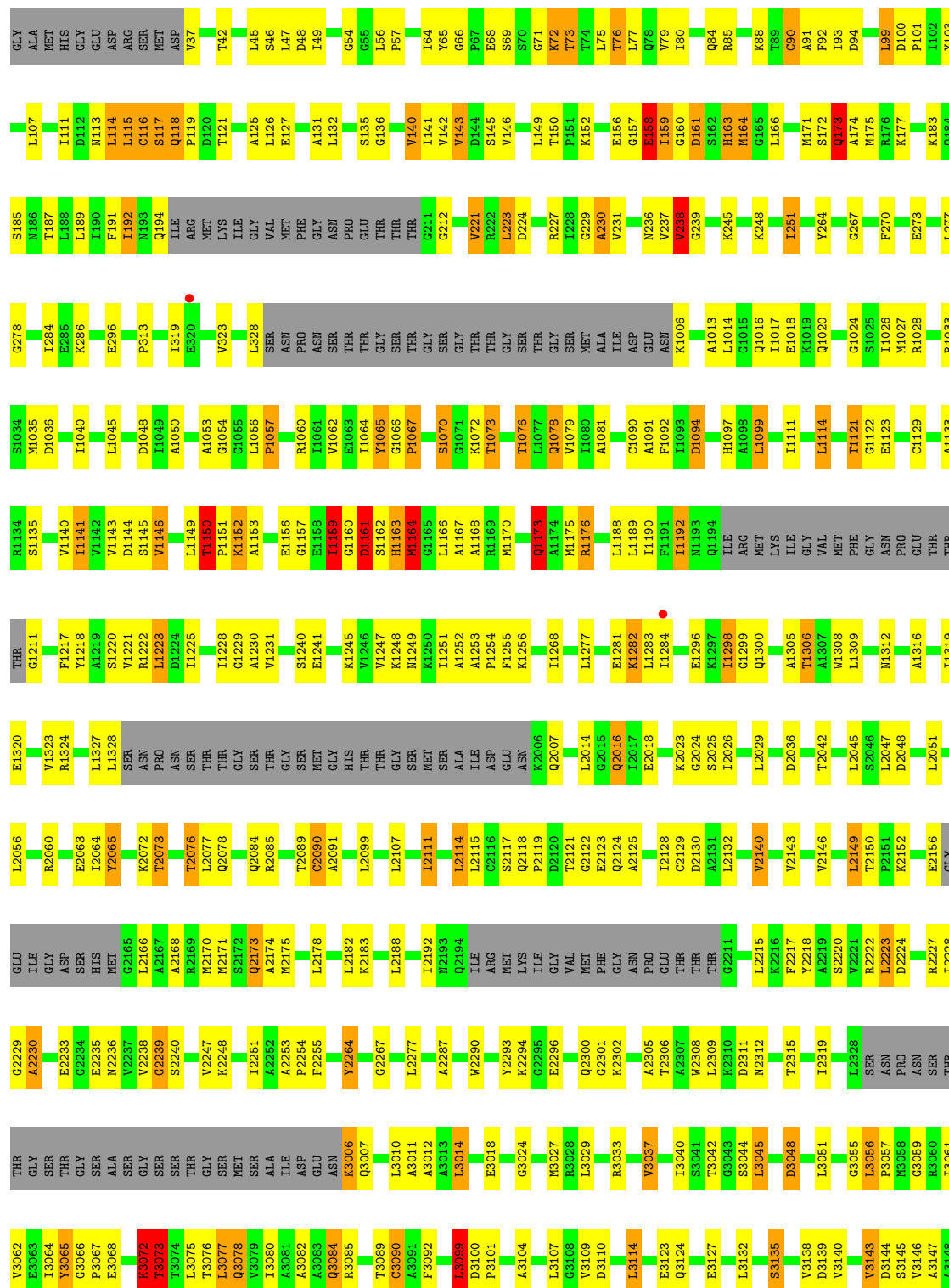
Chain E: 50% 28% 6% 14%

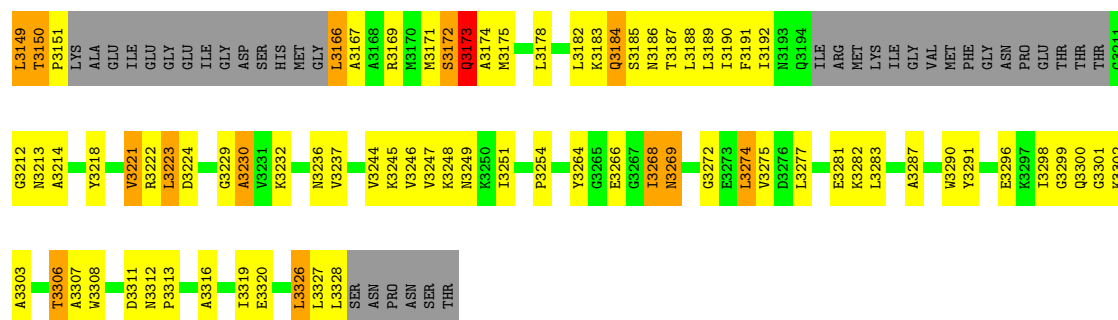






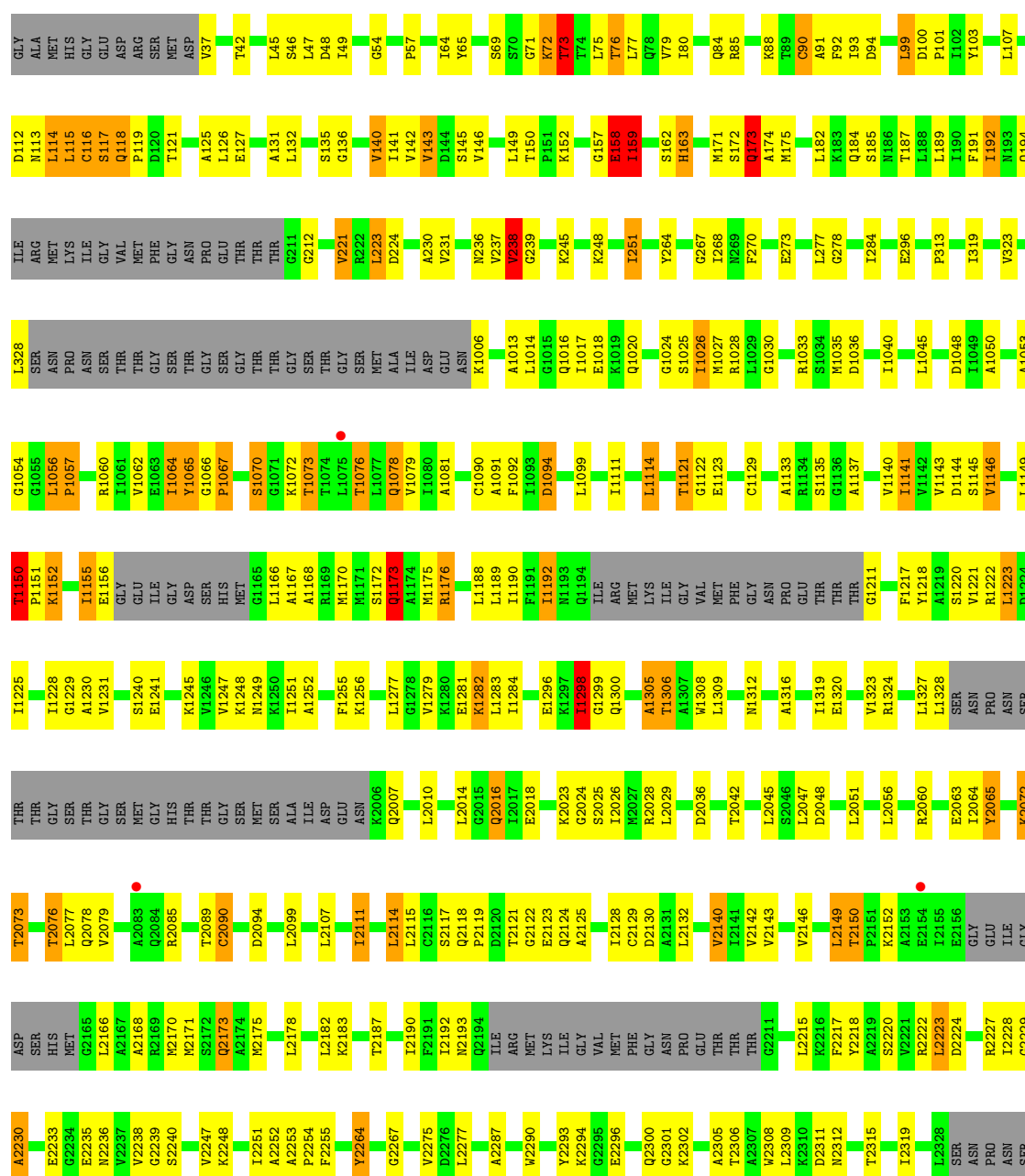
• Molecule 1: Protein recA

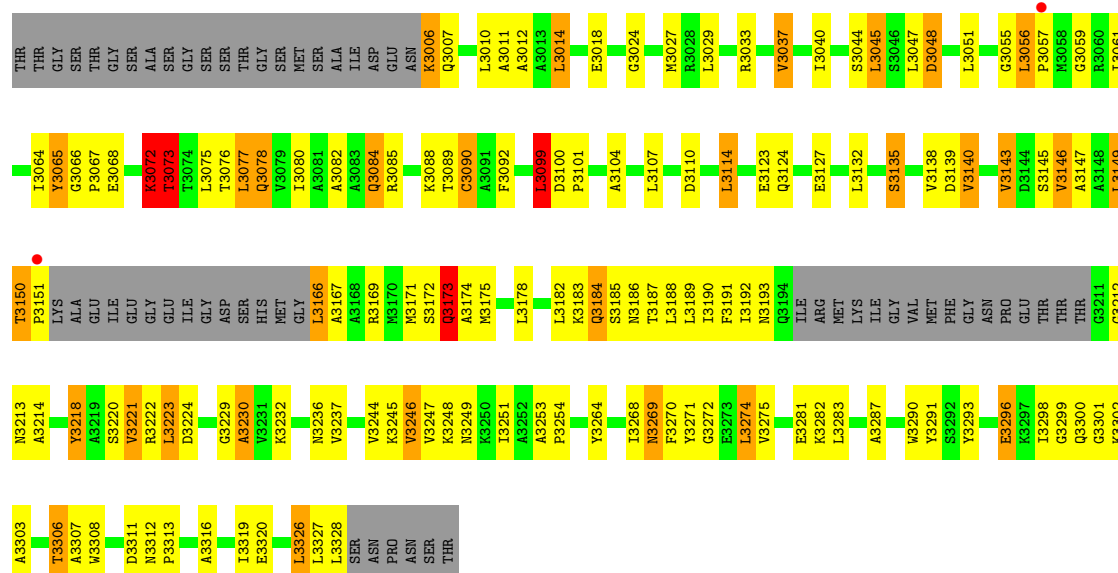




Molecule 1: Protein recA

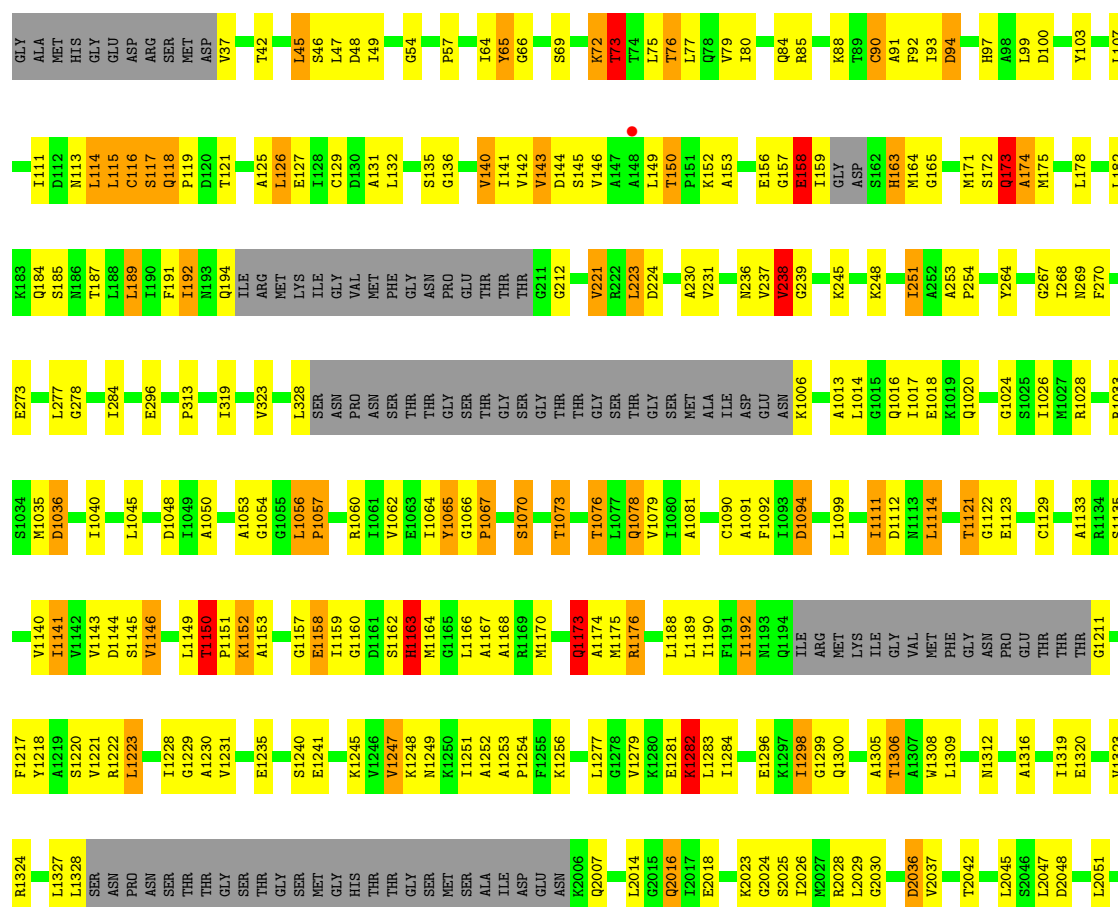
Chain G: 51% 28% 6% 14%





• Molecule 1: Protein recA

Chain H: 51% 28% 7% • 14%



L2056 P2057	GLU ILE GLY ASP SER HIS MET	G2229 A2230	SER ASN PRO ASN ASN THR THR GLY SER THR GLY ALA SER GLY SER THR GLY ASP GLU ASN	M3058 G3059 R3060 I3061 V3062 E3063 I3064 Y3065 G3066 P3067 E3068	V3143 D3144 S3145 V3146 A3147 A3148 L3149 T3150 P3151 LYS ALA GLU ILE GLU GLY ILE GLY ASP SER HIS MET GLY L3166 A3167 A3168 R3169 M3170 S3171 S3172 D3173 A3174 I3175 L3178	PRO GLU THR THR G3212 N3213 A3214 Y3218 V3221 R3222 L3223 D3224 G3229 A3230 V3231 K3232 N3236 V3237 Y3244 K3245 V3246 V3247 K3248 N3249 K3250 I3251 A3252 P3254 Y3264 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 I3319 E3320 L3326 L3327 L3328 SER ASN PRO ASN SER THR	L2066 P2067 R2068 E2063 I2064 Y2065 T2072 K2073 A2167 L2166 A2168 R2169 M2170 M2171 S2172 Q2173 A2174 M2175 L2178 L2182 K2183 L2188 I2192 N2193 L2114 L2115 C2116 S2117 Q2118 P2119 D2120 T2121 G2122 F2123 Q2124 A2125 L2128 C2129 D2130 A2131 L2132 V2140 V2143 V2146 L2149 T2150 R2222 L2223 K2152 E2156 GLY I2228	G2229 A2230 E2233 G2234 E2235 N2236 V2237 V2238 G2239 S2240 V2244 V2247 K2248 I2251 A2252 A2253 F2254 F2255 Y2264 G2267 V2275 D2276 L2277 A2287 W2290 Y2293 K2294 G2295 E2296 G2299 Q2300 G2301 K2302 A2303 N2304 T2305 T2306 H2307 L2308 L2309 K2310 D2311 N2312 T2315 I2319 L2328	SER ASN PRO ASN ASN THR THR GLY SER THR GLY ALA SER GLY SER THR GLY ASP GLU ASN Q3006 Q3007 L3010 A3011 A3012 A3013 L3014 E3018 G3024 M3027 R3028 L3029 R3033 V3037 I3040 S3041 T3042 G3043 S3044 L3045 D3048 G3055 L3056 P3057	M3058 G3059 R3060 I3061 V3062 E3063 I3064 Y3065 G3066 P3067 E3068 K3072 T3073 T3074 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 L3114 E3123 Q3124 E3127 L3132 L3133 S3135 V3138 D3139 V3140	V3143 D3144 S3145 V3146 A3147 A3148 L3149 T3150 P3151 LYS ALA GLU ILE GLU GLY ILE GLY ASP SER HIS MET GLY L3166 A3167 A3168 R3169 M3170 S3171 S3172 D3173 A3174 I3175 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 G3212 N3213 A3214 Y3218 V3221 R3222 L3223 D3224 G3229 A3230 V3231 K3232 N3236 V3237 Y3244 K3245 V3246 V3247 K3248 N3249 K3250 I3251 A3252 P3254 Y3264 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 I3319 E3320 L3326 L3327 L3328 SER ASN PRO ASN SER THR
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4 Data and refinement statistics

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 20.00 – 4.30	Depositor EDS
% Data completeness (in resolution range)	92.7 (20.00-4.30) 91.6 (20.00-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 4.28Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.261 0.275 , 0.285	Depositor DCC
R_{free} test set	1946 reflections (1.99%)	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)	0.19 , 94.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.99	19/9068 (0.2%)	1.14	55/12192 (0.5%)
1	B	0.90	3/8861 (0.0%)	1.08	31/11910 (0.3%)
1	C	0.92	7/8951 (0.1%)	1.09	40/12033 (0.3%)
1	D	0.86	3/8951 (0.0%)	1.08	36/12033 (0.3%)
1	E	0.85	5/8879 (0.1%)	1.08	34/11934 (0.3%)
1	F	0.92	8/8951 (0.1%)	1.09	34/12033 (0.3%)
1	G	0.91	6/8892 (0.1%)	1.09	37/11953 (0.3%)
1	H	0.87	9/8938 (0.1%)	1.09	35/12014 (0.3%)
All	All	0.90	60/71491 (0.1%)	1.09	302/96102 (0.3%)

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 (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	HIS	N-CA	11.76	1.61	1.46
1	A	159	ILE	CA-C	11.04	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	159	ILE	CA-CB	8.75	1.65	1.54
1	F	1159	ILE	CA-CB	8.70	1.66	1.54
1	H	2036	ASP	CA-C	8.61	1.63	1.53
1	A	1199	ILE	CA-CB	8.37	1.65	1.54
1	A	1210	THR	CA-CB	8.30	1.63	1.52
1	A	163	HIS	CA-C	8.04	1.63	1.52
1	A	1210	THR	CA-C	8.00	1.62	1.53
1	A	1208	THR	CA-CB	7.82	1.66	1.53
1	A	160	GLY	N-CA	7.11	1.53	1.44
1	A	3073	THR	CA-CB	6.97	1.64	1.53
1	C	1164	MET	CA-C	6.83	1.61	1.52
1	C	1164	MET	N-CA	6.77	1.54	1.46
1	A	1164	MET	CB-CG	6.74	1.72	1.52
1	A	1164	MET	CA-C	-6.68	1.43	1.52
1	A	159	ILE	CA-CB	6.61	1.62	1.55
1	B	3073	THR	CA-CB	6.17	1.63	1.53
1	H	158	GLU	CA-C	6.08	1.58	1.52
1	G	159	ILE	N-CA	6.05	1.53	1.46
1	H	1036	ASP	CA-C	5.99	1.60	1.53
1	H	163	HIS	N-CA	5.98	1.53	1.46
1	A	161	ASP	N-CA	5.83	1.52	1.46
1	H	1159	ILE	CA-CB	5.82	1.61	1.53
1	D	3073	THR	CA-CB	5.80	1.62	1.53
1	F	3268	ILE	C-N	5.75	1.40	1.33
1	H	2037	VAL	N-CA	5.72	1.53	1.46
1	H	3150	THR	CA-CB	5.70	1.62	1.52
1	F	159	ILE	CA-CB	5.69	1.62	1.54
1	A	3150	THR	CA-CB	5.61	1.62	1.52
1	B	73	THR	CA-CB	5.58	1.62	1.53
1	H	3073	THR	CA-CB	5.56	1.62	1.53
1	C	3150	THR	CA-CB	5.55	1.61	1.52
1	A	164	MET	N-CA	5.50	1.53	1.46
1	E	1036	ASP	CA-C	5.47	1.59	1.53
1	E	3150	THR	CA-CB	5.43	1.61	1.52
1	F	1268	ILE	C-N	5.39	1.40	1.33
1	C	73	THR	CA-CB	5.38	1.62	1.53
1	A	1159	ILE	CA-CB	5.37	1.61	1.54
1	E	3073	THR	CA-CB	5.36	1.62	1.53
1	D	3150	THR	CA-CB	5.35	1.61	1.52
1	G	3150	THR	CA-CB	5.35	1.61	1.52
1	G	268	ILE	C-N	-5.33	1.26	1.33
1	E	73	THR	CA-CB	5.32	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	73	THR	CA-CB	5.30	1.62	1.53
1	G	73	THR	CA-CB	5.28	1.62	1.53
1	F	1159	ILE	CA-C	5.28	1.59	1.52
1	B	3150	THR	CA-CB	5.27	1.61	1.52
1	G	3073	THR	CA-CB	5.26	1.61	1.53
1	C	1159	ILE	CA-CB	5.24	1.61	1.54
1	C	163	HIS	CA-C	5.23	1.59	1.52
1	F	3150	THR	CA-CB	5.22	1.61	1.52
1	C	1036	ASP	C-O	5.19	1.29	1.23
1	F	3073	THR	CA-CB	5.19	1.61	1.53
1	D	159	ILE	CA-CB	5.16	1.61	1.54
1	E	156	GLU	CA-C	5.09	1.59	1.52
1	F	164	MET	N-CA	5.07	1.52	1.46
1	A	1197	MET	CA-C	5.03	1.59	1.52
1	A	2166	LEU	CA-C	5.02	1.59	1.52
1	A	73	THR	CA-CB	5.00	1.61	1.53

All (302) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	HIS	N-CA-C	11.44	128.28	110.20
1	D	1163	HIS	N-CA-C	10.76	126.00	109.96
1	A	1150	THR	CA-C-N	9.40	130.64	120.11
1	A	1150	THR	C-N-CA	9.40	130.64	120.11
1	H	158	GLU	N-CA-C	9.23	124.49	112.12
1	H	2036	ASP	CA-C-N	9.19	135.68	122.45
1	H	2036	ASP	C-N-CA	9.19	135.68	122.45
1	A	1210	THR	CB-CA-C	9.13	124.76	111.88
1	H	1150	THR	CA-C-N	9.13	130.34	120.11
1	H	1150	THR	C-N-CA	9.13	130.34	120.11
1	C	1150	THR	CA-C-N	9.03	130.22	120.11
1	C	1150	THR	C-N-CA	9.03	130.22	120.11
1	E	1150	THR	CA-C-N	9.01	130.19	120.11
1	E	1150	THR	C-N-CA	9.01	130.19	120.11
1	G	1150	THR	CA-C-N	8.97	130.16	120.11
1	G	1150	THR	C-N-CA	8.97	130.16	120.11
1	B	1150	THR	CA-C-N	8.94	130.12	120.11
1	B	1150	THR	C-N-CA	8.94	130.12	120.11
1	D	1150	THR	CA-C-N	8.85	130.02	120.11
1	D	1150	THR	C-N-CA	8.85	130.02	120.11
1	F	1150	THR	CA-C-N	8.83	130.00	120.11
1	F	1150	THR	C-N-CA	8.83	130.00	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	156	GLU	N-CA-C	-8.53	101.97	112.38
1	G	158	GLU	N-CA-C	8.43	128.76	110.80
1	G	159	ILE	N-CA-C	8.39	121.13	109.55
1	H	2228	ILE	N-CA-C	8.23	118.56	111.90
1	A	2150	THR	CA-C-N	8.20	128.08	120.21
1	A	2150	THR	C-N-CA	8.20	128.08	120.21
1	A	1164	MET	CA-C-N	-8.13	105.48	121.41
1	A	1164	MET	C-N-CA	-8.13	105.48	121.41
1	C	2228	ILE	N-CA-C	8.12	118.48	111.90
1	B	2228	ILE	N-CA-C	8.11	118.47	111.90
1	F	2228	ILE	N-CA-C	8.11	118.47	111.90
1	G	2150	THR	CA-C-N	8.11	127.99	120.21
1	G	2150	THR	C-N-CA	8.11	127.99	120.21
1	B	2150	THR	CA-C-N	8.10	127.98	120.21
1	B	2150	THR	C-N-CA	8.10	127.98	120.21
1	E	2150	THR	CA-C-N	8.06	127.95	120.21
1	E	2150	THR	C-N-CA	8.06	127.95	120.21
1	E	2228	ILE	N-CA-C	8.04	118.41	111.90
1	G	1121	THR	N-CA-C	7.99	120.78	108.07
1	D	2228	ILE	N-CA-C	7.99	118.37	111.90
1	H	2150	THR	CA-C-N	7.97	127.86	120.21
1	H	2150	THR	C-N-CA	7.97	127.86	120.21
1	E	1121	THR	N-CA-C	7.93	120.68	108.07
1	H	1121	THR	N-CA-C	7.93	120.68	108.07
1	F	2150	THR	CA-C-N	7.91	127.81	120.21
1	F	2150	THR	C-N-CA	7.91	127.81	120.21
1	A	1121	THR	N-CA-C	7.90	120.63	108.07
1	B	1121	THR	N-CA-C	7.88	120.61	108.07
1	C	1121	THR	N-CA-C	7.87	120.59	108.07
1	C	2150	THR	CA-C-N	7.85	127.74	120.21
1	C	2150	THR	C-N-CA	7.85	127.74	120.21
1	D	2150	THR	CA-C-N	7.84	127.74	120.21
1	D	2150	THR	C-N-CA	7.84	127.74	120.21
1	G	2228	ILE	N-CA-C	7.84	118.25	111.90
1	F	3269	ASN	N-CA-C	7.83	120.23	109.11
1	D	1121	THR	N-CA-C	7.77	120.42	108.07
1	F	1121	THR	N-CA-C	7.67	120.27	108.07
1	A	3066	GLY	CA-C-N	7.64	129.39	119.84
1	A	3066	GLY	C-N-CA	7.64	129.39	119.84
1	F	3066	GLY	CA-C-N	7.63	129.37	119.84
1	F	3066	GLY	C-N-CA	7.63	129.37	119.84
1	B	3066	GLY	CA-C-N	7.62	129.36	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3066	GLY	C-N-CA	7.62	129.36	119.84
1	D	3066	GLY	CA-C-N	7.55	129.27	119.84
1	D	3066	GLY	C-N-CA	7.55	129.27	119.84
1	A	2228	ILE	N-CA-C	7.51	117.99	111.90
1	A	162	SER	CA-C-N	7.45	132.07	121.42
1	A	162	SER	C-N-CA	7.45	132.07	121.42
1	H	3066	GLY	CA-C-N	7.31	128.98	119.84
1	H	3066	GLY	C-N-CA	7.31	128.98	119.84
1	C	3066	GLY	CA-C-N	7.27	128.93	119.84
1	C	3066	GLY	C-N-CA	7.27	128.93	119.84
1	E	3056	LEU	CA-C-N	7.24	128.38	119.98
1	E	3056	LEU	C-N-CA	7.24	128.38	119.98
1	A	159	ILE	N-CA-C	7.15	117.90	107.75
1	E	3066	GLY	CA-C-N	7.15	128.78	119.84
1	E	3066	GLY	C-N-CA	7.15	128.78	119.84
1	D	3056	LEU	CA-C-N	7.15	128.27	119.98
1	D	3056	LEU	C-N-CA	7.15	128.27	119.98
1	C	3056	LEU	CA-C-N	7.10	128.21	119.98
1	C	3056	LEU	C-N-CA	7.10	128.21	119.98
1	A	1194	GLN	CA-C-N	-7.05	109.27	121.97
1	A	1194	GLN	C-N-CA	-7.05	109.27	121.97
1	C	1279	VAL	N-CA-C	-7.04	104.33	110.74
1	H	3056	LEU	CA-C-N	7.01	128.11	119.98
1	H	3056	LEU	C-N-CA	7.01	128.11	119.98
1	E	3269	ASN	N-CA-C	6.97	119.02	109.11
1	C	1164	MET	N-CA-C	6.91	125.52	110.80
1	G	3056	LEU	CA-C-N	6.91	128.00	119.98
1	G	3056	LEU	C-N-CA	6.91	128.00	119.98
1	G	3066	GLY	CA-C-N	6.84	128.39	119.84
1	G	3066	GLY	C-N-CA	6.84	128.39	119.84
1	H	3269	ASN	N-CA-C	6.80	118.76	109.11
1	A	1279	VAL	N-CA-C	-6.77	104.58	110.74
1	E	1279	VAL	N-CA-C	-6.75	104.60	110.74
1	A	3056	LEU	CA-C-N	6.69	127.74	119.98
1	A	3056	LEU	C-N-CA	6.69	127.74	119.98
1	F	1156	GLU	N-CA-C	-6.64	103.86	112.23
1	B	1056	LEU	CA-C-N	6.63	128.13	119.84
1	B	1056	LEU	C-N-CA	6.63	128.13	119.84
1	A	1164	MET	CB-CG-SD	6.60	132.50	112.70
1	G	1279	VAL	N-CA-C	-6.59	104.74	110.74
1	A	238	VAL	N-CA-C	6.56	122.99	109.34
1	A	150	THR	CA-C-N	6.53	126.56	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	THR	C-N-CA	6.53	126.56	119.89
1	C	150	THR	CA-C-N	6.53	126.55	119.89
1	C	150	THR	C-N-CA	6.53	126.55	119.89
1	F	238	VAL	N-CA-C	6.52	122.91	109.34
1	C	238	VAL	N-CA-C	6.52	122.90	109.34
1	C	2056	LEU	CA-C-N	6.50	126.86	119.83
1	C	2056	LEU	C-N-CA	6.50	126.86	119.83
1	E	238	VAL	N-CA-C	6.50	122.87	109.34
1	H	1279	VAL	N-CA-C	-6.48	104.84	110.74
1	A	3090	CYS	N-CA-C	6.47	120.04	109.24
1	G	150	THR	CA-C-N	6.47	126.49	119.89
1	G	150	THR	C-N-CA	6.47	126.49	119.89
1	H	150	THR	CA-C-N	6.44	126.46	119.89
1	H	150	THR	C-N-CA	6.44	126.46	119.89
1	F	1056	LEU	CA-C-N	6.43	127.87	119.84
1	F	1056	LEU	C-N-CA	6.43	127.87	119.84
1	G	238	VAL	N-CA-C	6.42	122.69	109.34
1	H	238	VAL	N-CA-C	6.41	122.68	109.34
1	D	3090	CYS	N-CA-C	6.41	119.94	109.24
1	B	238	VAL	N-CA-C	6.40	122.65	109.34
1	F	3090	CYS	N-CA-C	6.39	119.91	109.24
1	B	150	THR	CA-C-N	6.39	126.40	119.89
1	B	150	THR	C-N-CA	6.39	126.40	119.89
1	H	1056	LEU	CA-C-N	6.39	127.82	119.84
1	H	1056	LEU	C-N-CA	6.39	127.82	119.84
1	D	238	VAL	N-CA-C	6.37	122.59	109.34
1	F	1162	SER	N-CA-C	6.36	120.50	112.87
1	F	2056	LEU	CA-C-N	6.36	126.70	119.83
1	F	2056	LEU	C-N-CA	6.36	126.70	119.83
1	D	150	THR	CA-C-N	6.35	126.37	119.89
1	D	150	THR	C-N-CA	6.35	126.37	119.89
1	F	3056	LEU	CA-C-N	6.34	127.33	119.98
1	F	3056	LEU	C-N-CA	6.34	127.33	119.98
1	D	1056	LEU	CA-C-N	6.33	127.75	119.84
1	D	1056	LEU	C-N-CA	6.33	127.75	119.84
1	B	1279	VAL	N-CA-C	-6.33	104.98	110.74
1	E	2056	LEU	CA-C-N	6.33	126.66	119.83
1	E	2056	LEU	C-N-CA	6.33	126.66	119.83
1	A	1056	LEU	CA-C-N	6.32	127.74	119.84
1	A	1056	LEU	C-N-CA	6.32	127.74	119.84
1	C	1036	ASP	O-C-N	6.28	130.79	122.56
1	F	150	THR	CA-C-N	6.28	126.29	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	150	THR	C-N-CA	6.28	126.29	119.89
1	G	2056	LEU	CA-C-N	6.26	126.59	119.83
1	G	2056	LEU	C-N-CA	6.26	126.59	119.83
1	E	1056	LEU	CA-C-N	6.26	127.66	119.84
1	E	1056	LEU	C-N-CA	6.26	127.66	119.84
1	B	3056	LEU	CA-C-N	6.25	127.22	119.98
1	B	3056	LEU	C-N-CA	6.25	127.22	119.98
1	C	3139	ASP	N-CA-C	6.25	120.64	112.89
1	D	1279	VAL	N-CA-C	-6.20	105.10	110.74
1	C	3269	ASN	N-CA-C	6.19	118.44	109.71
1	B	2056	LEU	CA-C-N	6.19	126.51	119.83
1	B	2056	LEU	C-N-CA	6.19	126.51	119.83
1	A	3139	ASP	N-CA-C	6.19	120.90	113.23
1	D	2056	LEU	CA-C-N	6.17	126.50	119.83
1	D	2056	LEU	C-N-CA	6.17	126.50	119.83
1	H	3090	CYS	N-CA-C	6.17	119.55	109.24
1	A	2056	LEU	CA-C-N	6.17	126.50	119.83
1	A	2056	LEU	C-N-CA	6.17	126.50	119.83
1	E	150	THR	CA-C-N	6.17	126.18	119.89
1	E	150	THR	C-N-CA	6.17	126.18	119.89
1	E	1268	ILE	O-C-N	6.14	130.14	122.59
1	C	1056	LEU	CA-C-N	6.11	127.48	119.84
1	C	1056	LEU	C-N-CA	6.11	127.48	119.84
1	B	3090	CYS	N-CA-C	6.09	119.41	109.24
1	A	1210	THR	CA-C-N	6.05	133.26	121.41
1	A	1210	THR	C-N-CA	6.05	133.26	121.41
1	G	1056	LEU	CA-C-N	6.03	127.38	119.84
1	G	1056	LEU	C-N-CA	6.03	127.38	119.84
1	E	3090	CYS	N-CA-C	6.01	119.28	109.24
1	H	2056	LEU	CA-C-N	6.00	126.31	119.83
1	H	2056	LEU	C-N-CA	6.00	126.31	119.83
1	E	3083	ALA	N-CA-C	-5.96	104.75	112.68
1	E	236	ASN	N-CA-C	5.96	118.23	109.24
1	B	3150	THR	N-CA-CB	5.92	117.99	110.23
1	G	3090	CYS	N-CA-C	5.92	119.12	109.24
1	E	3139	ASP	N-CA-C	5.92	120.57	113.23
1	A	3269	ASN	N-CA-C	5.89	118.34	107.73
1	D	236	ASN	N-CA-C	5.86	118.09	109.24
1	C	3090	CYS	N-CA-C	5.85	119.01	109.24
1	D	3269	ASN	N-CA-C	5.85	118.26	107.73
1	C	1298	ILE	CB-CA-C	-5.84	105.92	111.06
1	H	236	ASN	N-CA-C	5.83	118.04	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	236	ASN	N-CA-C	5.80	117.99	109.24
1	C	3150	THR	N-CA-CB	5.79	117.81	110.23
1	B	236	ASN	N-CA-C	5.78	117.97	109.24
1	B	3269	ASN	N-CA-C	5.77	118.12	107.73
1	G	1305	ALA	N-CA-C	-5.76	104.69	110.97
1	C	236	ASN	N-CA-C	5.75	117.92	109.24
1	A	236	ASN	N-CA-C	5.75	117.92	109.24
1	G	3139	ASP	N-CA-C	5.72	120.33	113.23
1	F	3150	THR	N-CA-CB	5.72	117.73	110.23
1	G	3150	THR	N-CA-CB	5.70	117.70	110.23
1	C	90	CYS	N-CA-C	5.69	118.83	109.72
1	D	155	ILE	O-C-N	5.69	127.80	121.94
1	G	1094	ASP	N-CA-C	5.68	117.97	108.02
1	H	3139	ASP	N-CA-C	5.68	120.28	113.23
1	E	90	CYS	N-CA-C	5.68	118.81	109.72
1	H	1158	GLU	N-CA-C	5.65	122.84	110.80
1	A	158	GLU	N-CA-C	5.62	122.77	110.80
1	D	3139	ASP	N-CA-C	5.62	120.19	113.23
1	F	236	ASN	N-CA-C	5.61	117.71	109.24
1	B	3139	ASP	N-CA-C	5.60	119.83	112.89
1	A	90	CYS	N-CA-C	5.59	118.66	109.72
1	A	1194	GLN	O-C-N	-5.58	114.41	121.67
1	A	1210	THR	CA-C-O	5.57	130.68	122.38
1	E	3150	THR	N-CA-CB	5.56	117.52	110.23
1	H	90	CYS	N-CA-C	5.56	118.62	109.72
1	C	1268	ILE	O-C-N	-5.55	116.17	122.72
1	H	3150	THR	N-CA-CB	5.55	117.50	110.23
1	C	1094	ASP	N-CA-C	5.55	117.73	108.02
1	E	1094	ASP	N-CA-C	5.53	117.70	108.02
1	A	1094	ASP	N-CA-C	5.52	117.69	108.02
1	A	94	ASP	N-CA-C	5.52	117.52	108.52
1	D	2168	ALA	N-CA-C	-5.51	106.53	113.20
1	E	2007	GLN	CA-C-N	5.50	128.12	120.63
1	E	2007	GLN	C-N-CA	5.50	128.12	120.63
1	G	90	CYS	N-CA-C	5.50	118.52	109.72
1	D	3150	THR	N-CA-CB	5.48	117.41	110.23
1	A	1194	GLN	N-CA-C	5.47	120.85	114.62
1	B	90	CYS	N-CA-C	5.46	118.46	109.72
1	G	3027	MET	N-CA-C	5.46	116.44	108.14
1	G	2168	ALA	N-CA-C	-5.46	106.60	113.20
1	C	85	ARG	N-CA-C	-5.45	107.19	112.97
1	H	2007	GLN	CA-C-N	5.39	127.96	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	2007	GLN	C-N-CA	5.39	127.96	120.63
1	A	3150	THR	N-CA-CB	5.39	117.29	110.23
1	H	1094	ASP	N-CA-C	5.39	117.45	108.02
1	A	3027	MET	N-CA-C	5.38	116.33	108.14
1	E	3027	MET	N-CA-C	5.38	116.32	108.14
1	G	3269	ASN	N-CA-C	5.37	117.95	108.24
1	C	3083	ALA	N-CA-C	-5.36	105.56	112.68
1	F	3027	MET	N-CA-C	5.35	116.28	108.14
1	H	2168	ALA	N-CA-C	-5.35	106.72	113.20
1	A	2168	ALA	N-CA-C	-5.34	106.73	113.20
1	B	85	ARG	N-CA-C	-5.33	107.31	112.97
1	D	1094	ASP	N-CA-C	5.33	117.36	108.02
1	A	1164	MET	N-CA-CB	5.33	119.50	110.49
1	D	3083	ALA	N-CA-C	-5.33	105.59	112.68
1	E	2168	ALA	N-CA-C	-5.32	106.76	113.20
1	B	1094	ASP	N-CA-C	5.31	117.31	108.02
1	G	2007	GLN	CA-C-N	5.31	127.85	120.63
1	G	2007	GLN	C-N-CA	5.31	127.85	120.63
1	A	2007	GLN	CA-C-N	5.30	127.84	120.63
1	A	2007	GLN	C-N-CA	5.30	127.84	120.63
1	C	1268	ILE	CA-C-N	5.29	130.73	122.26
1	C	1268	ILE	C-N-CA	5.29	130.73	122.26
1	F	56	LEU	CA-C-N	5.29	126.46	119.84
1	F	56	LEU	C-N-CA	5.29	126.46	119.84
1	B	3027	MET	N-CA-C	5.28	116.17	108.14
1	C	2168	ALA	N-CA-C	-5.28	106.82	113.20
1	D	3027	MET	N-CA-C	5.27	116.15	108.14
1	D	2007	GLN	CA-C-N	5.27	127.80	120.63
1	D	2007	GLN	C-N-CA	5.27	127.80	120.63
1	G	1298	ILE	CB-CA-C	-5.27	106.42	111.06
1	C	3027	MET	N-CA-C	5.26	116.14	108.14
1	E	94	ASP	N-CA-C	5.23	117.04	108.52
1	F	2168	ALA	N-CA-C	-5.22	106.88	113.20
1	F	2007	GLN	CA-C-N	5.22	127.73	120.63
1	F	2007	GLN	C-N-CA	5.22	127.73	120.63
1	F	90	CYS	N-CA-C	5.21	118.06	109.72
1	F	85	ARG	N-CA-C	-5.19	107.47	112.97
1	G	3140	VAL	N-CA-C	5.19	114.70	108.06
1	B	2007	GLN	CA-C-N	5.18	127.67	120.63
1	B	2007	GLN	C-N-CA	5.18	127.67	120.63
1	E	85	ARG	N-CA-C	-5.18	107.48	112.97
1	D	90	CYS	N-CA-C	5.17	117.99	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	3027	MET	N-CA-C	5.16	115.99	108.14
1	C	56	LEU	CA-C-N	5.15	126.28	119.84
1	C	56	LEU	C-N-CA	5.15	126.28	119.84
1	C	1269	ASN	N-CA-C	5.15	117.48	108.52
1	D	1298	ILE	CB-CA-C	-5.15	106.53	111.06
1	A	2094	ASP	N-CA-C	5.14	117.09	107.99
1	B	2168	ALA	N-CA-C	-5.13	106.99	113.20
1	C	94	ASP	N-CA-C	5.13	116.88	108.52
1	F	3139	ASP	N-CA-C	5.13	119.59	113.23
1	A	3140	VAL	N-CA-C	5.12	114.61	108.06
1	A	1298	ILE	CB-CA-C	-5.11	106.56	111.06
1	A	85	ARG	N-CA-C	-5.11	107.56	112.97
1	G	85	ARG	N-CA-C	-5.10	107.56	112.97
1	B	94	ASP	N-CA-C	5.09	116.82	108.52
1	F	1094	ASP	N-CA-C	5.09	116.92	108.02
1	F	2239	GLY	N-CA-C	5.08	118.70	110.87
1	C	2094	ASP	N-CA-C	5.07	116.95	107.99
1	G	1064	ILE	CB-CA-C	-5.06	104.88	111.81
1	A	1164	MET	N-CA-C	-5.05	100.03	110.80
1	A	192	ILE	N-CA-C	5.05	115.24	108.17
1	E	3140	VAL	N-CA-C	5.05	114.53	108.06
1	G	2094	ASP	N-CA-C	5.04	116.92	107.99
1	A	56	LEU	CA-C-N	5.04	126.14	119.84
1	A	56	LEU	C-N-CA	5.04	126.14	119.84
1	H	85	ARG	N-CA-C	-5.02	107.65	112.97
1	D	56	LEU	CA-C-N	5.01	126.10	119.84
1	D	56	LEU	C-N-CA	5.01	126.10	119.84
1	H	94	ASP	N-CA-C	5.00	116.68	108.52

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

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Mol	Chain	Res	Type	Group
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	Mainchain,Peptide
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

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	330	1
1	B	8769	0	9070	295	0
1	C	8856	0	9139	310	1
1	D	8856	0	9139	294	0
1	E	8787	0	9082	326	0
1	F	8856	0	9139	332	0
1	G	8799	0	9090	293	0
1	H	8844	0	9131	324	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
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	2368	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 16.

All (2368) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:162:SER:C	1:A:165:GLY:HA3	1.93	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:ASN:ND2	1:A:1209:THR:HG23	1.88	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:A:163:HIS:C	1:A:165:GLY:H	1.80	0.85
1:A:162:SER:O	1:A:165:GLY:C	2.20	0.84
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
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: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:C:3177:LYS:HE2	1:F:173:GLN:CD	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:1160:GLY:HA3	1:F:1164:MET:HE3	1.68	0.76
1:G:1222:ARG:HB2	1:G:1248:LYS:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:156:GLU:CD	1:A:1176:ARG:HG3	2.11	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: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:E:2304:ASN:HB3	1:H:2300:GLN:CD	2.12	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
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:A:163:HIS:C	1:A:165:GLY:N	2.47	0.72
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1160:GLY:C	1:A:1161:ASP:OD1	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1146:VAL:HG11	1:E:1211:GLY:HA3	1.76	0.68
1:G:3044:SER:OG	1:G:3045:LEU:N	2.23	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: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:1305:ALA:O	1:G:1306:THR:C	2.38	0.67
1:G:2118:GLN:HE22	1:G:3249:ASN:H	1.42	0.67
1:A:1202:MET:HE2	1:A:1202:MET:HA	1.77	0.67
1:F:3185:SER:C	1:F:3187:THR:H	2.03	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
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:B:3185:SER:C	1:B:3187:THR:H	2.02	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:C:1305:ALA:O	1:C:1306:THR:C	2.37	0.66
1:F:1305:ALA:O	1:F:1306:THR:C	2.39	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:D:3185:SER:C	1:D:3187:THR:H	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1217:PHE:HA	1:D:1248:LYS:HE3	1.77	0.66
1:G:3185:SER:C	1:G:3187:THR:H	2.04	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:3185:SER:C	1:E:3187:THR:H	2.05	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:3185:SER:C	1:A:3187:THR:H	2.05	0.65
1:C:3185:SER:C	1:C:3187:THR:H	2.05	0.65
1:A:1217:PHE:HA	1:A:1248:LYS:HE3	1.79	0.65
1:A:1305:ALA:O	1:A:1306:THR:C	2.40	0.65
1:D:1305:ALA:O	1:D:1306:THR:C	2.40	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: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: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
1:A:2063:GLU:OE1	1:A:2222:ARG:HD2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1123:GLU:HB2	1:B:1152:LYS:CE	2.28	0.63
1:A:1163:HIS:O	1:A:1164:MET:C	2.41	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:B:156:GLU:CD	1:B:1176:ARG:HG3	2.23	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:H:3185:SER:C	1:H:3187:THR:H	2.05	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: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: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: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
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:B:1308:TRP:HE3	1:B:1309:LEU:HD23	1.63	0.62
1:D:1164:MET:HE2	1:D:1165:GLY:HA2	1.81	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:H:1305:ALA:O	1:H:1306:THR:C	2.43	0.62
1:B:1305:ALA:O	1:B:1306:THR:C	2.41	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3177:LYS:NZ	1:F:173:GLN:HG3	2.15	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:H:3018:GLU:HG2	1:H:3024:GLY:H	1.64	0.61
1:G:1155:ILE:C	1:G:1156:GLU:OE2	2.44	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: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
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:1305:ALA:O	1:E:1306:THR:C	2.43	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:ASN:HD21	1:A:1211:GLY:H	1.47	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:E:2300:GLN:NE2	1:H:2300:GLN:N	2.49	0.60
1:F:3065:TYR:C	1:F:3065:TYR:CD2	2.80	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:E:3065:TYR:HD2	1:E:3065:TYR:C	2.10	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:D:3065:TYR:HD2	1:D:3065:TYR:C	2.10	0.60
1:E:1053:ALA:HB2	1:E:1251:ILE:HG21	1.82	0.60
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:E:3065:TYR:C	1:E:3065:TYR:CD2	2.80	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:F:3065:TYR:C	1:F:3065:TYR:HD2	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3065:TYR:C	1:H:3065:TYR:CD2	2.81	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:D:3065:TYR:C	1:D:3065:TYR:CD2	2.81	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: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: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
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:G:3065:TYR:HD2	1:G:3065:TYR:C	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:3065:TYR:C	1:H:3065:TYR:HD2	2.10	0.58
1:A:1161:ASP:CG	1:A:1166:LEU:HD13	2.29	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:G:3065:TYR:C	1:G:3065:TYR:CD2	2.82	0.58
1:A:3065:TYR:HD2	1:A:3065:TYR:C	2.12	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:C:3065:TYR:HD2	1:C:3065:TYR:C	2.12	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:F:3100:ASP:O	1:F:3101:PRO:C	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1141:ILE:HG21	1:G:1189:LEU:HD12	1.86	0.57
1:B:1123:GLU:HB2	1:B:1152:LYS:HZ2	1.68	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:D:155:ILE:C	1:D:157:GLY:N	2.60	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:C:3065:TYR:C	1:C:3065:TYR:CD2	2.82	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:C:1065:TYR:C	1:C:1065:TYR:CD1	2.82	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: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:C:270:PHE:HA	1:C:273:GLU:HG2	1.84	0.57
1:E:1123:GLU:HB2	1:E:1152:LYS:HZ2	1.70	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
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:D:1123:GLU:HB2	1:D:1152:LYS:HZ1	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:THR:HA	1:G:79:VAL:HG12	1.87	0.57
1:A:1063:GLU:OE2	1:A:1209:THR:OG1	2.20	0.57
1:E:2217:PHE:O	1:E:2248:LYS:NZ	2.38	0.57
1:F:1065:TYR:C	1:F:1065:TYR:CD1	2.83	0.57
1:D:3100:ASP:O	1:D:3101:PRO:C	2.46	0.56
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:E:1065:TYR:CD1	1:E:1065:TYR:C	2.83	0.56
1:B:1065:TYR:CD1	1:B:1065:TYR:C	2.84	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:C:2155:ILE:C	1:C:2156:GLU:HG3	2.30	0.56
1:C:3177:LYS:CE	1:F:173:GLN:CD	2.76	0.56
1:D:1065:TYR:CD1	1:D:1065:TYR:C	2.83	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:1065:TYR:CD1	1:G:1065:TYR:C	2.84	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:H:1065:TYR:CD1	1:H:1065:TYR:C	2.83	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:1123:GLU:HB2	1:F:1152:LYS:NZ	2.21	0.56
1:F:1281:GLU:O	1:F:1283:LEU:N	2.39	0.56
1:G:3100:ASP:O	1:G:3101:PRO:C	2.49	0.56
1:H:1145:SER:HB2	1:H:1192:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3065:TYR:C	1:A:3065:TYR:CD2	2.82	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
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:A:1065:TYR:CD1	1:A:1065:TYR:C	2.84	0.56
1:B:1141:ILE:HG21	1:B:1189:LEU:HD12	1.87	0.56
1:B:3065:TYR:C	1:B:3065:TYR:CD2	2.84	0.56
1:F:237:VAL:O	1:F:239:GLY:N	2.33	0.56
1:B:3100:ASP:O	1:B:3101:PRO:C	2.47	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: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:C:164:MET:C	1:C:166:LEU:H	2.14	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:A:1067:PRO:O	1:A:1070:SER:OG	2.22	0.55
1:A:1123:GLU:HB2	1:A:1152:LYS:HZ2	1.72	0.55
1:B:1230:ALA:HA	1:B:1240:SER:HA	1.88	0.55
1:E:232:LYS:HZ3	1:F:3266:GLU:HG3	1.71	0.55
1:F:3072:LYS:CE	3:F:3400:ANP:O1B	2.50	0.55
1:H:1067:PRO:O	1:H:1070:SER:OG	2.23	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:A:1145:SER:O	1:A:1146:VAL:C	2.50	0.55
1:B:3065:TYR:C	1:B:3065:TYR:HD2	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:3065:TYR:HE2	1:B:3224:ASP:CG	2.15	0.55
1:C:42:THR:HA	1:C:79:VAL:HG12	1.89	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:E:2173:GLN:C	1:E:2175:MET:H	2.15	0.55
1:A:1123:GLU:HB2	1:A:1152:LYS:NZ	2.22	0.55
1:C:1141:ILE:HG21	1:C:1189:LEU:HD12	1.88	0.55
1:E:1153:ALA:O	1:E:1156:GLU:C	2.50	0.55
1:F:42:THR:HA	1:F:79:VAL:HG12	1.88	0.55
1:D:2173:GLN:C	1:D:2175:MET:H	2.15	0.55
1:E:42:THR:HA	1:E:79:VAL:HG12	1.88	0.55
1:F:118:GLN:NE2	1:F:1249:ASN:H	2.04	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: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: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:G:1123:GLU:HB2	1:G:1152:LYS:HZ1	1.72	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:2173:GLN:C	1:F:2175:MET:H	2.15	0.54
1:F:3268:ILE:HG22	1:F:3269:ASN:N	2.23	0.54
1:G:2173:GLN:C	1:G:2175:MET:H	2.15	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:1065:TYR:C	1:C:1065:TYR:HD1	2.16	0.54
1:C:1123:GLU:HB2	1:C:1152:LYS:NZ	2.22	0.54
1:C:3100:ASP:O	1:C:3101:PRO:C	2.50	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:F:1067:PRO:O	1:F:1070:SER:OG	2.23	0.54
1:F:3171:MET:C	1:F:3173:GLN:N	2.65	0.54
1:G:131:ALA:HB1	1:G:1017:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1078:GLN:O	1:G:1081:ALA:HB3	2.08	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:G:1067:PRO:O	1:G:1070:SER:OG	2.26	0.54
1:C:1057:PRO:HB2	1:C:1060:ARG:HG3	1.90	0.54
1:C:1123:GLU:HB2	1:C:1152:LYS:HZ2	1.73	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:H:1065:TYR:C	1:H:1065:TYR:HD1	2.16	0.54
1:H:3100:ASP:O	1:H:3101:PRO:C	2.51	0.54
1:B:1143:VAL:O	1:B:1192:ILE:HG13	2.09	0.53
1:B:2173:GLN:C	1:B:2175:MET:H	2.16	0.53
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:B:1067:PRO:O	1:B:1070:SER:OG	2.23	0.53
1:G:2029:LEU:HD23	1:G:2254:PRO:HD2	1.89	0.53
1:A:1166:LEU:C	1:A:1168:ALA:H	2.16	0.53
1:B:1092:PHE:HB2	1:B:1114:LEU:HD11	1.90	0.53
1:C:2173:GLN:C	1:C:2175:MET:H	2.16	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:G:3171:MET:C	1:G:3173:GLN:N	2.66	0.53
1:C:1166:LEU:C	1:C:1168:ALA:H	2.16	0.53
1:G:92:PHE:N	1:G:115:LEU:O	2.39	0.53
1:G:1166:LEU:C	1:G:1168:ALA:H	2.17	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:C:1229:GLY:O	1:C:1230:ALA:HB3	2.08	0.53
1:D:1166:LEU:C	1:D:1168:ALA:H	2.17	0.53
1:E:1166:LEU:C	1:E:1168:ALA:H	2.16	0.53
1:E:3064:ILE:HG12	1:E:3223:LEU:CB	2.33	0.53
1:E:3100:ASP:O	1:E:3101:PRO:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3171:MET:C	1:D:3173:GLN:N	2.66	0.53
1:E:1229:GLY:O	1:E:1230:ALA:HB3	2.08	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:A:2173:GLN:C	1:A:2175:MET:H	2.16	0.53
1:E:3171:MET:C	1:E:3173:GLN:N	2.66	0.53
1:G:3059:GLY:HA2	1:G:3187:THR:O	2.08	0.53
1:H:2173:GLN:C	1:H:2175:MET:H	2.15	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:A:3100:ASP:O	1:A:3101:PRO:C	2.52	0.53
1:C:1073:THR:HA	1:C:1076:THR:HB	1.91	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:B:1145:SER:O	1:B:1146:VAL:C	2.52	0.53
1:C:3065:TYR:HE2	1:C:3224:ASP:CG	2.17	0.53
1:D:1057:PRO:HB2	1:D:1060:ARG:HG3	1.90	0.53
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:E:1065:TYR:C	1:E:1065:TYR:HD1	2.17	0.53
1:F:1065:TYR:C	1:F:1065:TYR:HD1	2.17	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:A:3065:TYR:HE2	1:A:3224:ASP:CG	2.17	0.52
1:F:1308:TRP:CE3	1:F:1309:LEU:HD23	2.44	0.52
1:B:1166:LEU:C	1:B:1168:ALA:H	2.17	0.52
1:C:153:ALA:O	1:C:158:GLU:HB2	2.09	0.52
1:C:1327:LEU:C	1:C:1328:LEU:HD12	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1229:GLY:O	1:B:1230:ALA:HB3	2.08	0.52
1:B:2065:TYR:HE1	1:B:2224:ASP:CG	2.17	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:F:3065:TYR:HE2	1:F:3224:ASP:CG	2.18	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:D:3065:TYR:HE2	1:D:3224:ASP:CG	2.18	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:F:1123:GLU:HB2	1:F:1152:LYS:HZ2	1.75	0.52
1:G:1327:LEU:C	1:G:1328:LEU:HD12	2.34	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:3065:TYR:HE2	1:E:3224:ASP:CG	2.17	0.52
1:E:3300:GLN:N	1:H:1300:GLN:HE22	2.02	0.52
1:F:1166:LEU:C	1:F:1168:ALA:H	2.17	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:B:3171:MET:C	1:B:3173:GLN:N	2.66	0.52
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:1298:ILE:HG13	1:D:1299:GLY:N	2.24	0.52
1:H:3171:MET:C	1:H:3173:GLN:N	2.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:2149:LEU:O	1:H:2170:MET:HE1	2.10	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:C:3171:MET:C	1:C:3173:GLN:N	2.67	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:156:GLU:OE2	1:A:1176:ARG:HG3	2.07	0.51
1:A:1091:ALA:HB3	1:A:1141:ILE:HA	1.93	0.51
1:B:3249:ASN:OD1	1:B:3251:ILE:HG22	2.10	0.51
1:D:1145:SER:O	1:D:1146:VAL:C	2.53	0.51
1:E:1143:VAL:O	1:E:1192:ILE:HG13	2.10	0.51
1:F:2065:TYR:HE1	1:F:2224:ASP:CG	2.18	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:A:132:LEU:HB2	1:A:141:ILE:HD11	1.92	0.51
1:A:1193:ASN:HD21	1:A:1209:THR:C	2.19	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:125:ALA:C	1:F:127:GLU:H	2.17	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1166:LEU:C	1:H:1168:ALA:H	2.17	0.51
1:H:2178:LEU:O	1:H:2182:LEU:HG	2.10	0.51
1:A:1065:TYR:C	1:A:1065:TYR:HD1	2.18	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:E:2065:TYR:HE1	1:E:2224:ASP:CG	2.18	0.51
1:E:3042:THR:OG1	1:E:3048:ASP:OD1	2.27	0.51
1:H:114:LEU:O	1:H:1028:ARG:HA	2.10	0.51
1:H:1145:SER:O	1:H:1146:VAL:C	2.53	0.51
1:H:1222:ARG:HB2	1:H:1248:LYS:CB	2.38	0.51
1:D:1065:TYR:C	1:D:1065:TYR:HD1	2.17	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:3059:GLY:HA2	1:C:3187:THR:O	2.10	0.51
1:F:1145:SER:O	1:F:1146:VAL:C	2.53	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:F:1229:GLY:O	1:F:1230:ALA:HB3	2.10	0.51
1:G:1298:ILE:HG13	1:G:1299:GLY:N	2.23	0.51
1:G:3221:VAL:HA	1:G:3248:LYS:O	2.10	0.51
1:H:125:ALA:C	1:H:127:GLU:H	2.18	0.51
1:H:3065:TYR:HE2	1:H:3224:ASP:CG	2.18	0.51
1:H:3078:GLN:HG3	1:H:3268:ILE:HG13	1.93	0.51
1:B:1065:TYR:C	1:B:1065:TYR:HD1	2.17	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1327:LEU:C	1:A:1328:LEU:HD12	2.37	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:B:2149:LEU:O	1:B:2170:MET:HE1	2.11	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:1123:GLU:HB2	1:H:1152:LYS:HZ1	1.75	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:A:3171:MET:C	1:A:3173:GLN:N	2.67	0.50
1:B:1308:TRP:CE3	1:B:1309:LEU:HD23	2.46	0.50
1:C:1092:PHE:HB2	1:C:1114:LEU:HD11	1.92	0.50
1:C:2065:TYR:HE1	1:C:2224:ASP:CG	2.19	0.50
1:D:185:SER:HB2	1:D:187:THR:OG1	2.12	0.50
1:D:2149:LEU:O	1:D:2170:MET:HE1	2.10	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:E:2149:LEU:O	1:E:2170:MET:HE1	2.11	0.50
1:E:3145:SER:C	1:E:3147:ALA:N	2.68	0.50
1:F:1300:GLN:NE2	1:G:3300:GLN:H	2.10	0.50
1:G:3065:TYR:HE2	1:G:3224:ASP:CG	2.19	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:D:3123:GLU:O	1:D:3124:GLN:C	2.55	0.50
1:E:185:SER:HB2	1:E:187:THR:OG1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1145:SER:O	1:E:1146:VAL:C	2.54	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:125:ALA:C	1:G:127:GLU:H	2.20	0.50
1:G:1222:ARG:HB2	1:G:1248:LYS:CB	2.38	0.50
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:A:2065:TYR:HE1	1:A:2224:ASP:CG	2.19	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:1308:TRP:CE3	1:E:1309:LEU:HD23	2.45	0.50
1:E:1327:LEU:C	1:E:1328:LEU:HD12	2.37	0.50
1:F:3084:GLN:HG2	1:F:3110:ASP:H	1.76	0.50
1:G:1065:TYR:C	1:G:1065:TYR:HD1	2.18	0.50
1:G:1316:ALA:O	1:G:1319:ILE:N	2.44	0.50
1:G:3145:SER:C	1:G:3147:ALA:N	2.67	0.50
1:H:1143:VAL:O	1:H:1192:ILE:HG13	2.11	0.50
1:H:2065:TYR:HE1	1:H:2224:ASP:CG	2.20	0.50
1:H:2107:LEU:CD2	1:H:2267:GLY:HA3	2.41	0.50
1:A:2149:LEU:O	1:A:2170:MET:HE1	2.11	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:C:2149:LEU:O	1:C:2170:MET:HE1	2.12	0.50
1:D:3222:ARG:HG3	1:D:3248:LYS:HB3	1.93	0.50
1:E:125:ALA:C	1:E:127:GLU:H	2.20	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:G:2149:LEU:O	1:G:2170:MET:HE1	2.12	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:H:3145:SER:C	1:H:3147:ALA:N	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3123:GLU:O	1:G:3124:GLN:C	2.55	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
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:G:2305:ALA:O	1:G:2306:THR:C	2.55	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:F:2149:LEU:O	1:F:2170:MET:HE1	2.11	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:A:125:ALA:C	1:A:127:GLU:H	2.20	0.49
1:B:1327:LEU:C	1:B:1328:LEU:HD12	2.37	0.49
1:B:2065:TYR:CD1	1:B:2065:TYR:C	2.90	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3171:MET:O	1:F:3173:GLN:N	2.45	0.49
1:G:1145:SER:O	1:G:1146:VAL:C	2.55	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:1327:LEU:C	1:D:1328:LEU:HD12	2.37	0.49
1:D:2065:TYR:HE1	1:D:2224:ASP:CG	2.20	0.49
1:D:2264:TYR:H	1:D:2264:TYR:HD2	1.60	0.49
1:F:3298:ILE:HG13	1:F:3299:GLY:N	2.26	0.49
1:G:3145:SER:O	1:G:3147:ALA:N	2.45	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:G:2065:TYR:HE1	1:G:2224:ASP:CG	2.20	0.49
1:H:1091:ALA:HB3	1:H:1141:ILE:HA	1.92	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
1:D:2123:GLU:HG3	1:D:2170:MET:HG3	1.93	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: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:H:1327:LEU:C	1:H:1328:LEU:HD12	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:3185:SER:C	1:F:3187:THR:N	2.70	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:125:ALA:C	1:B:127:GLU:H	2.19	0.49
1:B:1066:GLY:O	1:B:1067:PRO:C	2.56	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:A:3145:SER:C	1:A:3147:ALA:N	2.68	0.49
1:C:1145:SER:O	1:C:1146:VAL:C	2.54	0.49
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:3222:ARG:HG3	1:H:3248:LYS:HB3	1.93	0.49
1:A:160:GLY:C	1:A:163:HIS:HB3	2.37	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:D:2305:ALA:O	1:D:2306:THR:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:2305:ALA:O	1:F:2306:THR:C	2.54	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:1308:TRP:CE3	1:A:1309:LEU:HD23	2.45	0.48
1:A:3123:GLU:O	1:A:3124:GLN:C	2.56	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:125:ALA:C	1:C:127:GLU:H	2.21	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
1:E:2299:GLY:HA2	1:H:2300:GLN:HE22	1.77	0.48
1:E:2300:GLN:CD	1:H:2304:ASN:HB3	2.38	0.48
1:F:1091:ALA:HB3	1:F:1141:ILE:HA	1.94	0.48
1:F:1327:LEU:C	1:F:1328:LEU:HD12	2.38	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: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:1067:PRO:O	1:C:1070:SER:OG	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3101:PRO:O	1:D:3104:ALA:HB3	2.13	0.48
1:E:1073:THR:HG22	3:E:1400:ANP:PA	2.54	0.48
1:E:1176:ARG:HA	1:E:1218:TYR:CE1	2.48	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: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:1164:MET:C	1:A:1166:LEU:N	2.72	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
1:G:3298:ILE:HG13	1:G:3299:GLY:N	2.28	0.48
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:B:2305:ALA:O	1:B:2306:THR:C	2.57	0.48
1:C:1319:ILE:O	1:C:1323:VAL:HG23	2.13	0.48
1:C:2305:ALA:O	1:C:2306:THR:C	2.57	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:E:1219:ALA:O	1:E:1248:LYS:NZ	2.45	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: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:A:1161:ASP:C	1:A:1163:HIS:N	2.70	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:C:3123:GLU:O	1:C:3124:GLN:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:GLY:HA3	1:D:284:ILE:HD12	1.96	0.48
1:F:3171:MET:C	1:F:3173:GLN:H	2.21	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:B:1166:LEU:O	1:B:1168:ALA:N	2.47	0.48
1:C:164:MET:C	1:C:166:LEU:N	2.71	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: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: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:C:1066:GLY:O	1:C:1067:PRO:C	2.56	0.48
1:D:1066:GLY:O	1:D:1067:PRO:C	2.57	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
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:H:3174:ALA:O	1:H:3178:LEU:HD12	2.14	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:F:3123:GLU:O	1:F:3124:GLN:C	2.56	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:F:3145:SER:C	1:F:3147:ALA:N	2.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3232:LYS:HZ2	1:C:1235:GLU:HG2	1.77	0.47
1:D:1166:LEU:O	1:D:1168:ALA:N	2.46	0.47
1:D:3145:SER:C	1:D:3147:ALA:N	2.72	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:A:2305:ALA:O	1:A:2306:THR:C	2.56	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:D:3042:THR:OG1	1:D:3048:ASP:OD1	2.28	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: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:3178:LEU:O	1:D:3182:LEU:HG	2.14	0.47
1:F:2065:TYR:C	1:F:2065:TYR:CD1	2.92	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:G:3185:SER:C	1:G:3187:THR:N	2.71	0.47
1:H:1066:GLY:O	1:H:1067:PRO:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2301:GLY:O	1:B:2302:LYS:C	2.57	0.47
1:B:3171:MET:C	1:B:3173:GLN:H	2.23	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:D:125:ALA:C	1:D:127:GLU:H	2.21	0.47
1:E:1067:PRO:O	1:E:1070:SER:OG	2.26	0.47
1:E:1166:LEU:O	1:E:1168:ALA:N	2.47	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: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:A:3185:SER:C	1:A:3187:THR:N	2.72	0.47
1:B:1144:ASP:HA	1:B:1145:SER:HB3	1.97	0.47
1:B:3145:SER:C	1:B:3147:ALA:N	2.69	0.47
1:C:2065:TYR:CD1	1:C:2065:TYR:C	2.92	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:1066:GLY:O	1:A:1067:PRO:C	2.58	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:3171:MET:C	1:A:3173:GLN:H	2.23	0.47
1:B:114:LEU:O	1:B:1028:ARG:HA	2.15	0.47
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: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:F:3306:THR:C	1:F:3308:TRP:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:3185:SER:C	1:H:3187:THR:N	2.72	0.47
1:A:278:GLY:HA3	1:A:284:ILE:HD12	1.95	0.47
1:B:2146:VAL:HA	1:B:2149:LEU:HD23	1.95	0.47
1:B:3123:GLU:O	1:B:3124:GLN:C	2.57	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: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:G:3073:THR:O	1:G:3076:THR:OG1	2.28	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:2114:LEU:HD22	1:D:2115:LEU:H	1.79	0.47
1:E:3123:GLU:O	1:E:3124:GLN:C	2.58	0.47
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: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:2065:TYR:CD1	1:H:2065:TYR:C	2.94	0.47
1:H:3114:LEU:HD13	1:H:3114:LEU:O	2.15	0.47
1:B:3174:ALA:O	1:B:3178:LEU:HD12	2.14	0.46
1:C:3145:SER:C	1:C:3147:ALA:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:75:LEU:HD23	1:F:75:LEU:C	2.40	0.46
1:F:2129:CYS:HB2	1:F:2178:LEU:HD11	1.96	0.46
1:G:3171:MET:C	1:G:3173:GLN:H	2.22	0.46
1:A:3287:ALA:HB3	1:A:3290:TRP:HB2	1.97	0.46
1:A:3306:THR:C	1:A:3308:TRP:H	2.22	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:G:1066:GLY:O	1:G:1067:PRO:C	2.57	0.46
1:H:2073:THR:HG23	1:H:2077:LEU:HD13	1.96	0.46
1:H:3123:GLU:O	1:H:3124:GLN:C	2.57	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:2305:ALA:O	1:E:2306:THR:C	2.57	0.46
1:E:3171:MET:C	1:E:3173:GLN:H	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:2305:ALA:O	1:H:2306:THR:C	2.57	0.46
1:H:3037:VAL:HG21	1:H:3251:ILE:HD11	1.98	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:1133:ALA:C	1:B:1135:SER:H	2.24	0.46
1:C:2014:LEU:C	1:C:2016:GLN:H	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:1193:ASN:ND2	1:A:1209:THR:C	2.74	0.46
1:B:3185:SER:C	1:B:3187:THR:N	2.70	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:2065:TYR:CD1	1:D:2065:TYR:C	2.94	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:1066:GLY:O	1:F:1067:PRO:C	2.59	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:1133:ALA:C	1:G:1135:SER:H	2.24	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: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:G:3274:LEU:O	1:G:3275:VAL:C	2.59	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:3048:ASP:OD1	1:E:3048:ASP:N	2.48	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3287:ALA:HB3	1:G:3290:TRP:HB2	1.97	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: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:2065:TYR:CD1	1:G:2065:TYR:C	2.93	0.46
1:G:3281:GLU:O	1:G:3283:LEU:N	2.49	0.46
1:H:1173:GLN:C	1:H:1175:MET:H	2.23	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:3037:VAL:HG21	1:A:3251:ILE:HD11	1.97	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:C:1062:VAL:HB	1:C:1190:ILE:HG12	1.98	0.46
1:C:2301:GLY:O	1:C:2302:LYS:C	2.59	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:2014:LEU:C	1:E:2016:GLN:H	2.24	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:A:3274:LEU:O	1:A:3275:VAL:C	2.59	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:75:LEU:HD23	1:C:75:LEU:C	2.40	0.46
1:C:1029:LEU:HD23	1:C:1254:PRO:HD2	1.98	0.46
1:C:2122:GLY:O	1:C:2123:GLU:C	2.59	0.46
1:C:3010:LEU:C	1:C:3012:ALA:H	2.24	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:3010:LEU:C	1:G:3012:ALA:H	2.24	0.46
1:G:3092:PHE:CE2	1:G:3099:LEU:HD22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:221:VAL:HA	1:H:248:LYS:O	2.15	0.46
1:A:75:LEU:HD23	1:A:75:LEU:C	2.42	0.45
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:A:2065:TYR:C	1:A:2065:TYR:CD1	2.93	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:C:3171:MET:C	1:C:3173:GLN:H	2.23	0.45
1:C:3274:LEU:O	1:C:3275:VAL:C	2.59	0.45
1:C:3306:THR:C	1:C:3308:TRP:H	2.24	0.45
1:D:1161:ASP:CB	1:F:183:LYS:HZ1	2.02	0.45
1:E:1150:THR:HA	1:E:1151:PRO:HD3	1.61	0.45
1:G:69:SER:N	3:G:400:ANP:O1B	2.49	0.45
1:A:2129:CYS:HB2	1:A:2178:LEU:HD11	1.97	0.45
1:A:3306:THR:C	1:A:3308:TRP:N	2.75	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:B:3274:LEU:O	1:B:3275:VAL:C	2.59	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:F:3010:LEU:C	1:F:3012:ALA:H	2.25	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:H:2064:ILE:O	1:H:2192:ILE:HA	2.16	0.45
1:H:2293:TYR:CE1	1:H:2319:ILE:HD11	2.52	0.45
1:A:3010:LEU:C	1:A:3012:ALA:H	2.24	0.45
1:B:2014:LEU:C	1:B:2016:GLN:H	2.23	0.45
1:B:2065:TYR:C	1:B:2065:TYR:HD1	2.24	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:D:3065:TYR:HD2	1:D:3065:TYR:O	1.99	0.45
1:E:1066:GLY:O	1:E:1067:PRO:C	2.59	0.45
1:E:1133:ALA:C	1:E:1135:SER:H	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:1133:ALA:C	1:C:1135:SER:H	2.24	0.45
1:C:3269:ASN:O	1:C:3270:PHE:C	2.60	0.45
1:D:1133:ALA:C	1:D:1135:SER:H	2.24	0.45
1:D:2301:GLY:O	1:D:2302:LYS:C	2.60	0.45
1:E:75:LEU:HD23	1:E:75:LEU:C	2.42	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:2301:GLY:O	1:G:2302:LYS:C	2.59	0.45
1:H:75:LEU:HD23	1:H:75:LEU:C	2.41	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: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:E:2065:TYR:CD1	1:E:2065:TYR:C	2.94	0.45
1:E:3010:LEU:C	1:E:3012:ALA:H	2.25	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:H:2229:GLY:O	1:H:2230:ALA:CB	2.65	0.45
1:A:2301:GLY:O	1:A:2302:LYS:C	2.59	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:F:2122:GLY:O	1:F:2123:GLU:C	2.58	0.45
1:G:3271:TYR:O	1:G:3275:VAL:HG23	2.17	0.45
1:A:75:LEU:HD23	1:A:75:LEU:O	2.16	0.45
1:A:2014:LEU:C	1:A:2016:GLN:H	2.24	0.45
1:B:2048:ASP:O	1:B:2051:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1170:MET:O	1:C:1170:MET:HG2	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:2014:LEU:C	1:F:2016:GLN:H	2.24	0.45
1:F:2287:ALA:HB3	1:F:2290:TRP:HB2	1.99	0.45
1:G:3151:PRO:HG2	1:H:3151:PRO:CB	2.47	0.45
1:H:1014:LEU:C	1:H:1016:GLN:N	2.75	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
1:H:1112:ASP:HA	1:H:2030:GLY:CA	2.47	0.45
1:H:2301:GLY:O	1:H:2302:LYS:C	2.60	0.45
1:A:2122:GLY:O	1:A:2123:GLU:C	2.59	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:E:3274:LEU:O	1:E:3275:VAL:C	2.60	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:3171:MET:C	1:H:3173:GLN:H	2.23	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:173:GLN:C	1:D:175:MET:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2090:CYS:CB	1:D:2140:VAL:HG13	2.47	0.45
1:D:3269:ASN:O	1:D:3270:PHE:C	2.59	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:2129:CYS:HB2	1:G:2178:LEU:HD11	1.99	0.45
1:G:3312:ASN:O	1:G:3313:PRO:C	2.60	0.45
1:H:1133:ALA:C	1:H:1135:SER:H	2.23	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
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:2014:LEU:C	1:G:2016:GLN:H	2.24	0.44
1:G:2253:ALA:HA	1:G:2254:PRO:HD3	1.83	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:1173:GLN:C	1:A:1175:MET:H	2.25	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:B:3010:LEU:C	1:B:3012:ALA:H	2.25	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:HI'	2.52	0.44
1:A:3319:ILE:O	1:A:3320:GLU:C	2.61	0.44
1:B:1062:VAL:HB	1:B:1190:ILE:HG12	1.98	0.44
1:B:1173:GLN:C	1:B:1175:MET:H	2.24	0.44
1:B:3140:VAL:HG23	1:B:3188:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2122:GLY:O	1:D:2123:GLU:C	2.61	0.44
1:E:1064:ILE:HG23	1:E:1223:LEU:HB3	1.99	0.44
1:E:2122:GLY:O	1:E:2123:GLU:C	2.60	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:H:3306:THR:C	1:H:3308:TRP:H	2.25	0.44
1:A:1133:ALA:C	1:A:1135:SER:H	2.25	0.44
1:A:3301:GLY:O	1:A:3302:LYS:C	2.60	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:B:3306:THR:C	1:B:3308:TRP:H	2.25	0.44
1:B:3312:ASN:O	1:B:3313:PRO:C	2.61	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
1:F:2128:ILE:HG22	1:F:2132:LEU:CD1	2.47	0.44
1:G:75:LEU:HD23	1:G:75:LEU:C	2.42	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:1207:GLU:O	1:A:1208:THR:C	2.61	0.44
1:A:3224:ASP:O	1:A:3244:VAL:HA	2.18	0.44
1:B:3269:ASN:O	1:B:3270:PHE:C	2.60	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:3269:ASN:O	1:D:3272:GLY:N	2.51	0.44
1:E:1173:GLN:C	1:E:1175:MET:H	2.26	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:F:173:GLN:C	1:F:175:MET:H	2.25	0.44
1:H:3040:ILE:O	1:H:3055:GLY:HA3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:3010:LEU:C	1:D:3012:ALA:H	2.25	0.44
1:D:3171:MET:C	1:D:3173:GLN:H	2.23	0.44
1:E:3306:THR:C	1:E:3308:TRP:H	2.25	0.44
1:F:2301:GLY:O	1:F:2302:LYS:C	2.60	0.44
1:F:3313:PRO:O	1:F:3316:ALA:HB3	2.17	0.44
1:G:90:CYS:HG	1:G:140:VAL:HG13	1.82	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:H:3269:ASN:O	1:H:3270:PHE:C	2.61	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:B:115:LEU:HA	1:B:1027:MET:O	2.18	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:3045:LEU:H	1:D:3273:GLU:CD	2.26	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:E:2301:GLY:O	1:E:2302:LYS:C	2.60	0.44
1:E:3145:SER:O	1:E:3146:VAL:C	2.60	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:145:SER:O	1:H:146:VAL:C	2.60	0.44
1:H:3101:PRO:O	1:H:3104:ALA:HB3	2.18	0.44
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:1173:GLN:C	1:C:1175:MET:H	2.26	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:75:LEU:HD23	1:D:75:LEU:C	2.42	0.44
1:D:3092:PHE:CE2	1:D:3099:LEU:HD22	2.53	0.44
1:E:3114:LEU:HD13	1:E:3114:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2122:GLY:O	1:G:2123:GLU:C	2.59	0.44
1:G:2229:GLY:O	1:G:2230:ALA:CB	2.66	0.44
1:G:3319:ILE:O	1:G:3320:GLU:C	2.60	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:D:1173:GLN:C	1:D:1175:MET:H	2.25	0.44
1:F:3042:THR:OG1	1:F:3048:ASP:OD1	2.27	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:1201:VAL:O	1:A:1202:MET:HE2	2.18	0.43
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:C:3145:SER:O	1:C:3146:VAL:C	2.61	0.43
1:D:3140:VAL:HG23	1:D:3188:LEU:HB3	1.99	0.43
1:E:156:GLU:C	1:E:158:GLU:H	2.26	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:1173:GLN:C	1:F:1175:MET:H	2.24	0.43
1:F:2300:GLN:H	1:G:2300:GLN:NE2	2.16	0.43
1:F:3306:THR:C	1:F:3308:TRP:N	2.76	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1153:ALA:O	1:H:1157:GLY:O	2.36	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:1014:LEU:C	1:B:1016:GLN:N	2.75	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:1153:ALA:O	1:D:1157:GLY:C	2.61	0.43
1:D:1305:ALA:O	1:D:1306:THR:O	2.35	0.43
1:F:1133:ALA:C	1:F:1135:SER:H	2.25	0.43
1:F:3312:ASN:O	1:F:3313:PRO:C	2.60	0.43
1:G:171:MET:O	1:G:175:MET:HB2	2.17	0.43
1:G:1173:GLN:C	1:G:1175:MET:H	2.26	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:2014:LEU:C	1:H:2016:GLN:H	2.26	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:3326:LEU:O	1:C:3327:LEU:HG	2.17	0.43
1:D:1014:LEU:C	1:D:1016:GLN:N	2.75	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: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:173:GLN:C	1:B:175:MET:H	2.26	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:1014:LEU:C	1:C:1016:GLN:N	2.77	0.43
1:C:2014:LEU:C	1:C:2016:GLN:N	2.76	0.43
1:D:1154:GLU:HG2	1:D:1159:ILE:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1014:LEU:C	1:F:1016:GLN:N	2.74	0.43
1:G:2128:ILE:HG22	1:G:2132:LEU:CD1	2.48	0.43
1:A:145:SER:O	1:A:146:VAL:C	2.62	0.43
1:A:2065:TYR:C	1:A:2065:TYR:HD1	2.27	0.43
1:A:3065:TYR:HD2	1:A:3065:TYR:O	2.00	0.43
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: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:C:3306:THR:C	1:C:3308:TRP:N	2.77	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: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: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:75:LEU:HD23	1:B:75:LEU:C	2.42	0.43
1:B:3144:ASP:OD1	1:B:3145:SER:HB2	2.19	0.43
1:B:3306:THR:C	1:B:3308:TRP:N	2.77	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:2014:LEU:C	1:D:2016:GLN:H	2.25	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:3274:LEU:O	1:F:3275:VAL:C	2.61	0.43
1:G:1014:LEU:C	1:G:1016:GLN:N	2.77	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:173:GLN:C	1:C:175:MET:H	2.26	0.43
1:D:3306:THR:C	1:D:3308:TRP:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:145:SER:O	1:G:146:VAL:C	2.61	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
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: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:E:3306:THR:C	1:E:3308:TRP:N	2.77	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:1014:LEU:C	1:A:1016:GLN:N	2.75	0.43
1:A:1305:ALA:O	1:A:1306:THR:O	2.37	0.43
1:A:2014:LEU:C	1:A:2016:GLN:N	2.77	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:D:3185:SER:C	1:D:3187:THR:N	2.71	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:173:GLN:C	1:G:175:MET:H	2.26	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:H:3010:LEU:C	1:H:3012:ALA:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:3306:THR:C	1:G:3308:TRP:H	2.27	0.43
1:H:173:GLN:C	1:H:175:MET:H	2.27	0.43
1:H:3224:ASP:O	1:H:3244:VAL:HA	2.19	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:2014:LEU:C	1:B:2016:GLN:N	2.76	0.42
1:B:2065:TYR:HD1	1:B:2065:TYR:O	2.02	0.42
1:B:2122:GLY:O	1:B:2123:GLU:C	2.62	0.42
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:D:3312:ASN:O	1:D:3313:PRO:C	2.61	0.42
1:E:3144:ASP:OD1	1:E:3145:SER:HB2	2.19	0.42
1:G:72:LYS:HE3	1:G:72:LYS:HB2	1.74	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:H:3312:ASN:O	1:H:3313:PRO:C	2.62	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:B:173:GLN:HB3	1:B:174:ALA:H	1.68	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:C:3301:GLY:O	1:C:3302:LYS:C	2.62	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:173:GLN:C	1:E:175:MET:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3040:ILE:O	1:G:3055:GLY:HA3	2.18	0.42
1:G:3269:ASN:O	1:G:3270:PHE:C	2.61	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:H:3268:ILE:HG22	1:H:3269:ASN:N	2.33	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:182:LEU:C	1:A:184:GLN:N	2.77	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
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:C	1:C:2065:TYR:HD1	2.26	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:E:3301:GLY:O	1:E:3302:LYS:C	2.62	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:3145:SER:O	1:G:3146:VAL:C	2.61	0.42
1:G:3182:LEU:C	1:G:3184:GLN:N	2.77	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:E:182:LEU:C	1:E:184:GLN:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1253:ALA:HA	1:F:1254:PRO:HD3	1.90	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:2173:GLN:C	1:G:2175:MET:N	2.77	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:G:3306:THR:C	1:G:3308:TRP:N	2.78	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:1123:GLU:HG3	1:A:1170:MET:HG3	2.02	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:D:3301:GLY:O	1:D:3302:LYS:C	2.63	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
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:G:182:LEU:C	1:G:184:GLN:N	2.77	0.42
1:G:2014:LEU:C	1:G:2016:GLN:N	2.78	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:3301:GLY:O	1:B:3302:LYS:C	2.63	0.42
1:C:76:THR:O	1:C:79:VAL:HG22	2.19	0.42
1:C:182:LEU:C	1:C:184:GLN:N	2.76	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:2173:GLN:C	1:F:2175:MET:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:90:CYS:HG	1:E:140:VAL:HG13	1.85	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
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:173:GLN:C	1:A:175:MET:H	2.27	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:171:MET:C	1:C:173:GLN:N	2.78	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:D:3319:ILE:O	1:D:3320:GLU:C	2.63	0.42
1:F:3132:LEU:HA	1:F:3135:SER:HB2	2.02	0.42
1:F:3182:LEU:C	1:F:3184:GLN:N	2.77	0.42
1:H:76:THR:O	1:H:79:VAL:HG22	2.20	0.42
1:H:2122:GLY:O	1:H:2123:GLU:C	2.61	0.42
1:A:2218:TYR:HD2	1:A:2218:TYR:HA	1.74	0.42
1:B:2173:GLN:C	1:B:2175:MET:N	2.78	0.42
1:B:3090:CYS:SG	1:B:3140:VAL:CG1	3.08	0.42
1:C:145:SER:O	1:C:146:VAL:C	2.61	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:C:3319:ILE:O	1:C:3320:GLU:C	2.61	0.42
1:D:2073:THR:HA	1:D:2076:THR:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1014:LEU:C	1:E:1016:GLN:N	2.78	0.42
1:E:2014:LEU:C	1:E:2016:GLN:N	2.77	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:1163:HIS:O	1:A:1165:GLY:N	2.52	0.42
1:A:2173:GLN:C	1:A:2175:MET:N	2.78	0.42
1:A:3269:ASN:O	1:A:3270:PHE:C	2.63	0.42
1:A:3312:ASN:O	1:A:3313:PRO:C	2.63	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: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: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:G:2065:TYR:C	1:G:2065:TYR:HD1	2.27	0.42
1:H:66:GLY:O	1:H:72:LYS:HE2	2.19	0.42
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: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:1301:GLY:O	1:A:1302:LYS:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:3274:LEU:O	1:D:3275:VAL:C	2.61	0.41
1:E:231:VAL:HB	1:E:239:GLY:HA3	2.02	0.41
1:E:3312:ASN:O	1:E:3313:PRO:C	2.63	0.41
1:F:114:LEU:O	1:F:1028:ARG:HA	2.21	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: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:2065:TYR:C	1:H:2065:TYR:HD1	2.27	0.41
1:A:1048:ASP:HB3	1:A:1054:GLY:HA2	2.01	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: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:D:3182:LEU:C	1:D:3184:GLN:N	2.78	0.41
1:E:2230:ALA:HA	1:E:2239:GLY:O	2.20	0.41
1:E:3319:ILE:O	1:E:3320:GLU:C	2.63	0.41
1:F:2065:TYR:C	1:F:2065:TYR:HD1	2.27	0.41
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:F:3319:ILE:O	1:F:3320:GLU:C	2.61	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:G:3147:ALA:C	1:G:3149:LEU:H	2.28	0.41
1:H:1121:THR:CG2	1:H:1152:LYS:HZ2	2.32	0.41
1:B:2223:LEU:HD12	1:B:2223:LEU:HA	1.85	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:1301:GLY:O	1:C:1302:LYS:C	2.63	0.41
1:C:2122:GLY:O	1:C:2125:ALA:HB3	2.19	0.41
1:C:2173:GLN:C	1:C:2175:MET:N	2.78	0.41
1:C:2254:PRO:HB2	1:C:2255:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1048:ASP:HB3	1:D:1054:GLY:HA2	2.00	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: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:3182:LEU:C	1:A:3184:GLN:N	2.79	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:2065:TYR:C	1:D:2065:TYR:HD1	2.28	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:E:3269:ASN:O	1:E:3270:PHE:C	2.62	0.41
1:F:57:PRO:CG	1:F:251:ILE:HG12	2.50	0.41
1:F:1121:THR:CG2	1:F:1152:LYS:HZ3	2.32	0.41
1:F:2014:LEU:C	1:F:2016:GLN:N	2.78	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:3301:GLY:O	1:G:3302:LYS:C	2.63	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:171:MET:C	1:A:173:GLN:N	2.78	0.41
1:A:1204:GLY:O	1:A:1205:ASN:CB	2.68	0.41
1:A:2111:ILE:HD13	1:A:2111:ILE:HA	1.75	0.41
1:B:111:ILE:HD13	1:B:111:ILE:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:145:SER:O	1:B:146:VAL:C	2.62	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:3056:LEU:CD1	1:C:3190:ILE:HD11	2.50	0.41
1:D:145:SER:O	1:D:146:VAL:C	2.63	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:D:3147:ALA:C	1:D:3149:LEU:H	2.28	0.41
1:E:1123:GLU:O	1:E:1124:GLN:C	2.64	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:F:2254:PRO:HB2	1:F:2255:PHE:CD2	2.55	0.41
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:2014:LEU:C	1:D:2016:GLN:N	2.78	0.41
1:E:1090:CYS:O	1:E:1114:LEU:HD22	2.20	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: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: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:H:3042:THR:OG1	1:H:3048:ASP:OD1	2.26	0.41
1:H:3147:ALA:C	1:H:3149:LEU:H	2.28	0.41
1:H:3306:THR:C	1:H:3308:TRP:N	2.78	0.41
1:H:3319:ILE:O	1:H:3320:GLU:C	2.63	0.41
1:A:100:ASP:HB3	1:A:103:TYR:HB3	2.02	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: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
1:F:1097:HIS:NE2	1:F:2248:LYS:HG3	2.36	0.41
1:F:3301:GLY:O	1:F:3302:LYS:C	2.63	0.41
1:H:141:ILE:HB	1:H:189:LEU:HG	2.03	0.41
1:H:2014:LEU:C	1:H:2016:GLN:N	2.79	0.41
1:H:3145:SER:O	1:H:3146:VAL:C	2.64	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:178:LEU:O	1:A:182:LEU:HG	2.21	0.41
1:A:1123:GLU:O	1:A:1124:GLN:C	2.64	0.41
1:A:2057:PRO:O	1:A:2188:LEU:HD13	2.21	0.41
1:B:182:LEU:C	1:B:184:GLN:N	2.79	0.41
1:B:1006:LYS:HG3	1:B:1007:GLN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2275:VAL:HG21	1:B:2306:THR:HA	2.02	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:2125:ALA:HA	1:C:2128:ILE:HD12	2.03	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:2065:TYR:C	1:E:2065:TYR:HD1	2.28	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:3075:LEU:HD23	1:E:3075:LEU:C	2.46	0.41
1:E:3232:LYS:HA	1:E:3236:ASN:O	2.21	0.41
1:F:145:SER:O	1:F:146:VAL:C	2.62	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
1:G:3044:SER:HB3	1:G:3047:LEU:HB2	2.03	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: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: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:3319:ILE:O	1:B:3320:GLU:C	2.64	0.41
1:C:1121:THR:CG2	1:C:1152:LYS:HZ3	2.34	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:D:3306:THR:C	1:D:3308:TRP:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:MET:C	1:E:173:GLN:N	2.79	0.41
1:E:1040:ILE:HD13	1:E:1040:ILE:HA	1.93	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:3246:VAL:O	1:G:3246:VAL:HG12	2.20	0.41
1:G:3327:LEU:O	1:G:3328:LEU:HD12	2.21	0.41
1:H:182:LEU:C	1:H:184:GLN:N	2.77	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:D:1166:LEU:C	1:D:1168:ALA:N	2.80	0.40
1:E:1062:VAL:O	1:E:1190:ILE:HA	2.21	0.40
1:E:3182:LEU:C	1:E:3184:GLN:N	2.79	0.40
1:F:2091:ALA:HA	1:F:2115:LEU:HB2	2.02	0.40
1:F:2125:ALA:HA	1:F:2128:ILE:HD12	2.03	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:3312:ASN:O	1:C:3313:PRO:C	2.63	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: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:2223:LEU:HD12	1:E:2223:LEU:HA	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1062:VAL:O	1:B:1190:ILE:HA	2.21	0.40
1:B:1166:LEU:C	1:B:1168:ALA:N	2.80	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
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:D:3145:SER:O	1:D:3146:VAL:C	2.64	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:E:2173:GLN:C	1:E:2175:MET:N	2.77	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:2084:GLN:HG3	1:F:2090:CYS:SG	2.61	0.40
1:F:2254:PRO:O	1:F:2255:PHE:HB2	2.20	0.40
1:F:3147:ALA:C	1:F:3149:LEU:H	2.29	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:157:GLY:C	1:H:158:GLU:HG2	2.46	0.40
1:H:3274:LEU:O	1:H:3275:VAL:C	2.63	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:B:3182:LEU:C	1:B:3184:GLN:N	2.77	0.40
1:C:1254:PRO:HB2	1:C:1255:PHE:CD2	2.57	0.40
1:D:182:LEU:C	1:D:184:GLN:N	2.78	0.40
1:D:2142:VAL:HG22	1:D:2190:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:SER:O	1:E:146:VAL:C	2.63	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:A:1161:ASP:C	1:A:1163:HIS:H	2.29	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:B:3182:LEU:C	1:B:3184:GLN:H	2.29	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:D:3083:ALA:C	1:D:3085:ARG:N	2.80	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:F:3075:LEU:O	1:F:3075:LEU:HD23	2.21	0.40
1:G:92:PHE:CE2	1:G:94:ASP:HB2	2.56	0.40
1:G:171:MET:C	1:G:173:GLN:N	2.79	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%)	1	16
1	B	1139/1357 (84%)	915 (80%)	172 (15%)	52 (5%)	2	17
1	C	1155/1357 (85%)	919 (80%)	178 (15%)	58 (5%)	1	16
1	D	1155/1357 (85%)	923 (80%)	179 (16%)	53 (5%)	2	17
1	E	1141/1357 (84%)	910 (80%)	178 (16%)	53 (5%)	2	17
1	F	1155/1357 (85%)	913 (79%)	188 (16%)	54 (5%)	2	16
1	G	1145/1357 (84%)	914 (80%)	179 (16%)	52 (4%)	2	17
1	H	1151/1357 (85%)	914 (79%)	180 (16%)	57 (5%)	1	16
All	All	9213/10856 (85%)	7331 (80%)	1445 (16%)	437 (5%)	2	16

All (437) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	LYS
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	791 (85%)	139 (15%)	3	14
1	B	908/1065 (85%)	775 (85%)	133 (15%)	3	14
1	C	917/1065 (86%)	777 (85%)	140 (15%)	3	13
1	D	917/1065 (86%)	783 (85%)	134 (15%)	3	14
1	E	910/1065 (85%)	778 (86%)	132 (14%)	3	15
1	F	917/1065 (86%)	784 (86%)	133 (14%)	3	15
1	G	911/1065 (86%)	777 (85%)	134 (15%)	3	14
1	H	916/1065 (86%)	780 (85%)	136 (15%)	3	14
All	All	7326/8520 (86%)	6245 (85%)	1081 (15%)	3	14

All (1081) 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	76	THR
1	A	113	ASN
1	A	114	LEU
1	A	115	LEU
1	A	116	CYS
1	A	117	SER
1	A	140	VAL
1	A	142	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	192	ILE
1	A	194	GLN
1	A	221	VAL
1	A	223	LEU
1	A	238	VAL
1	A	251	ILE
1	A	277	LEU

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Mol	Chain	Res	Type
1	A	296	GLU
1	A	328	LEU
1	A	1006	LYS
1	A	1026	ILE
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	1076	THR
1	A	1078	GLN
1	A	1079	VAL
1	A	1111	ILE
1	A	1114	LEU
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	1164	MET
1	A	1173	GLN
1	A	1176	ARG
1	A	1192	ILE
1	A	1199	ILE
1	A	1201	VAL
1	A	1207	GLU
1	A	1210	THR
1	A	1221	VAL
1	A	1223	LEU
1	A	1228	ILE
1	A	1231	VAL
1	A	1245	LYS
1	A	1247	VAL
1	A	1277	LEU
1	A	1282	LYS
1	A	1284	ILE
1	A	1296	GLU
1	A	1298	ILE

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Mol	Chain	Res	Type
1	A	1312	ASN
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	2072	LYS
1	A	2073	THR
1	A	2076	THR
1	A	2078	GLN
1	A	2079	VAL
1	A	2085	ARG
1	A	2089	THR
1	A	2090	CYS
1	A	2111	ILE
1	A	2114	LEU
1	A	2130	ASP
1	A	2140	VAL
1	A	2143	VAL
1	A	2149	LEU
1	A	2150	THR
1	A	2152	LYS
1	A	2166	LEU
1	A	2183	LYS
1	A	2223	LEU
1	A	2235	GLU
1	A	2236	ASN
1	A	2247	VAL
1	A	2251	ILE
1	A	2264	TYR
1	A	2277	LEU
1	A	2296	GLU
1	A	2311	ASP
1	A	2312	ASN
1	A	2315	THR
1	A	3006	LYS
1	A	3037	VAL
1	A	3045	LEU
1	A	3048	ASP
1	A	3061	ILE
1	A	3062	VAL

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Mol	Chain	Res	Type
1	A	3065	TYR
1	A	3068	GLU
1	A	3072	LYS
1	A	3073	THR
1	A	3077	LEU
1	A	3078	GLN
1	A	3084	GLN
1	A	3089	THR
1	A	3099	LEU
1	A	3107	LEU
1	A	3114	LEU
1	A	3127	GLU
1	A	3135	SER
1	A	3143	VAL
1	A	3173	GLN
1	A	3183	LYS
1	A	3184	GLN
1	A	3189	LEU
1	A	3221	VAL
1	A	3223	LEU
1	A	3237	VAL
1	A	3245	LYS
1	A	3246	VAL
1	A	3247	VAL
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	76	THR
1	B	113	ASN
1	B	114	LEU
1	B	115	LEU
1	B	116	CYS
1	B	117	SER
1	B	140	VAL
1	B	142	VAL
1	B	143	VAL

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Mol	Chain	Res	Type
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	192	ILE
1	B	194	GLN
1	B	221	VAL
1	B	223	LEU
1	B	238	VAL
1	B	251	ILE
1	B	277	LEU
1	B	296	GLU
1	B	328	LEU
1	B	1006	LYS
1	B	1025	SER
1	B	1026	ILE
1	B	1033	ARG
1	B	1035	MET
1	B	1036	ASP
1	B	1045	LEU
1	B	1065	TYR
1	B	1070	SER
1	B	1073	THR
1	B	1076	THR
1	B	1078	GLN
1	B	1079	VAL
1	B	1111	ILE
1	B	1114	LEU
1	B	1129	CYS
1	B	1141	ILE
1	B	1149	LEU
1	B	1150	THR
1	B	1152	LYS
1	B	1173	GLN
1	B	1176	ARG
1	B	1192	ILE
1	B	1221	VAL
1	B	1223	LEU
1	B	1228	ILE
1	B	1231	VAL

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Mol	Chain	Res	Type
1	B	1245	LYS
1	B	1247	VAL
1	B	1277	LEU
1	B	1282	LYS
1	B	1284	ILE
1	B	1296	GLU
1	B	1298	ILE
1	B	1312	ASN
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	2072	LYS
1	B	2073	THR
1	B	2076	THR
1	B	2078	GLN
1	B	2079	VAL
1	B	2085	ARG
1	B	2089	THR
1	B	2090	CYS
1	B	2111	ILE
1	B	2114	LEU
1	B	2130	ASP
1	B	2140	VAL
1	B	2143	VAL
1	B	2149	LEU
1	B	2150	THR
1	B	2152	LYS
1	B	2166	LEU
1	B	2183	LYS
1	B	2223	LEU
1	B	2235	GLU
1	B	2236	ASN
1	B	2247	VAL
1	B	2251	ILE
1	B	2264	TYR
1	B	2277	LEU
1	B	2296	GLU
1	B	2311	ASP
1	B	2312	ASN

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Mol	Chain	Res	Type
1	B	2315	THR
1	B	3006	LYS
1	B	3037	VAL
1	B	3045	LEU
1	B	3048	ASP
1	B	3061	ILE
1	B	3062	VAL
1	B	3065	TYR
1	B	3068	GLU
1	B	3072	LYS
1	B	3073	THR
1	B	3077	LEU
1	B	3078	GLN
1	B	3084	GLN
1	B	3089	THR
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	3173	GLN
1	B	3183	LYS
1	B	3184	GLN
1	B	3189	LEU
1	B	3221	VAL
1	B	3223	LEU
1	B	3237	VAL
1	B	3245	LYS
1	B	3246	VAL
1	B	3247	VAL
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	76	THR
1	C	113	ASN

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Mol	Chain	Res	Type
1	C	114	LEU
1	C	115	LEU
1	C	116	CYS
1	C	117	SER
1	C	140	VAL
1	C	142	VAL
1	C	143	VAL
1	C	149	LEU
1	C	159	ILE
1	C	162	SER
1	C	163	HIS
1	C	164	MET
1	C	173	GLN
1	C	189	LEU
1	C	192	ILE
1	C	194	GLN
1	C	221	VAL
1	C	223	LEU
1	C	238	VAL
1	C	251	ILE
1	C	277	LEU
1	C	296	GLU
1	C	328	LEU
1	C	1006	LYS
1	C	1025	SER
1	C	1026	ILE
1	C	1033	ARG
1	C	1035	MET
1	C	1036	ASP
1	C	1045	LEU
1	C	1065	TYR
1	C	1070	SER
1	C	1073	THR
1	C	1076	THR
1	C	1078	GLN
1	C	1079	VAL
1	C	1111	ILE
1	C	1114	LEU
1	C	1129	CYS
1	C	1141	ILE
1	C	1149	LEU
1	C	1150	THR

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Mol	Chain	Res	Type
1	C	1152	LYS
1	C	1158	GLU
1	C	1159	ILE
1	C	1163	HIS
1	C	1164	MET
1	C	1173	GLN
1	C	1176	ARG
1	C	1192	ILE
1	C	1221	VAL
1	C	1223	LEU
1	C	1228	ILE
1	C	1231	VAL
1	C	1245	LYS
1	C	1247	VAL
1	C	1277	LEU
1	C	1282	LYS
1	C	1284	ILE
1	C	1296	GLU
1	C	1298	ILE
1	C	1312	ASN
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	2072	LYS
1	C	2073	THR
1	C	2076	THR
1	C	2078	GLN
1	C	2079	VAL
1	C	2085	ARG
1	C	2089	THR
1	C	2090	CYS
1	C	2111	ILE
1	C	2114	LEU
1	C	2130	ASP
1	C	2140	VAL
1	C	2143	VAL
1	C	2149	LEU
1	C	2150	THR
1	C	2152	LYS

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Mol	Chain	Res	Type
1	C	2156	GLU
1	C	2166	LEU
1	C	2183	LYS
1	C	2223	LEU
1	C	2235	GLU
1	C	2236	ASN
1	C	2247	VAL
1	C	2251	ILE
1	C	2264	TYR
1	C	2277	LEU
1	C	2296	GLU
1	C	2311	ASP
1	C	2312	ASN
1	C	2315	THR
1	C	3006	LYS
1	C	3037	VAL
1	C	3045	LEU
1	C	3048	ASP
1	C	3061	ILE
1	C	3062	VAL
1	C	3065	TYR
1	C	3068	GLU
1	C	3072	LYS
1	C	3073	THR
1	C	3077	LEU
1	C	3078	GLN
1	C	3084	GLN
1	C	3089	THR
1	C	3099	LEU
1	C	3107	LEU
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	3183	LYS
1	C	3184	GLN
1	C	3189	LEU
1	C	3221	VAL
1	C	3223	LEU
1	C	3237	VAL

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Mol	Chain	Res	Type
1	C	3245	LYS
1	C	3246	VAL
1	C	3247	VAL
1	C	3274	LEU
1	C	3296	GLU
1	C	3311	ASP
1	C	3326	LEU
1	D	37	VAL
1	D	45	LEU
1	D	65	TYR
1	D	72	LYS
1	D	73	THR
1	D	76	THR
1	D	113	ASN
1	D	114	LEU
1	D	115	LEU
1	D	116	CYS
1	D	117	SER
1	D	140	VAL
1	D	142	VAL
1	D	143	VAL
1	D	149	LEU
1	D	158	GLU
1	D	159	ILE
1	D	161	ASP
1	D	164	MET
1	D	173	GLN
1	D	189	LEU
1	D	192	ILE
1	D	194	GLN
1	D	221	VAL
1	D	223	LEU
1	D	238	VAL
1	D	251	ILE
1	D	277	LEU
1	D	296	GLU
1	D	328	LEU
1	D	1006	LYS
1	D	1026	ILE
1	D	1033	ARG
1	D	1035	MET
1	D	1036	ASP

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Mol	Chain	Res	Type
1	D	1045	LEU
1	D	1065	TYR
1	D	1070	SER
1	D	1073	THR
1	D	1076	THR
1	D	1078	GLN
1	D	1079	VAL
1	D	1111	ILE
1	D	1114	LEU
1	D	1129	CYS
1	D	1141	ILE
1	D	1149	LEU
1	D	1150	THR
1	D	1152	LYS
1	D	1159	ILE
1	D	1164	MET
1	D	1173	GLN
1	D	1176	ARG
1	D	1192	ILE
1	D	1221	VAL
1	D	1223	LEU
1	D	1228	ILE
1	D	1231	VAL
1	D	1245	LYS
1	D	1247	VAL
1	D	1277	LEU
1	D	1282	LYS
1	D	1284	ILE
1	D	1296	GLU
1	D	1298	ILE
1	D	1312	ASN
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	2072	LYS
1	D	2073	THR
1	D	2076	THR
1	D	2078	GLN
1	D	2085	ARG

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Mol	Chain	Res	Type
1	D	2089	THR
1	D	2090	CYS
1	D	2111	ILE
1	D	2114	LEU
1	D	2130	ASP
1	D	2140	VAL
1	D	2143	VAL
1	D	2149	LEU
1	D	2152	LYS
1	D	2166	LEU
1	D	2183	LYS
1	D	2223	LEU
1	D	2235	GLU
1	D	2236	ASN
1	D	2247	VAL
1	D	2251	ILE
1	D	2264	TYR
1	D	2277	LEU
1	D	2296	GLU
1	D	2311	ASP
1	D	2312	ASN
1	D	2315	THR
1	D	3006	LYS
1	D	3037	VAL
1	D	3045	LEU
1	D	3048	ASP
1	D	3061	ILE
1	D	3062	VAL
1	D	3065	TYR
1	D	3068	GLU
1	D	3072	LYS
1	D	3073	THR
1	D	3077	LEU
1	D	3078	GLN
1	D	3084	GLN
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

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Mol	Chain	Res	Type
1	D	3166	LEU
1	D	3173	GLN
1	D	3183	LYS
1	D	3184	GLN
1	D	3189	LEU
1	D	3221	VAL
1	D	3223	LEU
1	D	3237	VAL
1	D	3245	LYS
1	D	3246	VAL
1	D	3247	VAL
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	76	THR
1	E	113	ASN
1	E	114	LEU
1	E	115	LEU
1	E	116	CYS
1	E	117	SER
1	E	140	VAL
1	E	142	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	192	ILE
1	E	194	GLN
1	E	221	VAL
1	E	223	LEU
1	E	238	VAL

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Mol	Chain	Res	Type
1	E	251	ILE
1	E	277	LEU
1	E	296	GLU
1	E	328	LEU
1	E	1006	LYS
1	E	1026	ILE
1	E	1033	ARG
1	E	1035	MET
1	E	1036	ASP
1	E	1045	LEU
1	E	1065	TYR
1	E	1070	SER
1	E	1073	THR
1	E	1076	THR
1	E	1078	GLN
1	E	1079	VAL
1	E	1111	ILE
1	E	1114	LEU
1	E	1141	ILE
1	E	1149	LEU
1	E	1150	THR
1	E	1152	LYS
1	E	1173	GLN
1	E	1176	ARG
1	E	1192	ILE
1	E	1221	VAL
1	E	1223	LEU
1	E	1228	ILE
1	E	1231	VAL
1	E	1245	LYS
1	E	1247	VAL
1	E	1277	LEU
1	E	1282	LYS
1	E	1284	ILE
1	E	1296	GLU
1	E	1298	ILE
1	E	1312	ASN
1	E	2016	GLN
1	E	2023	LYS
1	E	2025	SER
1	E	2036	ASP
1	E	2045	LEU

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Mol	Chain	Res	Type
1	E	2065	TYR
1	E	2072	LYS
1	E	2073	THR
1	E	2076	THR
1	E	2078	GLN
1	E	2079	VAL
1	E	2085	ARG
1	E	2089	THR
1	E	2090	CYS
1	E	2111	ILE
1	E	2114	LEU
1	E	2130	ASP
1	E	2140	VAL
1	E	2143	VAL
1	E	2149	LEU
1	E	2150	THR
1	E	2152	LYS
1	E	2166	LEU
1	E	2183	LYS
1	E	2223	LEU
1	E	2235	GLU
1	E	2236	ASN
1	E	2247	VAL
1	E	2251	ILE
1	E	2264	TYR
1	E	2277	LEU
1	E	2296	GLU
1	E	2311	ASP
1	E	2312	ASN
1	E	2315	THR
1	E	3006	LYS
1	E	3037	VAL
1	E	3045	LEU
1	E	3048	ASP
1	E	3061	ILE
1	E	3065	TYR
1	E	3068	GLU
1	E	3072	LYS
1	E	3073	THR
1	E	3077	LEU
1	E	3078	GLN
1	E	3084	GLN

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Mol	Chain	Res	Type
1	E	3089	THR
1	E	3099	LEU
1	E	3107	LEU
1	E	3114	LEU
1	E	3127	GLU
1	E	3135	SER
1	E	3143	VAL
1	E	3173	GLN
1	E	3183	LYS
1	E	3184	GLN
1	E	3189	LEU
1	E	3221	VAL
1	E	3223	LEU
1	E	3237	VAL
1	E	3245	LYS
1	E	3246	VAL
1	E	3247	VAL
1	E	3274	LEU
1	E	3296	GLU
1	E	3311	ASP
1	E	3326	LEU
1	F	37	VAL
1	F	45	LEU
1	F	65	TYR
1	F	72	LYS
1	F	73	THR
1	F	76	THR
1	F	113	ASN
1	F	114	LEU
1	F	115	LEU
1	F	116	CYS
1	F	117	SER
1	F	140	VAL
1	F	142	VAL
1	F	143	VAL
1	F	149	LEU
1	F	158	GLU
1	F	173	GLN
1	F	189	LEU
1	F	192	ILE
1	F	194	GLN
1	F	221	VAL

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Mol	Chain	Res	Type
1	F	223	LEU
1	F	238	VAL
1	F	251	ILE
1	F	277	LEU
1	F	296	GLU
1	F	328	LEU
1	F	1006	LYS
1	F	1026	ILE
1	F	1033	ARG
1	F	1035	MET
1	F	1036	ASP
1	F	1045	LEU
1	F	1065	TYR
1	F	1070	SER
1	F	1073	THR
1	F	1076	THR
1	F	1078	GLN
1	F	1079	VAL
1	F	1111	ILE
1	F	1114	LEU
1	F	1129	CYS
1	F	1141	ILE
1	F	1149	LEU
1	F	1150	THR
1	F	1152	LYS
1	F	1159	ILE
1	F	1161	ASP
1	F	1163	HIS
1	F	1173	GLN
1	F	1176	ARG
1	F	1192	ILE
1	F	1221	VAL
1	F	1223	LEU
1	F	1228	ILE
1	F	1231	VAL
1	F	1245	LYS
1	F	1247	VAL
1	F	1277	LEU
1	F	1282	LYS
1	F	1284	ILE
1	F	1296	GLU
1	F	1298	ILE

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Mol	Chain	Res	Type
1	F	1312	ASN
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	2072	LYS
1	F	2073	THR
1	F	2076	THR
1	F	2078	GLN
1	F	2085	ARG
1	F	2089	THR
1	F	2090	CYS
1	F	2111	ILE
1	F	2114	LEU
1	F	2130	ASP
1	F	2140	VAL
1	F	2143	VAL
1	F	2149	LEU
1	F	2152	LYS
1	F	2166	LEU
1	F	2183	LYS
1	F	2223	LEU
1	F	2235	GLU
1	F	2236	ASN
1	F	2247	VAL
1	F	2251	ILE
1	F	2264	TYR
1	F	2277	LEU
1	F	2296	GLU
1	F	2311	ASP
1	F	2312	ASN
1	F	2315	THR
1	F	3006	LYS
1	F	3037	VAL
1	F	3045	LEU
1	F	3048	ASP
1	F	3061	ILE
1	F	3062	VAL
1	F	3065	TYR
1	F	3068	GLU

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Mol	Chain	Res	Type
1	F	3072	LYS
1	F	3073	THR
1	F	3077	LEU
1	F	3078	GLN
1	F	3084	GLN
1	F	3089	THR
1	F	3099	LEU
1	F	3107	LEU
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	3183	LYS
1	F	3184	GLN
1	F	3189	LEU
1	F	3221	VAL
1	F	3223	LEU
1	F	3237	VAL
1	F	3245	LYS
1	F	3246	VAL
1	F	3247	VAL
1	F	3274	LEU
1	F	3277	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	76	THR
1	G	113	ASN
1	G	114	LEU
1	G	115	LEU
1	G	116	CYS
1	G	117	SER
1	G	140	VAL
1	G	142	VAL
1	G	143	VAL

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Mol	Chain	Res	Type
1	G	149	LEU
1	G	159	ILE
1	G	162	SER
1	G	163	HIS
1	G	173	GLN
1	G	189	LEU
1	G	192	ILE
1	G	194	GLN
1	G	221	VAL
1	G	223	LEU
1	G	238	VAL
1	G	251	ILE
1	G	277	LEU
1	G	296	GLU
1	G	328	LEU
1	G	1006	LYS
1	G	1025	SER
1	G	1026	ILE
1	G	1033	ARG
1	G	1035	MET
1	G	1036	ASP
1	G	1045	LEU
1	G	1065	TYR
1	G	1070	SER
1	G	1073	THR
1	G	1076	THR
1	G	1078	GLN
1	G	1079	VAL
1	G	1111	ILE
1	G	1114	LEU
1	G	1129	CYS
1	G	1141	ILE
1	G	1149	LEU
1	G	1150	THR
1	G	1152	LYS
1	G	1173	GLN
1	G	1176	ARG
1	G	1192	ILE
1	G	1221	VAL
1	G	1223	LEU
1	G	1228	ILE
1	G	1231	VAL

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Mol	Chain	Res	Type
1	G	1245	LYS
1	G	1247	VAL
1	G	1277	LEU
1	G	1282	LYS
1	G	1284	ILE
1	G	1296	GLU
1	G	1298	ILE
1	G	1312	ASN
1	G	2016	GLN
1	G	2023	LYS
1	G	2025	SER
1	G	2036	ASP
1	G	2045	LEU
1	G	2065	TYR
1	G	2072	LYS
1	G	2073	THR
1	G	2076	THR
1	G	2078	GLN
1	G	2079	VAL
1	G	2085	ARG
1	G	2089	THR
1	G	2090	CYS
1	G	2111	ILE
1	G	2114	LEU
1	G	2130	ASP
1	G	2140	VAL
1	G	2143	VAL
1	G	2149	LEU
1	G	2150	THR
1	G	2152	LYS
1	G	2166	LEU
1	G	2183	LYS
1	G	2223	LEU
1	G	2235	GLU
1	G	2236	ASN
1	G	2247	VAL
1	G	2251	ILE
1	G	2264	TYR
1	G	2277	LEU
1	G	2296	GLU
1	G	2311	ASP
1	G	2312	ASN

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Mol	Chain	Res	Type
1	G	2315	THR
1	G	3006	LYS
1	G	3037	VAL
1	G	3045	LEU
1	G	3048	ASP
1	G	3061	ILE
1	G	3065	TYR
1	G	3068	GLU
1	G	3072	LYS
1	G	3073	THR
1	G	3077	LEU
1	G	3078	GLN
1	G	3084	GLN
1	G	3089	THR
1	G	3099	LEU
1	G	3107	LEU
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	3183	LYS
1	G	3184	GLN
1	G	3189	LEU
1	G	3218	TYR
1	G	3221	VAL
1	G	3223	LEU
1	G	3237	VAL
1	G	3245	LYS
1	G	3246	VAL
1	G	3247	VAL
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	76	THR

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Mol	Chain	Res	Type
1	H	113	ASN
1	H	114	LEU
1	H	115	LEU
1	H	116	CYS
1	H	117	SER
1	H	140	VAL
1	H	142	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	192	ILE
1	H	194	GLN
1	H	221	VAL
1	H	223	LEU
1	H	238	VAL
1	H	251	ILE
1	H	277	LEU
1	H	296	GLU
1	H	328	LEU
1	H	1006	LYS
1	H	1026	ILE
1	H	1033	ARG
1	H	1035	MET
1	H	1036	ASP
1	H	1045	LEU
1	H	1065	TYR
1	H	1070	SER
1	H	1073	THR
1	H	1076	THR
1	H	1078	GLN
1	H	1079	VAL
1	H	1111	ILE
1	H	1114	LEU
1	H	1129	CYS
1	H	1141	ILE
1	H	1149	LEU
1	H	1150	THR
1	H	1152	LYS

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Mol	Chain	Res	Type
1	H	1162	SER
1	H	1163	HIS
1	H	1173	GLN
1	H	1176	ARG
1	H	1192	ILE
1	H	1221	VAL
1	H	1223	LEU
1	H	1228	ILE
1	H	1231	VAL
1	H	1245	LYS
1	H	1247	VAL
1	H	1277	LEU
1	H	1282	LYS
1	H	1284	ILE
1	H	1296	GLU
1	H	1298	ILE
1	H	1312	ASN
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	2072	LYS
1	H	2073	THR
1	H	2076	THR
1	H	2078	GLN
1	H	2079	VAL
1	H	2085	ARG
1	H	2089	THR
1	H	2090	CYS
1	H	2111	ILE
1	H	2114	LEU
1	H	2130	ASP
1	H	2140	VAL
1	H	2143	VAL
1	H	2149	LEU
1	H	2150	THR
1	H	2152	LYS
1	H	2156	GLU
1	H	2166	LEU
1	H	2183	LYS

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Mol	Chain	Res	Type
1	H	2223	LEU
1	H	2235	GLU
1	H	2236	ASN
1	H	2247	VAL
1	H	2251	ILE
1	H	2264	TYR
1	H	2277	LEU
1	H	2296	GLU
1	H	2311	ASP
1	H	2312	ASN
1	H	2315	THR
1	H	3006	LYS
1	H	3037	VAL
1	H	3045	LEU
1	H	3048	ASP
1	H	3061	ILE
1	H	3062	VAL
1	H	3065	TYR
1	H	3068	GLU
1	H	3072	LYS
1	H	3073	THR
1	H	3077	LEU
1	H	3078	GLN
1	H	3084	GLN
1	H	3089	THR
1	H	3099	LEU
1	H	3107	LEU
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	3183	LYS
1	H	3184	GLN
1	H	3189	LEU
1	H	3221	VAL
1	H	3223	LEU
1	H	3237	VAL
1	H	3245	LYS
1	H	3246	VAL
1	H	3247	VAL

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Mol	Chain	Res	Type
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 (153) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	181	ASN
1	A	1084	GLN
1	A	1124	GLN
1	A	1193	ASN
1	A	1213	ASN
1	A	1300	GLN
1	A	2118	GLN
1	A	2181	ASN
1	A	2236	ASN
1	A	2300	GLN
1	A	3084	GLN
1	A	3097	HIS
1	A	3124	GLN
1	A	3181	ASN
1	A	3236	ASN
1	A	3257	GLN
1	A	3304	ASN
1	B	173	GLN
1	B	181	ASN
1	B	194	GLN
1	B	1084	GLN
1	B	1118	GLN
1	B	1124	GLN
1	B	1300	GLN
1	B	2118	GLN
1	B	2181	ASN
1	B	2236	ASN
1	B	2300	GLN
1	B	3084	GLN
1	B	3097	HIS
1	B	3124	GLN
1	B	3181	ASN
1	B	3236	ASN

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Mol	Chain	Res	Type
1	B	3257	GLN
1	B	3300	GLN
1	B	3304	ASN
1	C	173	GLN
1	C	181	ASN
1	C	194	GLN
1	C	1084	GLN
1	C	1118	GLN
1	C	1124	GLN
1	C	1300	GLN
1	C	2118	GLN
1	C	2181	ASN
1	C	2236	ASN
1	C	2300	GLN
1	C	3084	GLN
1	C	3124	GLN
1	C	3181	ASN
1	C	3236	ASN
1	C	3257	GLN
1	C	3300	GLN
1	C	3304	ASN
1	D	173	GLN
1	D	181	ASN
1	D	194	GLN
1	D	1084	GLN
1	D	1118	GLN
1	D	1124	GLN
1	D	1300	GLN
1	D	2118	GLN
1	D	2181	ASN
1	D	2213	ASN
1	D	2236	ASN
1	D	3084	GLN
1	D	3124	GLN
1	D	3181	ASN
1	D	3236	ASN
1	D	3257	GLN
1	D	3300	GLN
1	D	3304	ASN
1	E	173	GLN
1	E	181	ASN
1	E	1084	GLN

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Mol	Chain	Res	Type
1	E	1097	HIS
1	E	1118	GLN
1	E	1124	GLN
1	E	1300	GLN
1	E	2118	GLN
1	E	2181	ASN
1	E	2236	ASN
1	E	2300	GLN
1	E	3084	GLN
1	E	3097	HIS
1	E	3124	GLN
1	E	3181	ASN
1	E	3236	ASN
1	E	3257	GLN
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	194	GLN
1	F	1084	GLN
1	F	1124	GLN
1	F	1163	HIS
1	F	1213	ASN
1	F	1300	GLN
1	F	2118	GLN
1	F	2181	ASN
1	F	2213	ASN
1	F	2236	ASN
1	F	2300	GLN
1	F	3084	GLN
1	F	3097	HIS
1	F	3124	GLN
1	F	3181	ASN
1	F	3236	ASN
1	F	3257	GLN
1	F	3300	GLN
1	F	3304	ASN
1	G	173	GLN
1	G	181	ASN
1	G	1084	GLN

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Mol	Chain	Res	Type
1	G	1118	GLN
1	G	1124	GLN
1	G	1300	GLN
1	G	2118	GLN
1	G	2181	ASN
1	G	2236	ASN
1	G	2300	GLN
1	G	3084	GLN
1	G	3097	HIS
1	G	3124	GLN
1	G	3181	ASN
1	G	3236	ASN
1	G	3257	GLN
1	G	3300	GLN
1	G	3304	ASN
1	H	163	HIS
1	H	173	GLN
1	H	181	ASN
1	H	194	GLN
1	H	1084	GLN
1	H	1124	GLN
1	H	1213	ASN
1	H	1300	GLN
1	H	2118	GLN
1	H	2181	ASN
1	H	2236	ASN
1	H	2300	GLN
1	H	3084	GLN
1	H	3097	HIS
1	H	3124	GLN
1	H	3181	ASN
1	H	3236	ASN
1	H	3257	GLN
1	H	3300	GLN
1	H	3304	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	G	2400	-	33,33,33	2.22	10 (30%)	45,52,52	2.26	12 (26%)
3	ANP	C	3400	-	33,33,33	2.32	8 (24%)	45,52,52	2.48	13 (28%)
3	ANP	D	1400	-	33,33,33	2.18	9 (27%)	45,52,52	2.30	13 (28%)
3	ANP	H	2400	-	33,33,33	2.17	12 (36%)	45,52,52	2.25	12 (26%)
3	ANP	H	1400	-	33,33,33	2.27	9 (27%)	45,52,52	2.25	13 (28%)
3	ANP	B	400	-	33,33,33	2.21	9 (27%)	45,52,52	2.10	14 (31%)
3	ANP	A	400	-	33,33,33	2.26	12 (36%)	45,52,52	2.13	12 (26%)
3	ANP	C	400	-	33,33,33	2.06	10 (30%)	45,52,52	2.14	12 (26%)
3	ANP	F	3400	-	33,33,33	2.14	9 (27%)	45,52,52	2.48	12 (26%)
3	ANP	A	3400	-	33,33,33	2.16	7 (21%)	45,52,52	2.55	13 (28%)
3	ANP	C	2400	-	33,33,33	2.12	11 (33%)	45,52,52	2.26	12 (26%)
3	ANP	D	2400	-	33,33,33	2.19	9 (27%)	45,52,52	2.26	12 (26%)
3	ANP	G	3400	-	33,33,33	2.27	8 (24%)	45,52,52	2.51	14 (31%)
3	ANP	C	1400	-	33,33,33	2.27	10 (30%)	45,52,52	2.31	13 (28%)
3	ANP	H	400	-	33,33,33	2.14	10 (30%)	45,52,52	2.11	12 (26%)
3	ANP	H	3400	-	33,33,33	2.25	9 (27%)	45,52,52	2.68	14 (31%)
3	ANP	G	1400	-	33,33,33	2.17	11 (33%)	45,52,52	2.26	13 (28%)
3	ANP	B	3400	-	33,33,33	2.15	9 (27%)	45,52,52	2.59	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	E	400	-	33,33,33	2.18	12 (36%)	45,52,52	2.16	13 (28%)
3	ANP	F	2400	-	33,33,33	2.09	12 (36%)	45,52,52	2.26	12 (26%)
3	ANP	F	1400	-	33,33,33	2.27	11 (33%)	45,52,52	2.31	12 (26%)
3	ANP	D	3400	-	33,33,33	2.18	8 (24%)	45,52,52	2.56	13 (28%)
3	ANP	E	2400	-	33,33,33	2.23	10 (30%)	45,52,52	2.25	12 (26%)
3	ANP	E	1400	-	33,33,33	2.26	11 (33%)	45,52,52	2.32	12 (26%)
3	ANP	B	2400	-	33,33,33	2.17	12 (36%)	45,52,52	2.28	12 (26%)
3	ANP	E	3400	2	33,33,33	2.00	9 (27%)	45,52,52	2.59	16 (35%)
3	ANP	G	400	-	33,33,33	2.16	9 (27%)	45,52,52	2.13	12 (26%)
3	ANP	D	400	-	33,33,33	2.26	12 (36%)	45,52,52	2.07	12 (26%)
3	ANP	A	2400	-	33,33,33	2.20	9 (27%)	45,52,52	2.28	12 (26%)
3	ANP	A	1400	-	33,33,33	2.12	10 (30%)	45,52,52	2.30	12 (26%)
3	ANP	F	400	-	33,33,33	2.15	10 (30%)	45,52,52	2.08	12 (26%)
3	ANP	B	1400	-	33,33,33	2.17	9 (27%)	45,52,52	2.31	12 (26%)

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	G	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	C	3400	-	1/1/7/8	8/18/38/38	0/3/3/3
3	ANP	D	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	H	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	H	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	B	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	A	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	C	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	F	3400	-	1/1/7/8	8/18/38/38	0/3/3/3
3	ANP	A	3400	-	1/1/7/8	7/18/38/38	0/3/3/3
3	ANP	C	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	D	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	G	3400	-	1/1/7/8	8/18/38/38	0/3/3/3
3	ANP	C	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	H	400	-	1/1/7/8	9/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	H	3400	-	1/1/7/8	7/18/38/38	0/3/3/3
3	ANP	G	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	B	3400	-	1/1/7/8	8/18/38/38	0/3/3/3
3	ANP	E	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	F	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	F	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	D	3400	-	1/1/7/8	8/18/38/38	0/3/3/3
3	ANP	E	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	E	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	B	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	E	3400	2	1/1/7/8	8/18/38/38	0/3/3/3
3	ANP	G	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	D	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	A	2400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	A	1400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	F	400	-	1/1/7/8	9/18/38/38	0/3/3/3
3	ANP	B	1400	-	1/1/7/8	9/18/38/38	0/3/3/3

All (316) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3400	ANP	C5-C4	6.30	1.50	1.39
3	D	3400	ANP	C5-C4	6.10	1.50	1.39
3	G	3400	ANP	C5-C4	6.04	1.49	1.39
3	C	3400	ANP	C5-C4	6.03	1.49	1.39
3	C	3400	ANP	PG-N3B	5.90	1.78	1.63
3	B	400	ANP	C5-C4	5.85	1.49	1.39
3	F	400	ANP	C5-C4	5.78	1.49	1.39
3	H	1400	ANP	C5-C4	5.73	1.49	1.39
3	D	400	ANP	C5-C4	5.73	1.49	1.39
3	F	3400	ANP	C5-C4	5.63	1.49	1.39
3	E	2400	ANP	C5-C4	5.62	1.49	1.39
3	F	1400	ANP	C5-C4	5.61	1.49	1.39
3	G	2400	ANP	C5-C4	5.61	1.49	1.39
3	H	3400	ANP	C5-C4	5.61	1.49	1.39
3	D	1400	ANP	C5-C4	5.59	1.49	1.39
3	B	3400	ANP	C5-C4	5.57	1.49	1.39
3	H	3400	ANP	PG-N3B	5.54	1.77	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2400	ANP	C5-C4	5.53	1.48	1.39
3	E	1400	ANP	C5-C4	5.51	1.48	1.39
3	B	1400	ANP	C5-C4	5.50	1.48	1.39
3	G	3400	ANP	PG-N3B	5.49	1.77	1.63
3	C	400	ANP	C5-C4	5.49	1.48	1.39
3	A	400	ANP	C5-C4	5.48	1.48	1.39
3	G	400	ANP	C5-C4	5.47	1.48	1.39
3	D	2400	ANP	C5-C4	5.47	1.48	1.39
3	C	2400	ANP	C5-C4	5.46	1.48	1.39
3	C	3400	ANP	PB-N3B	5.45	1.77	1.63
3	F	2400	ANP	C5-C4	5.45	1.48	1.39
3	A	2400	ANP	C5-C4	5.43	1.48	1.39
3	C	1400	ANP	C5-C4	5.40	1.48	1.39
3	G	1400	ANP	C5-C4	5.38	1.48	1.39
3	G	3400	ANP	PB-N3B	5.33	1.77	1.63
3	B	2400	ANP	C5-C4	5.30	1.48	1.39
3	A	1400	ANP	C5-C4	5.30	1.48	1.39
3	H	1400	ANP	PG-N3B	5.30	1.77	1.63
3	H	400	ANP	C5-C4	5.29	1.48	1.39
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	400	ANP	C5-C4	5.17	1.48	1.39
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	E	3400	ANP	C5-C4	5.09	1.48	1.39
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	D	3400	ANP	C5-C6	4.29	1.52	1.41
3	B	400	ANP	PB-N3B	4.29	1.74	1.63
3	C	3400	ANP	C5-C6	4.28	1.52	1.41
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	H	3400	ANP	C5-C6	4.13	1.52	1.41
3	A	3400	ANP	PG-O1G	4.11	1.52	1.46
3	G	3400	ANP	PG-O1G	4.09	1.52	1.46
3	A	3400	ANP	C5-C6	4.05	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	400	ANP	PB-N3B	3.96	1.73	1.63
3	C	1400	ANP	PG-O1G	3.94	1.52	1.46
3	C	3400	ANP	PG-O1G	3.89	1.52	1.46
3	G	1400	ANP	PG-O1G	3.89	1.52	1.46
3	C	1400	ANP	PB-O1B	3.86	1.52	1.46
3	G	2400	ANP	PB-O1B	3.86	1.52	1.46
3	A	400	ANP	PG-O1G	3.85	1.52	1.46
3	F	1400	ANP	PG-O1G	3.82	1.52	1.46
3	B	3400	ANP	C5-C6	3.82	1.51	1.41
3	E	1400	ANP	PG-O1G	3.79	1.51	1.46
3	E	3400	ANP	C5-C6	3.78	1.51	1.41
3	D	3400	ANP	PG-O1G	3.76	1.51	1.46
3	F	3400	ANP	C5-C6	3.76	1.51	1.41
3	A	2400	ANP	PG-O1G	3.73	1.51	1.46
3	H	1400	ANP	PB-O1B	3.72	1.51	1.46
3	H	1400	ANP	PG-O1G	3.70	1.51	1.46
3	G	3400	ANP	C5-C6	3.68	1.51	1.41
3	E	400	ANP	PG-O1G	3.64	1.51	1.46
3	F	1400	ANP	C5-C6	3.64	1.51	1.41
3	F	3400	ANP	PG-O1G	3.63	1.51	1.46
3	B	1400	ANP	PG-O1G	3.61	1.51	1.46
3	H	3400	ANP	PG-O1G	3.61	1.51	1.46
3	A	1400	ANP	C5-C6	3.60	1.51	1.41
3	E	2400	ANP	PG-O1G	3.58	1.51	1.46
3	B	3400	ANP	PG-O1G	3.58	1.51	1.46
3	B	2400	ANP	PG-O1G	3.56	1.51	1.46
3	B	1400	ANP	PB-O1B	3.56	1.51	1.46
3	B	400	ANP	PB-O1B	3.55	1.51	1.46
3	E	1400	ANP	C5-C6	3.55	1.50	1.41
3	D	1400	ANP	PB-O1B	3.55	1.51	1.46
3	E	2400	ANP	PB-O1B	3.54	1.51	1.46
3	F	1400	ANP	PB-O1B	3.53	1.51	1.46
3	G	1400	ANP	PB-O1B	3.53	1.51	1.46
3	B	400	ANP	PG-O1G	3.52	1.51	1.46
3	H	1400	ANP	C5-C6	3.51	1.50	1.41
3	A	2400	ANP	PB-O1B	3.50	1.51	1.46
3	H	400	ANP	PG-O1G	3.50	1.51	1.46
3	E	3400	ANP	PG-O1G	3.49	1.51	1.46
3	C	1400	ANP	C5-C6	3.49	1.50	1.41
3	C	2400	ANP	PG-O1G	3.49	1.51	1.46
3	D	400	ANP	PB-O1B	3.48	1.51	1.46
3	D	1400	ANP	C5-C6	3.47	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1400	ANP	PB-O1B	3.46	1.51	1.46
3	D	2400	ANP	PG-O1G	3.46	1.51	1.46
3	B	2400	ANP	PB-O1B	3.46	1.51	1.46
3	G	400	ANP	PG-O1G	3.44	1.51	1.46
3	B	1400	ANP	C5-C6	3.44	1.50	1.41
3	H	2400	ANP	PG-O1G	3.44	1.51	1.46
3	H	2400	ANP	PB-O1B	3.42	1.51	1.46
3	G	2400	ANP	PG-O1G	3.42	1.51	1.46
3	D	400	ANP	PG-O1G	3.38	1.51	1.46
3	G	1400	ANP	C5-C6	3.38	1.50	1.41
3	D	1400	ANP	PG-O1G	3.35	1.51	1.46
3	G	400	ANP	C5-C6	3.34	1.50	1.41
3	A	1400	ANP	PG-O1G	3.34	1.51	1.46
3	A	400	ANP	PB-O3A	3.32	1.63	1.59
3	G	2400	ANP	C5-C6	3.31	1.50	1.41
3	E	2400	ANP	C5-C6	3.30	1.50	1.41
3	D	2400	ANP	PB-O1B	3.30	1.51	1.46
3	E	1400	ANP	PB-O1B	3.28	1.51	1.46
3	H	400	ANP	C5-C6	3.28	1.50	1.41
3	D	2400	ANP	C5-C6	3.28	1.50	1.41
3	C	400	ANP	C5-C6	3.28	1.50	1.41
3	F	400	ANP	PG-O1G	3.28	1.51	1.46
3	C	2400	ANP	C5-C6	3.27	1.50	1.41
3	B	2400	ANP	C5-C6	3.26	1.50	1.41
3	D	400	ANP	C5-C6	3.26	1.50	1.41
3	F	2400	ANP	PG-O1G	3.26	1.51	1.46
3	G	3400	ANP	C8-N7	3.23	1.37	1.31
3	E	400	ANP	C5-C6	3.22	1.50	1.41
3	B	400	ANP	C5-C6	3.22	1.50	1.41
3	C	400	ANP	PB-O1B	3.21	1.51	1.46
3	A	2400	ANP	C5-C6	3.20	1.49	1.41
3	A	400	ANP	C5-C6	3.20	1.49	1.41
3	G	400	ANP	PB-O1B	3.20	1.51	1.46
3	F	1400	ANP	PB-O3A	3.19	1.63	1.59
3	A	3400	ANP	C8-N7	3.18	1.37	1.31
3	H	2400	ANP	C5-C6	3.15	1.49	1.41
3	F	2400	ANP	C5-C6	3.15	1.49	1.41
3	H	400	ANP	PB-O1B	3.14	1.50	1.46
3	F	400	ANP	C5-C6	3.14	1.49	1.41
3	C	1400	ANP	PB-O3A	3.12	1.63	1.59
3	C	2400	ANP	PB-O1B	3.10	1.50	1.46
3	A	400	ANP	PB-O1B	3.10	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	400	ANP	PB-O1B	3.09	1.50	1.46
3	E	400	ANP	PB-O1B	3.08	1.50	1.46
3	E	1400	ANP	PB-O3A	2.99	1.62	1.59
3	C	400	ANP	PG-O1G	2.95	1.50	1.46
3	G	3400	ANP	PB-O1B	2.94	1.50	1.46
3	D	400	ANP	PB-O3A	2.93	1.62	1.59
3	F	2400	ANP	PB-O1B	2.90	1.50	1.46
3	A	1400	ANP	PB-O3A	2.85	1.62	1.59
3	G	1400	ANP	PB-O3A	2.82	1.62	1.59
3	B	400	ANP	C8-N7	2.82	1.37	1.31
3	H	1400	ANP	C8-N7	2.77	1.37	1.31
3	E	1400	ANP	PA-O3A	2.75	1.62	1.59
3	F	400	ANP	PB-O3A	2.74	1.62	1.59
3	D	3400	ANP	C8-N7	2.73	1.36	1.31
3	F	400	ANP	C8-N7	2.73	1.36	1.31
3	D	2400	ANP	PB-O3A	2.72	1.62	1.59
3	B	3400	ANP	C8-N7	2.69	1.36	1.31
3	G	2400	ANP	C8-N7	2.68	1.36	1.31
3	D	1400	ANP	PB-O3A	2.68	1.62	1.59
3	D	2400	ANP	C8-N7	2.68	1.36	1.31
3	F	3400	ANP	PB-O1B	2.68	1.50	1.46
3	A	2400	ANP	C8-N7	2.67	1.36	1.31
3	E	400	ANP	PB-O3A	2.66	1.62	1.59
3	D	1400	ANP	C8-N7	2.65	1.36	1.31
3	F	3400	ANP	PB-O2B	-2.63	1.49	1.56
3	A	3400	ANP	PB-O2B	-2.63	1.49	1.56
3	C	3400	ANP	C8-N7	2.63	1.36	1.31
3	H	3400	ANP	C8-N7	2.62	1.36	1.31
3	E	1400	ANP	C8-N7	2.61	1.36	1.31
3	A	400	ANP	C8-N7	2.60	1.36	1.31
3	H	2400	ANP	C8-N7	2.60	1.36	1.31
3	C	3400	ANP	PB-O1B	2.60	1.50	1.46
3	H	1400	ANP	PB-O3A	2.60	1.62	1.59
3	F	3400	ANP	C8-N7	2.60	1.36	1.31
3	F	1400	ANP	C8-N7	2.60	1.36	1.31
3	E	2400	ANP	PB-O3A	2.60	1.62	1.59
3	B	1400	ANP	C8-N7	2.59	1.36	1.31
3	E	2400	ANP	C8-N7	2.57	1.36	1.31
3	F	2400	ANP	C8-N7	2.56	1.36	1.31
3	A	400	ANP	PA-O3A	2.54	1.62	1.59
3	B	2400	ANP	PB-O3A	2.53	1.62	1.59
3	E	3400	ANP	C8-N7	2.53	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1400	ANP	C8-N7	2.53	1.36	1.31
3	B	3400	ANP	C5-N7	-2.53	1.34	1.39
3	B	400	ANP	PB-O3A	2.52	1.62	1.59
3	C	2400	ANP	C8-N7	2.52	1.36	1.31
3	H	400	ANP	PB-O3A	2.51	1.62	1.59
3	A	2400	ANP	PB-O3A	2.48	1.62	1.59
3	A	1400	ANP	C8-N7	2.48	1.36	1.31
3	A	400	ANP	PG-O2G	-2.48	1.50	1.56
3	C	400	ANP	C8-N7	2.47	1.36	1.31
3	B	2400	ANP	C8-N7	2.47	1.36	1.31
3	C	1400	ANP	C8-N7	2.46	1.36	1.31
3	E	3400	ANP	PB-O1B	2.45	1.49	1.46
3	D	400	ANP	C8-N7	2.43	1.36	1.31
3	C	400	ANP	PG-O2G	-2.36	1.50	1.56
3	G	400	ANP	PG-O2G	-2.36	1.50	1.56
3	B	3400	ANP	PB-O2B	-2.35	1.50	1.56
3	B	400	ANP	PG-O2G	-2.35	1.50	1.56
3	H	400	ANP	C8-N7	2.33	1.36	1.31
3	H	3400	ANP	PB-O1B	2.31	1.49	1.46
3	G	400	ANP	C8-N7	2.29	1.36	1.31
3	G	2400	ANP	PB-O3A	2.28	1.61	1.59
3	D	3400	ANP	PB-O2B	-2.27	1.50	1.56
3	E	400	ANP	C8-N7	2.26	1.36	1.31
3	C	400	ANP	C5-N7	-2.26	1.35	1.39
3	H	2400	ANP	PB-O3A	2.22	1.61	1.59
3	F	1400	ANP	PG-O2G	-2.21	1.50	1.56
3	B	1400	ANP	C1'-N9	2.20	1.52	1.46
3	G	2400	ANP	PG-O3G	-2.20	1.51	1.56
3	D	400	ANP	PA-O3A	2.20	1.61	1.59
3	E	400	ANP	PG-O2G	-2.19	1.51	1.56
3	E	400	ANP	PG-O3G	-2.19	1.51	1.56
3	E	2400	ANP	PG-O3G	-2.19	1.51	1.56
3	B	1400	ANP	PB-O2B	-2.19	1.51	1.56
3	F	2400	ANP	PG-O2G	-2.19	1.51	1.56
3	H	400	ANP	PG-O2G	-2.18	1.51	1.56
3	F	400	ANP	C5-N7	-2.16	1.35	1.39
3	F	3400	ANP	PG-O2G	-2.16	1.51	1.56
3	A	400	ANP	PG-O3G	-2.14	1.51	1.56
3	F	2400	ANP	C1'-N9	2.14	1.52	1.46
3	F	2400	ANP	PB-O3A	2.14	1.61	1.59
3	H	2400	ANP	PB-O2B	-2.13	1.51	1.56
3	E	400	ANP	PA-O3A	2.13	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1400	ANP	PG-O2G	-2.12	1.51	1.56
3	E	3400	ANP	PB-O2B	-2.12	1.51	1.56
3	D	400	ANP	PG-O3G	-2.11	1.51	1.56
3	D	3400	ANP	PG-O2G	-2.11	1.51	1.56
3	B	3400	ANP	C2-N3	2.10	1.37	1.33
3	H	2400	ANP	C1'-N9	2.10	1.52	1.46
3	F	400	ANP	PG-O2G	-2.10	1.51	1.56
3	C	1400	ANP	PG-O3G	-2.10	1.51	1.56
3	E	400	ANP	C5-N7	-2.10	1.35	1.39
3	C	2400	ANP	C1'-N9	2.10	1.52	1.46
3	E	2400	ANP	C1'-N9	2.09	1.52	1.46
3	H	3400	ANP	PB-O2B	-2.09	1.51	1.56
3	H	400	ANP	C5-N7	-2.09	1.35	1.39
3	H	1400	ANP	C1'-N9	2.09	1.52	1.46
3	D	400	ANP	PB-O2B	-2.08	1.51	1.56
3	E	1400	ANP	PB-O2B	-2.08	1.51	1.56
3	G	1400	ANP	C1'-N9	2.08	1.52	1.46
3	C	3400	ANP	PB-O2B	-2.08	1.51	1.56
3	H	2400	ANP	PG-O3G	-2.07	1.51	1.56
3	G	2400	ANP	C1'-N9	2.07	1.52	1.46
3	A	2400	ANP	PG-O3G	-2.07	1.51	1.56
3	F	2400	ANP	PB-O2B	-2.07	1.51	1.56
3	H	2400	ANP	PG-O2G	-2.07	1.51	1.56
3	C	2400	ANP	PB-O3A	2.06	1.61	1.59
3	D	2400	ANP	C1'-N9	2.06	1.52	1.46
3	A	400	ANP	C5-N7	-2.06	1.35	1.39
3	C	1400	ANP	C1'-N9	2.06	1.52	1.46
3	D	400	ANP	PG-O2G	-2.06	1.51	1.56
3	H	3400	ANP	C4-N3	2.05	1.38	1.34
3	B	2400	ANP	PB-O2B	-2.05	1.51	1.56
3	D	1400	ANP	C1'-N9	2.05	1.52	1.46
3	B	2400	ANP	C1'-N9	2.05	1.52	1.46
3	A	1400	ANP	PG-O3G	-2.05	1.51	1.56
3	E	3400	ANP	PG-O2G	-2.04	1.51	1.56
3	F	1400	ANP	PG-O3G	-2.04	1.51	1.56
3	G	1400	ANP	PG-O2G	-2.04	1.51	1.56
3	F	1400	ANP	PB-O2B	-2.04	1.51	1.56
3	E	1400	ANP	PG-O2G	-2.03	1.51	1.56
3	G	400	ANP	PG-O3G	-2.03	1.51	1.56
3	G	3400	ANP	PB-O2B	-2.03	1.51	1.56
3	C	2400	ANP	PG-O3G	-2.02	1.51	1.56
3	C	2400	ANP	PG-O2G	-2.02	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2400	ANP	PG-O3G	-2.01	1.51	1.56
3	G	1400	ANP	PG-O3G	-2.01	1.51	1.56
3	B	2400	ANP	PG-O2G	-2.01	1.51	1.56
3	F	2400	ANP	C5-N7	-2.01	1.35	1.39
3	C	400	ANP	PG-O3G	-2.00	1.51	1.56

All (406) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3400	ANP	O1G-PG-N3B	-7.84	100.23	111.77
3	H	3400	ANP	C5-C4-N3	-7.72	116.08	126.72
3	B	3400	ANP	C5-C4-N3	-7.61	116.24	126.72
3	E	3400	ANP	C5-C4-N3	-7.57	116.29	126.72
3	F	3400	ANP	O1G-PG-N3B	-7.45	100.81	111.77
3	A	3400	ANP	C5-C4-N3	-7.44	116.47	126.72
3	H	3400	ANP	O1G-PG-N3B	-7.29	101.03	111.77
3	G	3400	ANP	C5-C4-N3	-7.28	116.70	126.72
3	D	3400	ANP	C5-C4-N3	-7.27	116.71	126.72
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	F	1400	ANP	C5-C4-N3	-7.07	116.98	126.72
3	A	1400	ANP	C5-C4-N3	-7.04	117.03	126.72
3	C	3400	ANP	C5-C4-N3	-7.03	117.03	126.72
3	B	2400	ANP	C5-C4-N3	-7.03	117.04	126.72
3	D	2400	ANP	C5-C4-N3	-7.03	117.04	126.72
3	D	1400	ANP	C5-C4-N3	-7.02	117.05	126.72
3	E	1400	ANP	C5-C4-N3	-7.02	117.05	126.72
3	E	3400	ANP	O1G-PG-N3B	-7.02	101.44	111.77
3	A	2400	ANP	C5-C4-N3	-7.00	117.07	126.72
3	G	1400	ANP	C5-C4-N3	-6.99	117.09	126.72
3	G	2400	ANP	C5-C4-N3	-6.97	117.12	126.72
3	F	3400	ANP	C5-C4-N3	-6.96	117.14	126.72
3	C	2400	ANP	C5-C4-N3	-6.93	117.18	126.72
3	B	1400	ANP	C5-C4-N3	-6.91	117.20	126.72
3	F	2400	ANP	C5-C4-N3	-6.91	117.20	126.72
3	C	1400	ANP	C5-C4-N3	-6.91	117.21	126.72
3	H	1400	ANP	C5-C4-N3	-6.88	117.24	126.72
3	E	2400	ANP	C5-C4-N3	-6.83	117.31	126.72
3	D	3400	ANP	O1G-PG-N3B	-6.82	101.72	111.77
3	H	2400	ANP	C5-C4-N3	-6.81	117.34	126.72
3	A	400	ANP	C5-C4-N3	-6.59	117.64	126.72
3	C	3400	ANP	O1G-PG-N3B	-6.58	102.08	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	400	ANP	C5-C4-N3	-6.53	117.73	126.72
3	C	400	ANP	C5-C4-N3	-6.42	117.87	126.72
3	B	400	ANP	C5-C4-N3	-6.40	117.90	126.72
3	H	400	ANP	C5-C4-N3	-6.40	117.91	126.72
3	F	400	ANP	C5-C4-N3	-6.37	117.95	126.72
3	G	400	ANP	C5-C4-N3	-6.32	118.01	126.72
3	D	400	ANP	C5-C4-N3	-6.11	118.31	126.72
3	H	3400	ANP	C4-C5-N7	-5.71	104.06	110.58
3	A	3400	ANP	C4-C5-N7	-5.48	104.32	110.58
3	B	3400	ANP	C4-C5-N7	-5.37	104.44	110.58
3	E	3400	ANP	C4-C5-N7	-5.34	104.48	110.58
3	B	2400	ANP	N3-C4-N9	5.27	136.13	127.17
3	C	2400	ANP	N3-C4-N9	5.24	136.08	127.17
3	A	1400	ANP	N3-C4-N9	5.23	136.07	127.17
3	A	2400	ANP	N3-C4-N9	5.23	136.06	127.17
3	E	2400	ANP	N3-C4-N9	5.22	136.04	127.17
3	F	2400	ANP	N3-C4-N9	5.22	136.04	127.17
3	D	2400	ANP	N3-C4-N9	5.21	136.02	127.17
3	G	2400	ANP	N3-C4-N9	5.21	136.02	127.17
3	D	1400	ANP	N3-C4-N9	5.20	136.02	127.17
3	H	2400	ANP	N3-C4-N9	5.20	136.01	127.17
3	E	1400	ANP	N3-C4-N9	5.16	135.95	127.17
3	D	3400	ANP	C4-C5-N7	-5.13	104.71	110.58
3	H	1400	ANP	N3-C4-N9	5.12	135.88	127.17
3	B	1400	ANP	N3-C4-N9	5.11	135.87	127.17
3	F	1400	ANP	N3-C4-N9	5.10	135.83	127.17
3	C	1400	ANP	N3-C4-N9	5.09	135.83	127.17
3	C	3400	ANP	C4-C5-N7	-5.06	104.80	110.58
3	G	1400	ANP	N3-C4-N9	5.01	135.70	127.17
3	H	3400	ANP	N3-C4-N9	5.00	135.67	127.17
3	A	2400	ANP	O1G-PG-N3B	-4.92	104.53	111.77
3	D	3400	ANP	N3-C4-N9	4.91	135.51	127.17
3	E	400	ANP	N3-C4-N9	4.87	135.46	127.17
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	G	3400	ANP	C4-C5-N7	-4.82	105.07	110.58
3	B	1400	ANP	O1G-PG-N3B	-4.80	104.71	111.77
3	A	3400	ANP	N3-C4-N9	4.80	135.32	127.17
3	H	400	ANP	N3-C4-N9	4.79	135.32	127.17
3	C	400	ANP	N3-C4-N9	4.78	135.29	127.17
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3400	ANP	N3-C4-N9	4.76	135.27	127.17
3	G	3400	ANP	O1B-PB-N3B	-4.75	104.77	111.77
3	A	400	ANP	N3-C4-N9	4.75	135.25	127.17
3	B	400	ANP	N3-C4-N9	4.75	135.25	127.17
3	E	2400	ANP	O1G-PG-N3B	-4.75	104.78	111.77
3	G	400	ANP	N3-C4-N9	4.75	135.24	127.17
3	F	3400	ANP	C4-C5-N7	-4.74	105.16	110.58
3	C	3400	ANP	N3-C4-N9	4.74	135.23	127.17
3	G	3400	ANP	N3-C4-N9	4.73	135.21	127.17
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	D	400	ANP	N3-C4-N9	4.69	135.14	127.17
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	F	3400	ANP	N3-C4-N9	4.64	135.07	127.17
3	C	1400	ANP	O1G-PG-N3B	-4.61	104.97	111.77
3	F	400	ANP	N3-C4-N9	4.57	134.93	127.17
3	A	1400	ANP	C2-N3-C4	4.56	122.98	111.83
3	H	3400	ANP	O2B-PB-O1B	4.55	119.62	109.87
3	B	3400	ANP	N3-C4-N9	4.54	134.88	127.17
3	A	2400	ANP	C2-N3-C4	4.54	122.91	111.83
3	F	1400	ANP	C2-N3-C4	4.54	122.91	111.83
3	E	1400	ANP	C2-N3-C4	4.53	122.89	111.83
3	F	2400	ANP	C2-N3-C4	4.52	122.87	111.83
3	H	3400	ANP	C2-N3-C4	4.52	122.86	111.83
3	B	2400	ANP	C2-N3-C4	4.52	122.86	111.83
3	G	1400	ANP	C2-N3-C4	4.51	122.85	111.83
3	D	1400	ANP	C2-N3-C4	4.51	122.84	111.83
3	C	1400	ANP	C2-N3-C4	4.51	122.83	111.83
3	E	3400	ANP	O2B-PB-O1B	4.50	119.51	109.87
3	C	2400	ANP	C2-N3-C4	4.45	122.70	111.83
3	G	2400	ANP	C2-N3-C4	4.45	122.70	111.83
3	B	1400	ANP	C2-N3-C4	4.45	122.69	111.83
3	D	2400	ANP	C2-N3-C4	4.44	122.67	111.83
3	H	2400	ANP	C2-N3-C4	4.42	122.63	111.83
3	F	2400	ANP	O2B-PB-O1B	4.42	119.34	109.87
3	E	2400	ANP	C2-N3-C4	4.41	122.60	111.83
3	H	1400	ANP	C2-N3-C4	4.41	122.59	111.83
3	C	3400	ANP	O2B-PB-O1B	4.38	119.27	109.87
3	E	2400	ANP	O2B-PB-O1B	4.37	119.23	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2400	ANP	O2B-PB-O1B	4.36	119.22	109.87
3	D	400	ANP	O1G-PG-N3B	-4.35	105.37	111.77
3	D	2400	ANP	O2B-PB-O1B	4.34	119.17	109.87
3	B	2400	ANP	O2B-PB-O1B	4.33	119.15	109.87
3	B	3400	ANP	C2-N3-C4	4.33	122.40	111.83
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	D	1400	ANP	O1G-PG-N3B	-4.29	105.45	111.77
3	A	2400	ANP	O2B-PB-O1B	4.27	119.03	109.87
3	D	3400	ANP	C2-N3-C4	4.27	122.25	111.83
3	A	3400	ANP	O1B-PB-N3B	-4.25	105.51	111.77
3	C	400	ANP	O2B-PB-O1B	4.24	118.97	109.87
3	G	3400	ANP	C2-N3-C4	4.22	122.14	111.83
3	G	2400	ANP	O2B-PB-O1B	4.22	118.92	109.87
3	C	3400	ANP	O1B-PB-N3B	-4.21	105.56	111.77
3	E	3400	ANP	C2-N3-C4	4.21	122.12	111.83
3	C	400	ANP	O1G-PG-N3B	-4.19	105.59	111.77
3	A	1400	ANP	O2B-PB-O1B	4.18	118.84	109.87
3	H	2400	ANP	O2B-PB-O1B	4.17	118.81	109.87
3	E	1400	ANP	O2B-PB-O1B	4.16	118.79	109.87
3	F	400	ANP	O2B-PB-O1B	4.15	118.77	109.87
3	C	3400	ANP	C2-N3-C4	4.15	121.96	111.83
3	D	1400	ANP	O2B-PB-O1B	4.15	118.76	109.87
3	A	400	ANP	C2-N3-C4	4.14	121.94	111.83
3	D	3400	ANP	O2B-PB-O1B	4.14	118.74	109.87
3	E	400	ANP	C2-N3-C4	4.13	121.92	111.83
3	H	1400	ANP	O1G-PG-N3B	-4.13	105.69	111.77
3	C	400	ANP	C2-N3-C4	4.13	121.91	111.83
3	H	400	ANP	C2-N3-C4	4.11	121.87	111.83
3	B	1400	ANP	O2B-PB-O1B	4.10	118.67	109.87
3	F	3400	ANP	C2-N3-C4	4.09	121.82	111.83
3	G	400	ANP	O2B-PB-O1B	4.08	118.63	109.87
3	F	1400	ANP	O2B-PB-O1B	4.07	118.60	109.87
3	E	1400	ANP	C4-C5-N7	-4.06	105.94	110.58
3	B	400	ANP	C2-N3-C4	4.06	121.75	111.83
3	A	3400	ANP	C2-N3-C4	4.04	121.70	111.83
3	G	1400	ANP	O1G-PG-N3B	-4.03	105.84	111.77
3	A	1400	ANP	O1G-PG-N3B	-4.01	105.86	111.77
3	F	3400	ANP	O2B-PB-O1B	4.01	118.46	109.87
3	G	1400	ANP	O2B-PB-O1B	4.00	118.45	109.87
3	H	1400	ANP	O2B-PB-O1B	4.00	118.44	109.87
3	F	3400	ANP	O1B-PB-N3B	-4.00	105.89	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	400	ANP	C2-N3-C4	3.98	121.56	111.83
3	E	400	ANP	O1G-PG-N3B	-3.97	105.93	111.77
3	E	400	ANP	C4-C5-N7	-3.97	106.05	110.58
3	C	1400	ANP	O3A-PB-N3B	3.95	117.54	106.59
3	B	3400	ANP	O2B-PB-O1B	3.94	118.32	109.87
3	D	1400	ANP	C4-C5-N7	-3.94	106.08	110.58
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	D	400	ANP	C2-N3-C4	3.91	121.38	111.83
3	G	1400	ANP	O3A-PB-N3B	3.91	117.44	106.59
3	F	400	ANP	C2-N3-C4	3.91	121.38	111.83
3	F	1400	ANP	C4-C5-N7	-3.90	106.12	110.58
3	F	400	ANP	O1G-PG-N3B	-3.89	106.04	111.77
3	C	1400	ANP	O2B-PB-O1B	3.88	118.18	109.87
3	F	2400	ANP	N3-C2-N1	-3.88	122.72	128.58
3	H	400	ANP	O1G-PG-N3B	-3.86	106.08	111.77
3	B	1400	ANP	O3A-PB-N3B	3.85	117.28	106.59
3	A	1400	ANP	C4-C5-N7	-3.85	106.18	110.58
3	H	3400	ANP	C5-N7-C8	3.84	109.49	103.45
3	A	1400	ANP	O3A-PB-N3B	3.83	117.22	106.59
3	G	2400	ANP	O3A-PB-N3B	3.81	117.16	106.59
3	A	400	ANP	C4-C5-N7	-3.80	106.24	110.58
3	E	400	ANP	O2B-PB-O1B	3.80	118.02	109.87
3	F	1400	ANP	O3A-PB-N3B	3.80	117.13	106.59
3	H	2400	ANP	N3-C2-N1	-3.79	122.84	128.58
3	A	2400	ANP	N3-C2-N1	-3.79	122.85	128.58
3	H	1400	ANP	O3A-PB-N3B	3.76	117.03	106.59
3	C	1400	ANP	C4-C5-N7	-3.76	106.28	110.58
3	B	1400	ANP	C4-C5-N7	-3.75	106.30	110.58
3	B	400	ANP	O2B-PB-O1B	3.74	117.89	109.87
3	E	1400	ANP	N3-C2-N1	-3.74	122.92	128.58
3	H	1400	ANP	C4-C5-N7	-3.74	106.31	110.58
3	G	400	ANP	C4-C5-N7	-3.73	106.31	110.58
3	G	3400	ANP	O2B-PB-O1B	3.73	117.87	109.87
3	H	400	ANP	O2B-PB-O1B	3.73	117.86	109.87
3	E	2400	ANP	N3-C2-N1	-3.73	122.94	128.58
3	D	400	ANP	O2B-PB-O1B	3.73	117.86	109.87
3	C	2400	ANP	N3-C2-N1	-3.72	122.95	128.58
3	H	400	ANP	C4-C5-N7	-3.72	106.33	110.58
3	D	1400	ANP	O3A-PB-N3B	3.69	116.83	106.59
3	B	2400	ANP	N3-C2-N1	-3.69	122.99	128.58
3	G	2400	ANP	N3-C2-N1	-3.68	123.01	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	ANP	O2B-PB-O1B	3.68	117.75	109.87
3	C	2400	ANP	O3A-PB-N3B	3.67	116.77	106.59
3	A	3400	ANP	O2B-PB-O1B	3.67	117.73	109.87
3	C	1400	ANP	N3-C2-N1	-3.66	123.05	128.58
3	D	1400	ANP	N3-C2-N1	-3.65	123.06	128.58
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	H	2400	ANP	O1B-PB-N3B	-3.64	106.42	111.77
3	F	400	ANP	C4-C5-N7	-3.63	106.43	110.58
3	G	1400	ANP	C4-C5-N7	-3.63	106.43	110.58
3	B	1400	ANP	N3-C2-N1	-3.63	123.09	128.58
3	D	2400	ANP	N3-C2-N1	-3.62	123.10	128.58
3	B	400	ANP	N3-C2-N1	-3.61	123.11	128.58
3	E	400	ANP	N3-C2-N1	-3.61	123.11	128.58
3	G	1400	ANP	N3-C2-N1	-3.60	123.12	128.58
3	C	400	ANP	C4-C5-N7	-3.60	106.47	110.58
3	A	2400	ANP	O3A-PB-N3B	3.60	116.56	106.59
3	B	3400	ANP	O1B-PB-N3B	-3.58	106.50	111.77
3	B	2400	ANP	O3A-PB-N3B	3.57	116.50	106.59
3	E	2400	ANP	O3A-PB-N3B	3.57	116.50	106.59
3	A	400	ANP	N3-C2-N1	-3.56	123.19	128.58
3	H	400	ANP	N3-C2-N1	-3.56	123.19	128.58
3	A	1400	ANP	N3-C2-N1	-3.56	123.19	128.58
3	F	1400	ANP	N3-C2-N1	-3.55	123.21	128.58
3	C	400	ANP	N3-C2-N1	-3.55	123.22	128.58
3	H	1400	ANP	N3-C2-N1	-3.53	123.24	128.58
3	A	3400	ANP	C5-N7-C8	3.51	108.97	103.45
3	E	1400	ANP	O3A-PB-N3B	3.51	116.33	106.59
3	C	1400	ANP	O1B-PB-N3B	-3.51	106.60	111.77
3	D	2400	ANP	O3A-PB-N3B	3.50	116.29	106.59
3	B	400	ANP	C4-C5-N7	-3.50	106.58	110.58
3	D	400	ANP	N3-C2-N1	-3.46	123.34	128.58
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	D	2400	ANP	C4-C5-N7	-3.44	106.64	110.58
3	B	1400	ANP	O1B-PB-N3B	-3.44	106.71	111.77
3	E	1400	ANP	O1B-PB-N3B	-3.44	106.71	111.77
3	A	3400	ANP	O2G-PG-O3G	3.43	116.80	107.59
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	400	ANP	C4-C5-N7	-3.38	106.72	110.58
3	C	2400	ANP	C4-C5-N7	-3.38	106.72	110.58
3	G	1400	ANP	O1B-PB-N3B	-3.38	106.80	111.77
3	B	2400	ANP	C4-C5-N7	-3.38	106.72	110.58
3	F	1400	ANP	O1B-PB-N3B	-3.36	106.82	111.77
3	G	2400	ANP	C4-C5-N7	-3.36	106.74	110.58
3	F	400	ANP	N3-C2-N1	-3.34	123.52	128.58
3	A	2400	ANP	C4-C5-N7	-3.33	106.77	110.58
3	G	400	ANP	N3-C2-N1	-3.32	123.55	128.58
3	E	3400	ANP	C5-N7-C8	3.32	108.67	103.45
3	A	1400	ANP	O1B-PB-N3B	-3.31	106.90	111.77
3	D	3400	ANP	C5-N7-C8	3.28	108.61	103.45
3	E	2400	ANP	C4-C5-N7	-3.27	106.84	110.58
3	D	1400	ANP	O1B-PB-N3B	-3.27	106.96	111.77
3	F	2400	ANP	C4-C5-N7	-3.23	106.89	110.58
3	H	2400	ANP	C4-C5-N7	-3.22	106.90	110.58
3	F	2400	ANP	O1B-PB-N3B	-3.21	107.05	111.77
3	C	3400	ANP	C5-N7-C8	3.20	108.47	103.45
3	H	3400	ANP	O2G-PG-O3G	3.16	116.08	107.59
3	B	3400	ANP	C5-N7-C8	3.14	108.39	103.45
3	C	1400	ANP	C3'-C2'-C1'	3.14	107.41	101.46
3	H	3400	ANP	N3-C2-N1	-3.13	123.84	128.58
3	C	3400	ANP	O2G-PG-O3G	3.09	115.89	107.59
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	F	3400	ANP	C5-N7-C8	3.06	108.27	103.45
3	F	1400	ANP	C3'-C2'-C1'	3.05	107.23	101.46
3	G	1400	ANP	C3'-C2'-C1'	3.04	107.21	101.46
3	A	1400	ANP	C3'-C2'-C1'	3.02	107.18	101.46
3	B	1400	ANP	C3'-C2'-C1'	3.02	107.18	101.46
3	F	3400	ANP	O2G-PG-O3G	3.02	115.69	107.59
3	G	3400	ANP	C5-N7-C8	2.98	108.14	103.45
3	B	2400	ANP	C3'-C2'-C1'	2.97	107.08	101.46
3	G	400	ANP	O3A-PB-N3B	2.95	114.78	106.59
3	A	2400	ANP	C3'-C2'-C1'	2.95	107.03	101.46
3	D	3400	ANP	O2G-PG-O3G	2.93	115.47	107.59
3	B	3400	ANP	O2G-PG-O3G	2.93	115.46	107.59
3	G	3400	ANP	O2G-PG-O3G	2.93	115.45	107.59
3	F	2400	ANP	C3'-C2'-C1'	2.91	106.97	101.46
3	G	3400	ANP	N3-C2-N1	-2.91	124.17	128.58
3	H	3400	ANP	C6-C5-N7	2.91	137.70	132.09
3	D	2400	ANP	C3'-C2'-C1'	2.88	106.92	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2400	ANP	C3'-C2'-C1'	2.88	106.91	101.46
3	H	2400	ANP	C3'-C2'-C1'	2.87	106.90	101.46
3	E	400	ANP	O3A-PB-N3B	2.86	114.52	106.59
3	E	1400	ANP	C5-N7-C8	2.85	107.94	103.45
3	C	2400	ANP	C3'-C2'-C1'	2.85	106.86	101.46
3	D	1400	ANP	C3'-C2'-C1'	2.82	106.81	101.46
3	G	2400	ANP	C3'-C2'-C1'	2.82	106.81	101.46
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	H	400	ANP	C3'-C2'-C1'	2.81	106.78	101.46
3	B	3400	ANP	C5-C4-N9	2.81	108.87	105.81
3	F	400	ANP	O3A-PB-N3B	2.81	114.38	106.59
3	F	400	ANP	C3'-C2'-C1'	2.80	106.77	101.46
3	C	400	ANP	C3'-C2'-C1'	2.80	106.76	101.46
3	E	3400	ANP	O2G-PG-O3G	2.79	115.09	107.59
3	F	3400	ANP	N3-C2-N1	-2.78	124.37	128.58
3	E	400	ANP	C5-N7-C8	2.77	107.81	103.45
3	H	1400	ANP	C3'-C2'-C1'	2.77	106.70	101.46
3	D	1400	ANP	C5-N7-C8	2.76	107.79	103.45
3	G	400	ANP	C3'-C2'-C1'	2.75	106.66	101.46
3	E	400	ANP	C3'-C2'-C1'	2.74	106.65	101.46
3	D	3400	ANP	N3-C2-N1	-2.74	124.43	128.58
3	C	3400	ANP	N3-C2-N1	-2.73	124.44	128.58
3	E	1400	ANP	C3'-C2'-C1'	2.71	106.58	101.46
3	A	1400	ANP	C5-N7-C8	2.70	107.69	103.45
3	A	400	ANP	C3'-C2'-C1'	2.68	106.54	101.46
3	B	3400	ANP	N3-C2-N1	-2.68	124.53	128.58
3	D	3400	ANP	C6-C5-N7	2.68	137.25	132.09
3	B	400	ANP	O3A-PB-N3B	2.65	113.94	106.59
3	B	400	ANP	C3'-C2'-C1'	2.64	106.47	101.46
3	B	1400	ANP	C5-N7-C8	2.63	107.59	103.45
3	A	3400	ANP	C6-C5-N7	2.62	137.14	132.09
3	A	400	ANP	O3A-PB-N3B	2.60	113.82	106.59
3	D	400	ANP	C3'-C2'-C1'	2.59	106.37	101.46
3	H	3400	ANP	O2A-PA-O3A	2.59	114.28	107.27
3	H	1400	ANP	C5-N7-C8	2.59	107.52	103.45
3	A	400	ANP	C5-N7-C8	2.58	107.51	103.45
3	C	1400	ANP	C5-N7-C8	2.57	107.48	103.45
3	E	3400	ANP	C6-C5-N7	2.56	137.03	132.09
3	A	1400	ANP	C6-C5-N7	2.55	137.00	132.09
3	B	1400	ANP	C6-C5-N7	2.53	136.97	132.09
3	E	1400	ANP	C6-C5-N7	2.53	136.97	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	400	ANP	C5-N7-C8	2.53	107.42	103.45
3	B	3400	ANP	C6-C5-N7	2.53	136.96	132.09
3	D	1400	ANP	C6-C5-N7	2.52	136.96	132.09
3	F	1400	ANP	C5-N7-C8	2.51	107.40	103.45
3	H	400	ANP	C5-N7-C8	2.51	107.39	103.45
3	F	3400	ANP	C6-C5-N7	2.50	136.90	132.09
3	C	3400	ANP	C6-C5-N7	2.49	136.90	132.09
3	G	3400	ANP	C6-C5-N7	2.49	136.89	132.09
3	H	1400	ANP	C6-C5-N7	2.48	136.87	132.09
3	F	1400	ANP	C6-C5-N7	2.47	136.86	132.09
3	G	3400	ANP	C4'-O4'-C1'	-2.47	104.02	109.47
3	C	1400	ANP	C6-C5-N7	2.45	136.82	132.09
3	E	3400	ANP	O2A-PA-O3A	2.44	113.88	107.27
3	E	3400	ANP	C5-C4-N9	2.41	108.44	105.81
3	G	1400	ANP	C6-C5-N7	2.38	136.68	132.09
3	A	3400	ANP	N3-C2-N1	-2.37	125.00	128.58
3	G	1400	ANP	C5-N7-C8	2.34	107.13	103.45
3	D	400	ANP	O2G-PG-O3G	2.34	113.88	107.59
3	F	400	ANP	C5-N7-C8	2.34	107.12	103.45
3	B	400	ANP	C5-N7-C8	2.33	107.11	103.45
3	E	3400	ANP	N3-C2-N1	-2.33	125.06	128.58
3	C	400	ANP	C5-N7-C8	2.33	107.11	103.45
3	B	2400	ANP	C5-N7-C8	2.31	107.08	103.45
3	C	2400	ANP	C5-N7-C8	2.31	107.08	103.45
3	D	2400	ANP	C5-N7-C8	2.30	107.07	103.45
3	D	3400	ANP	C4'-O4'-C1'	-2.30	104.39	109.47
3	F	400	ANP	O2G-PG-O3G	2.30	113.76	107.59
3	H	3400	ANP	C4'-O4'-C1'	-2.30	104.40	109.47
3	D	400	ANP	C5-N7-C8	2.29	107.04	103.45
3	E	2400	ANP	C5-N7-C8	2.28	107.03	103.45
3	A	2400	ANP	C5-N7-C8	2.28	107.03	103.45
3	B	3400	ANP	O2A-PA-O3A	2.28	113.43	107.27
3	C	3400	ANP	C4'-O4'-C1'	-2.28	104.44	109.47
3	G	400	ANP	O2G-PG-O3G	2.28	113.70	107.59
3	H	2400	ANP	C5-N7-C8	2.25	106.99	103.45
3	D	3400	ANP	O2A-PA-O3A	2.24	113.34	107.27
3	G	2400	ANP	C5-N7-C8	2.24	106.97	103.45
3	H	3400	ANP	C5-C4-N9	2.24	108.25	105.81
3	E	400	ANP	C6-C5-N7	2.23	136.40	132.09
3	A	400	ANP	C6-C5-N7	2.23	136.39	132.09
3	E	3400	ANP	C4'-O4'-C1'	-2.22	104.56	109.47
3	C	3400	ANP	O2A-PA-O3A	2.22	113.26	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2400	ANP	C6-C5-N7	2.20	136.33	132.09
3	A	3400	ANP	C5-C4-N9	2.20	108.21	105.81
3	F	3400	ANP	C4'-O4'-C1'	-2.20	104.61	109.47
3	A	400	ANP	O2G-PG-O3G	2.19	113.47	107.59
3	F	2400	ANP	C5-N7-C8	2.17	106.87	103.45
3	B	3400	ANP	C4'-O4'-C1'	-2.17	104.68	109.47
3	H	400	ANP	C6-C5-N7	2.17	136.27	132.09
3	E	2400	ANP	C6-C5-N7	2.16	136.26	132.09
3	H	1400	ANP	O2G-PG-O3G	2.16	113.38	107.59
3	E	3400	ANP	O3A-PB-N3B	2.16	112.57	106.59
3	H	400	ANP	O2G-PG-O3G	2.15	113.37	107.59
3	G	400	ANP	C6-C5-N7	2.15	136.23	132.09
3	D	1400	ANP	O2G-PG-O3G	2.15	113.36	107.59
3	D	400	ANP	C2-N1-C6	2.14	122.24	118.73
3	A	2400	ANP	C6-C5-N7	2.13	136.20	132.09
3	B	400	ANP	C2-N1-C6	2.13	122.23	118.73
3	B	3400	ANP	C3'-C2'-C1'	2.13	105.49	101.46
3	B	2400	ANP	C6-C5-N7	2.13	136.19	132.09
3	G	2400	ANP	C6-C5-N7	2.13	136.19	132.09
3	H	2400	ANP	C6-C5-N7	2.13	136.19	132.09
3	C	400	ANP	C6-C5-N7	2.12	136.18	132.09
3	G	3400	ANP	O3A-PB-N3B	2.12	112.48	106.59
3	F	2400	ANP	C6-C5-N7	2.11	136.16	132.09
3	C	1400	ANP	O2G-PG-O3G	2.11	113.27	107.59
3	B	400	ANP	O2G-PG-O3G	2.11	113.26	107.59
3	D	2400	ANP	C6-C5-N7	2.11	136.16	132.09
3	C	400	ANP	O3'-C3'-C4'	2.09	117.09	111.08
3	G	3400	ANP	C5-C4-N9	2.09	108.09	105.81
3	G	1400	ANP	O2G-PG-O3G	2.09	113.20	107.59
3	A	3400	ANP	C4'-O4'-C1'	-2.06	104.91	109.47
3	F	400	ANP	C6-C5-N7	2.06	136.06	132.09
3	B	400	ANP	C6-C5-N7	2.05	136.05	132.09
3	B	400	ANP	O1B-PB-N3B	-2.05	108.75	111.77
3	B	3400	ANP	O4'-C4'-C5'	2.04	115.88	109.33
3	E	400	ANP	O2G-PG-O3G	2.04	113.08	107.59
3	E	400	ANP	O3'-C3'-C4'	2.03	116.90	111.08
3	E	3400	ANP	O4'-C4'-C5'	2.02	115.79	109.33

All (32) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	400	ANP	C4'

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Mol	Chain	Res	Type	Atom
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'
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 (278) 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	1400	ANP	PB-N3B-PG-O1G

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

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

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Mol	Chain	Res	Type	Atoms
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	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-O2A
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	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-O2B
3	G	1400	ANP	C5'-O5'-PA-O2A
3	G	1400	ANP	C5'-O5'-PA-O3A
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
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	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-O2A
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	1400	ANP	PB-N3B-PG-O1G
3	H	1400	ANP	PG-N3B-PB-O1B

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

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Mol	Chain	Res	Type	Atoms
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
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	C2'-C1'-N9-C8
3	B	3400	ANP	C2'-C1'-N9-C8
3	C	3400	ANP	C2'-C1'-N9-C8
3	D	3400	ANP	C2'-C1'-N9-C8
3	E	3400	ANP	C2'-C1'-N9-C8

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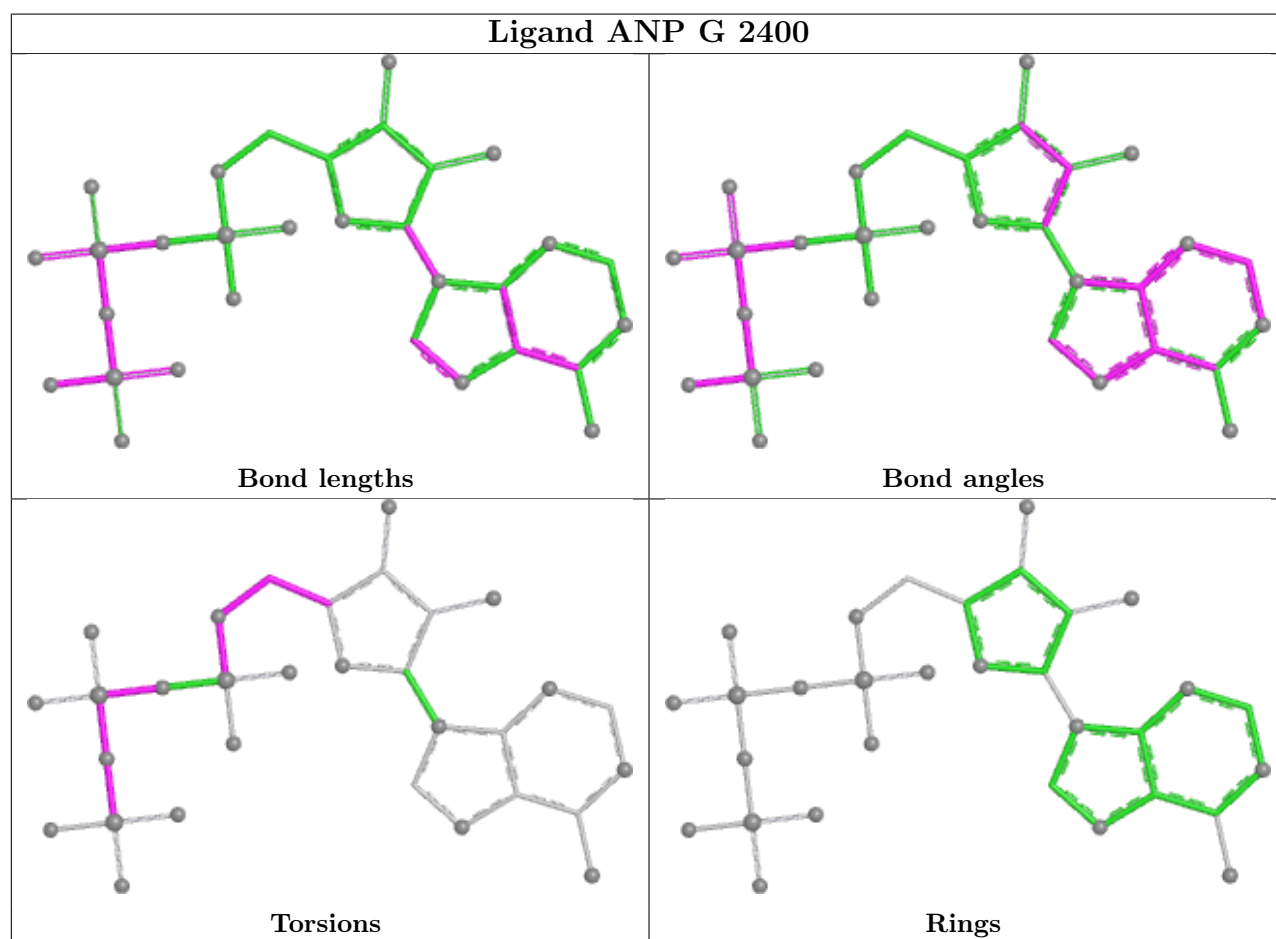
Mol	Chain	Res	Type	Atoms
3	F	3400	ANP	C2'-C1'-N9-C8
3	G	3400	ANP	C2'-C1'-N9-C8
3	H	3400	ANP	C2'-C1'-N9-C8
3	E	3400	ANP	C5'-O5'-PA-O2A
3	H	3400	ANP	C5'-O5'-PA-O2A
3	E	3400	ANP	C4'-C5'-O5'-PA
3	H	3400	ANP	C4'-C5'-O5'-PA
3	A	3400	ANP	C4'-C5'-O5'-PA
3	C	3400	ANP	C4'-C5'-O5'-PA
3	D	3400	ANP	C4'-C5'-O5'-PA
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	B	3400	ANP	PB-O3A-PA-O1A
3	C	3400	ANP	PB-O3A-PA-O1A
3	D	3400	ANP	PB-O3A-PA-O1A
3	E	3400	ANP	PB-O3A-PA-O1A
3	F	3400	ANP	PB-O3A-PA-O1A
3	G	3400	ANP	PB-O3A-PA-O1A

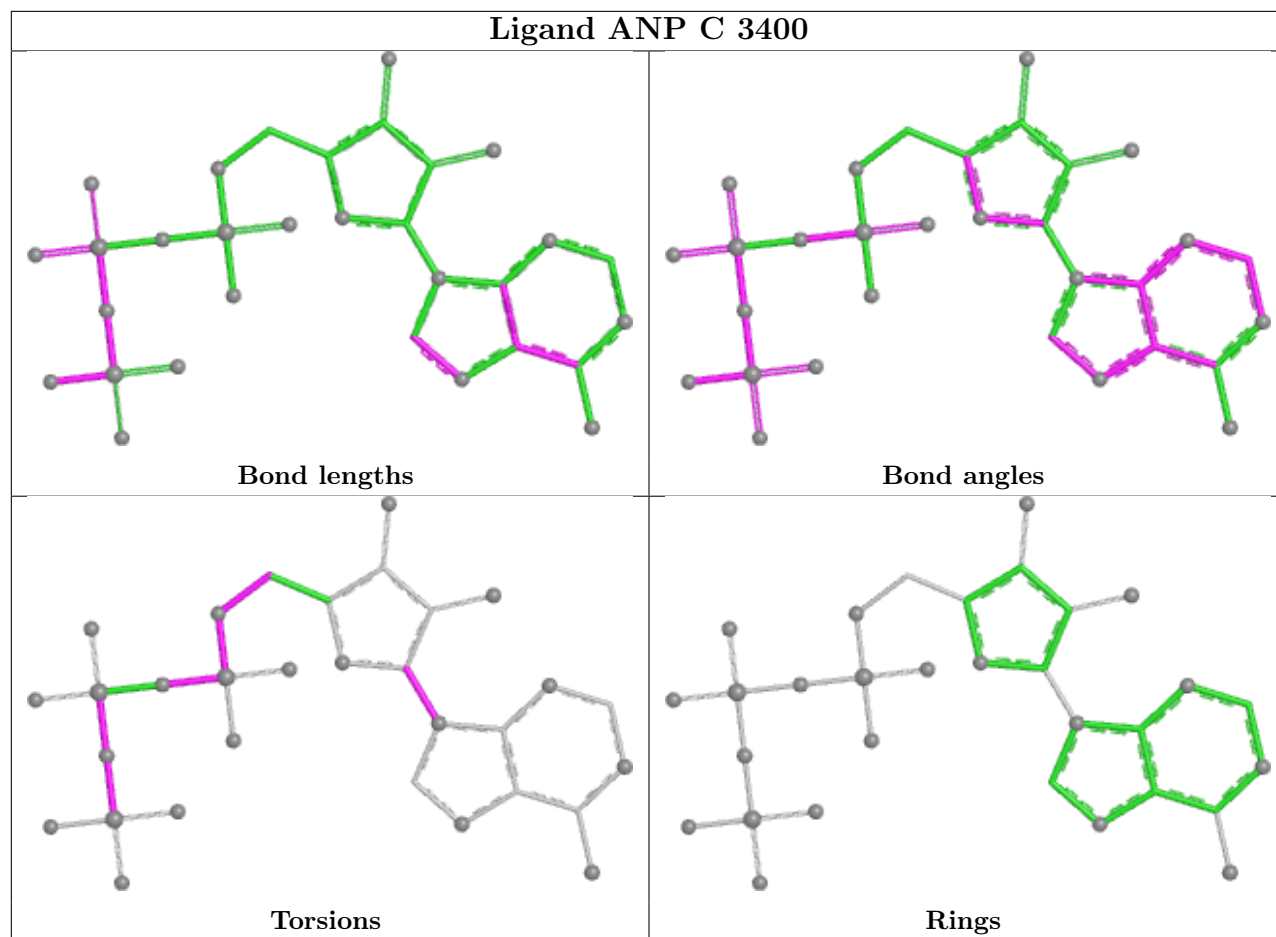
There are no ring outliers.

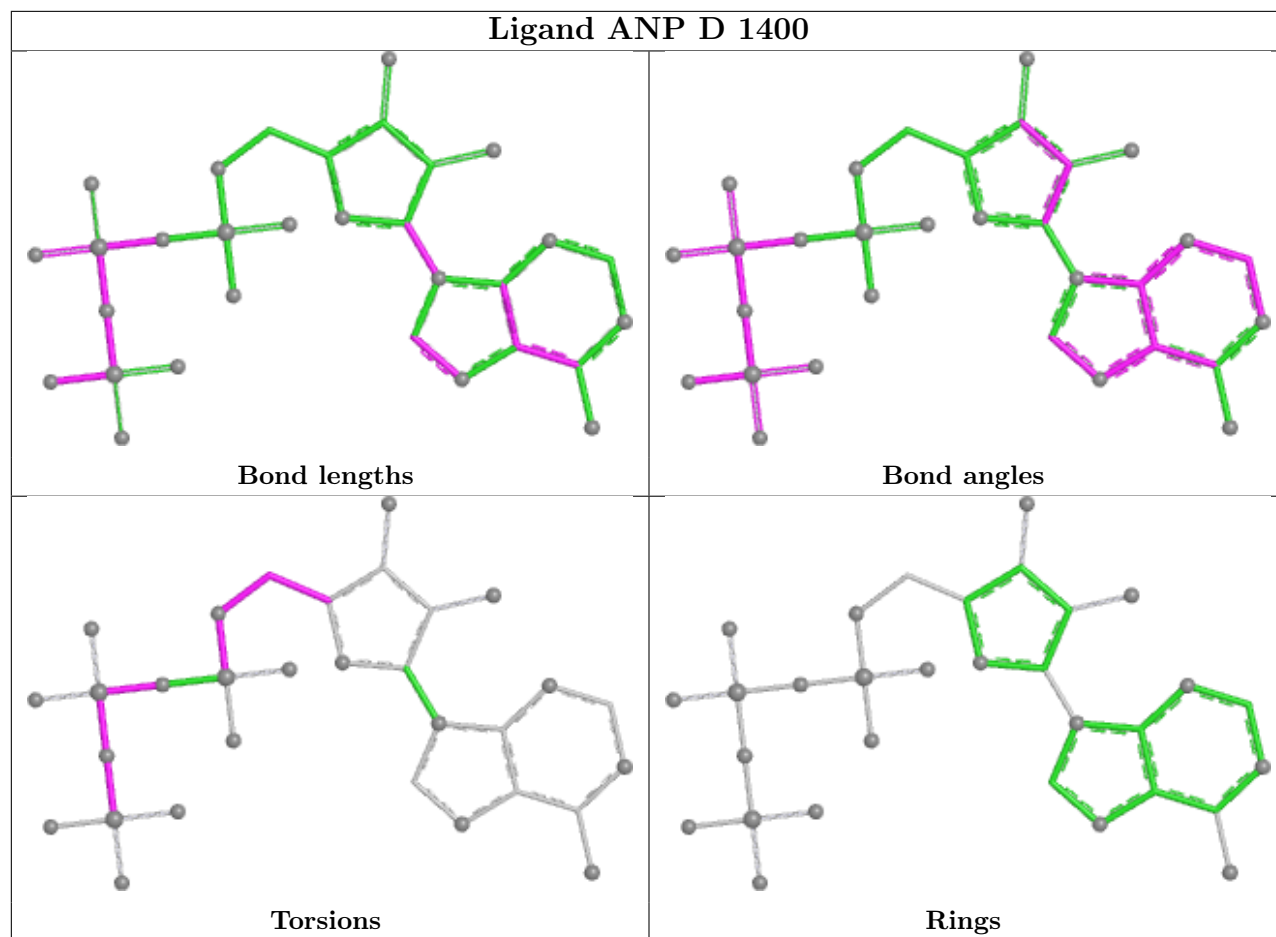
17 monomers are involved in 34 short contacts:

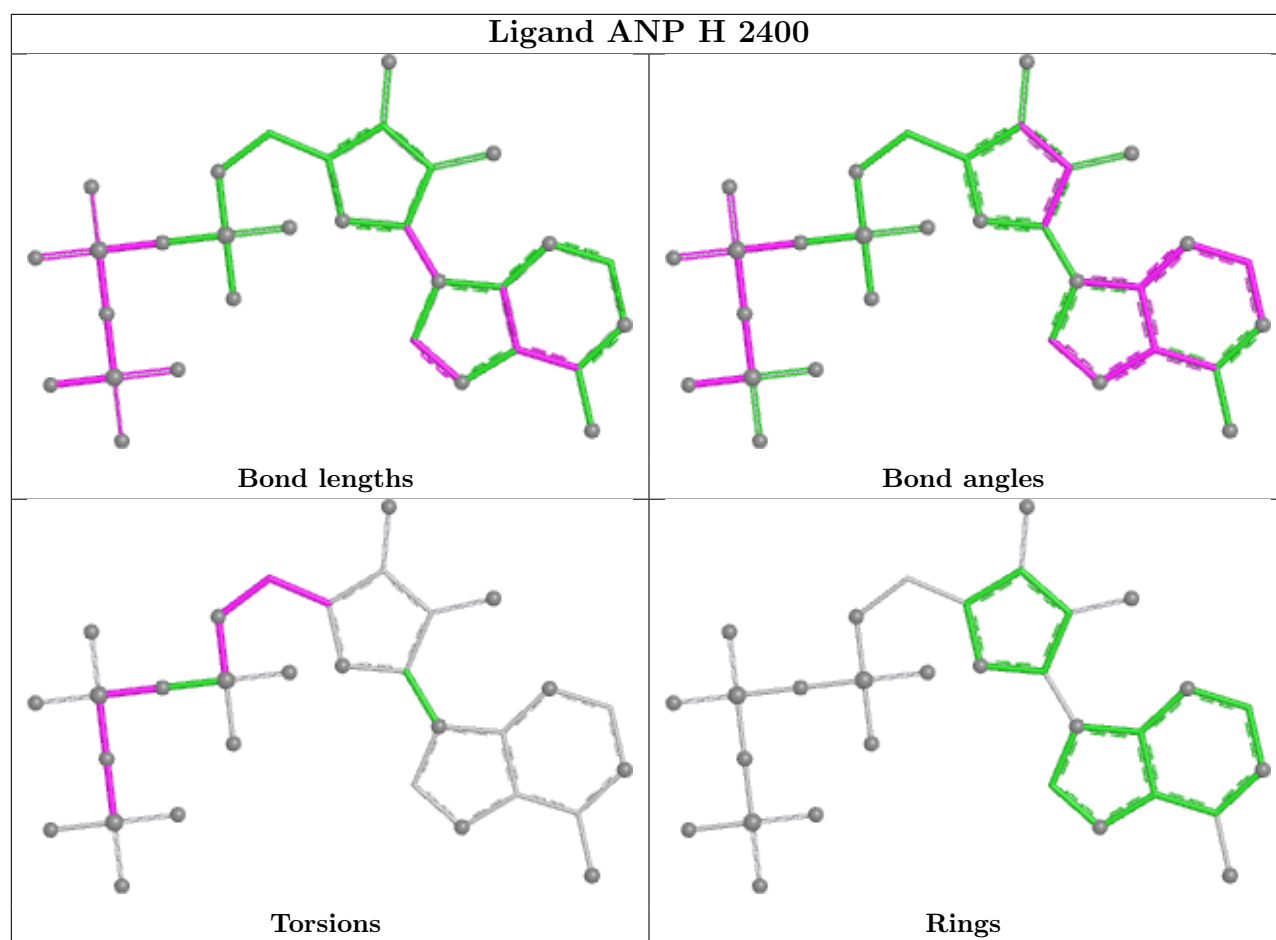
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3400	ANP	2	0
3	B	400	ANP	1	0
3	A	400	ANP	1	0
3	C	400	ANP	1	0
3	F	3400	ANP	3	0
3	A	3400	ANP	3	0
3	G	3400	ANP	2	0
3	H	400	ANP	1	0
3	H	3400	ANP	3	0
3	B	3400	ANP	1	0
3	E	400	ANP	1	0
3	D	3400	ANP	2	0
3	E	1400	ANP	1	0
3	E	3400	ANP	1	0
3	G	400	ANP	2	0
3	A	1400	ANP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

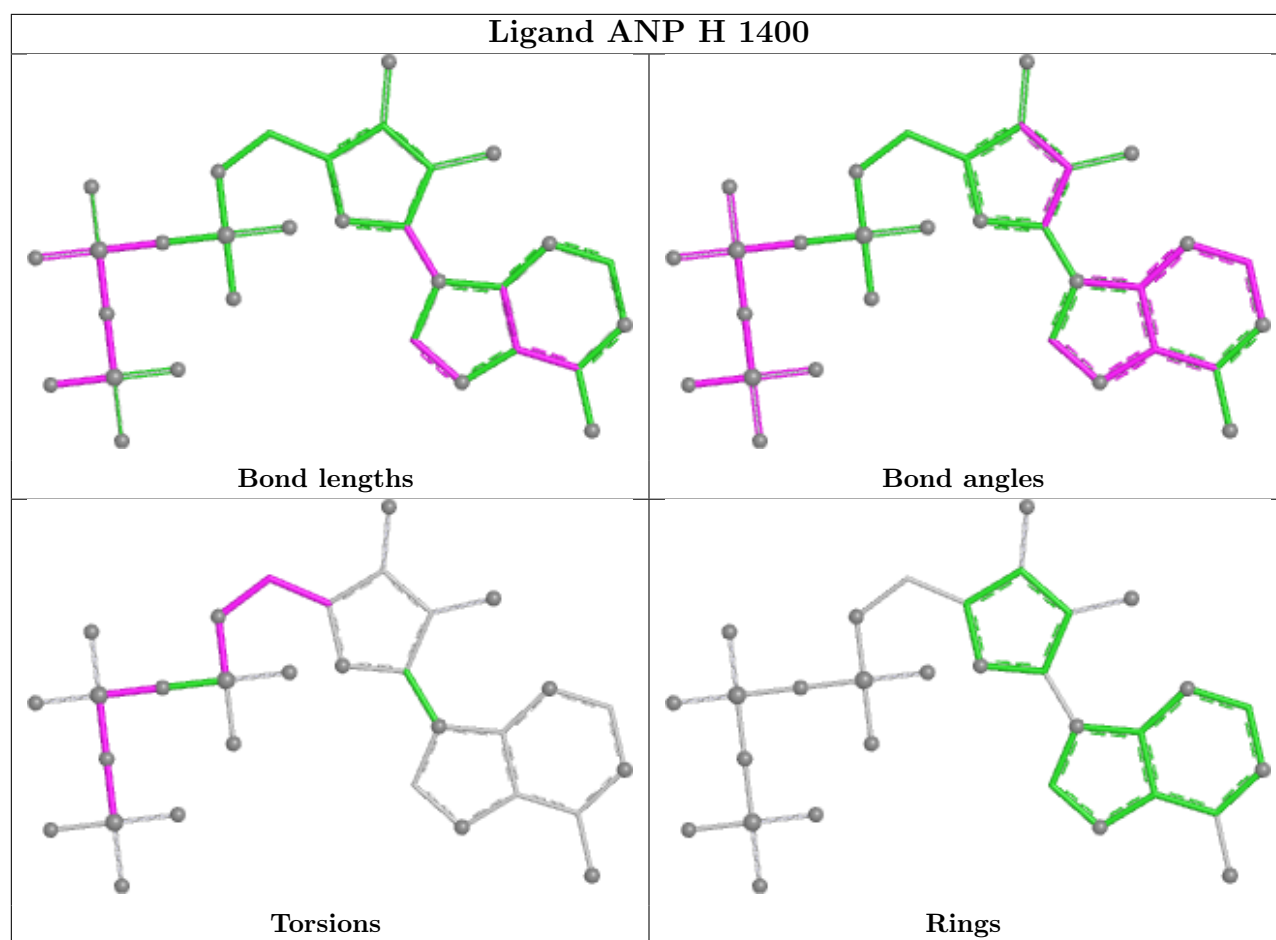
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

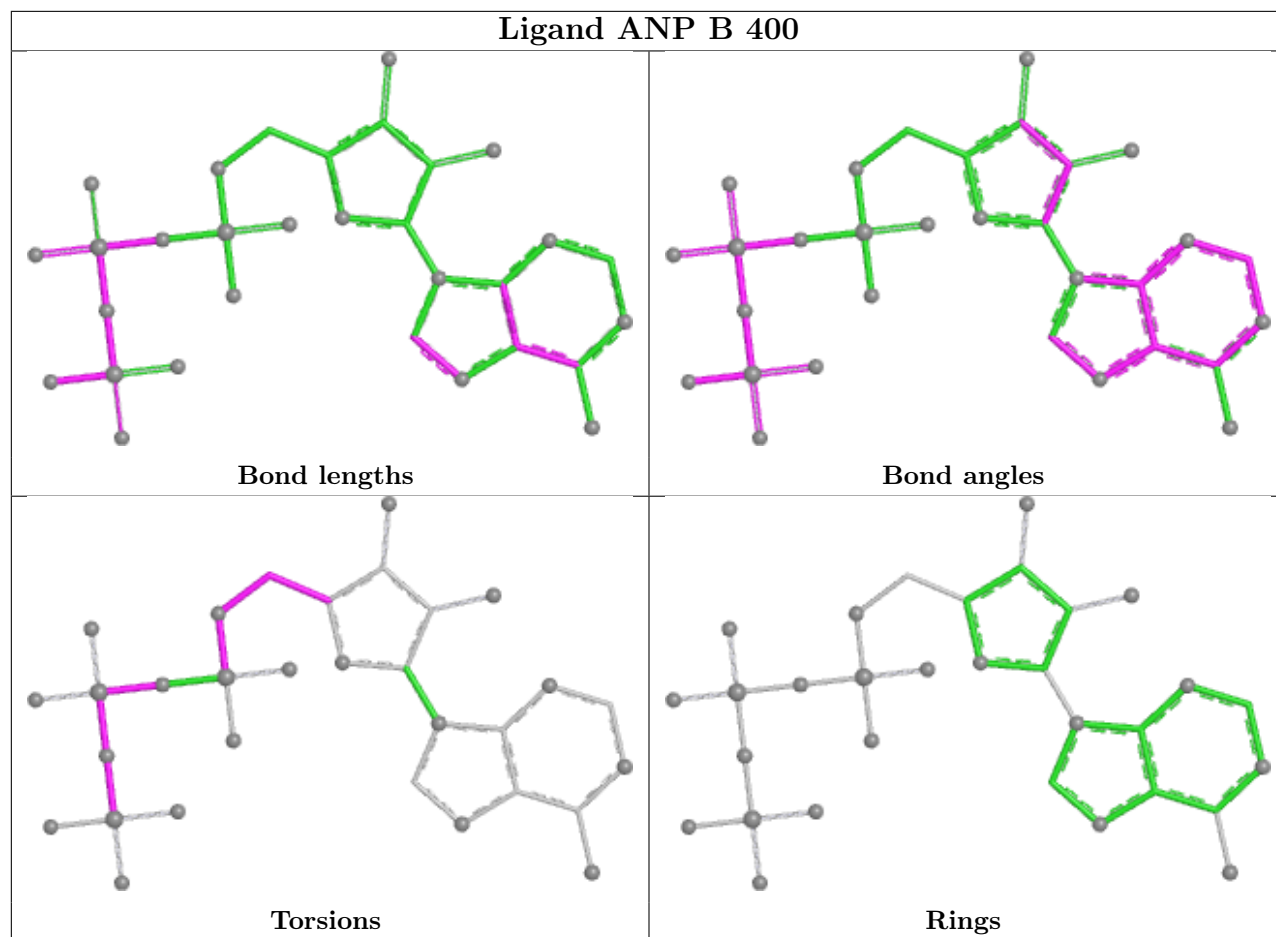


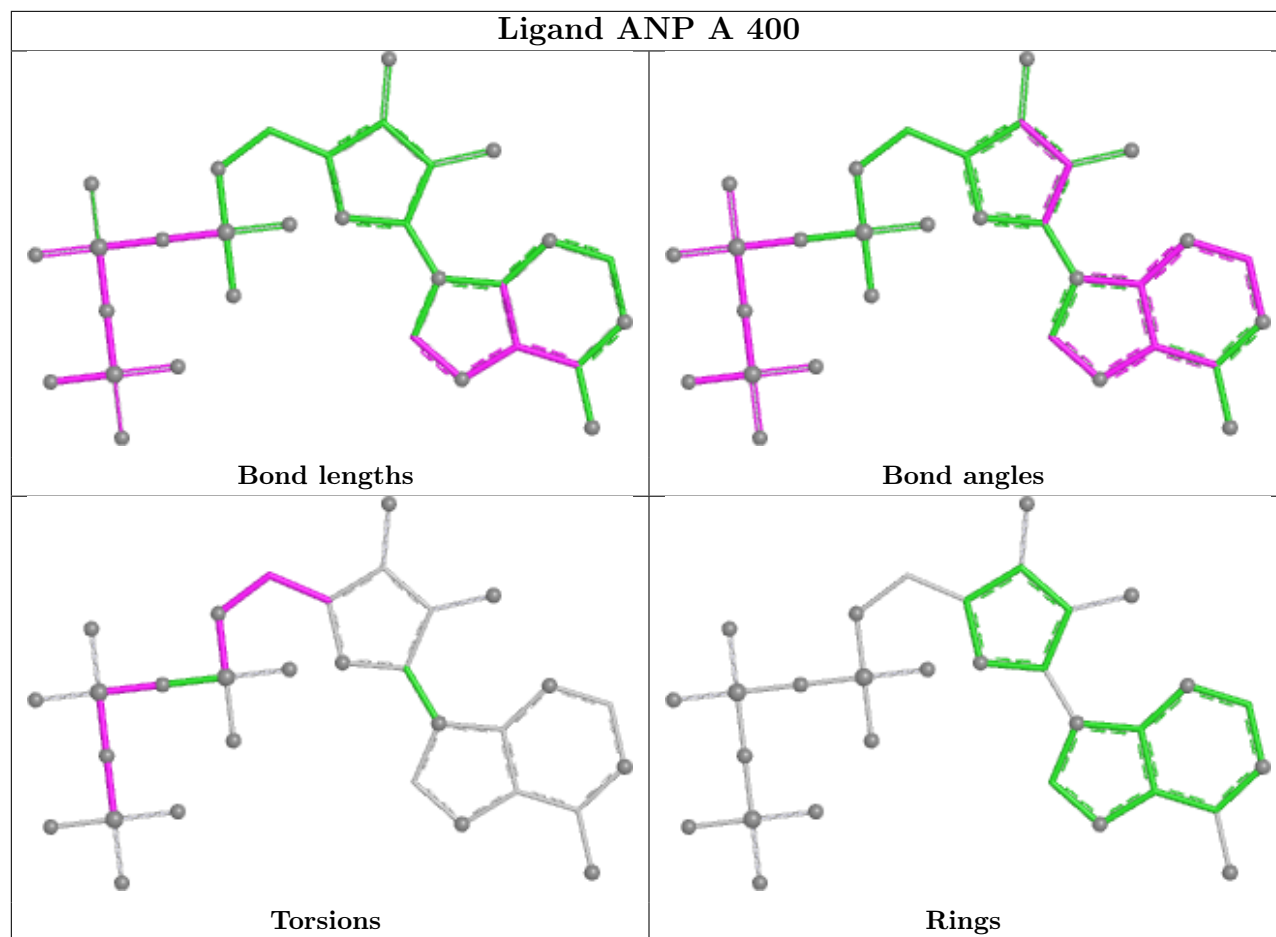


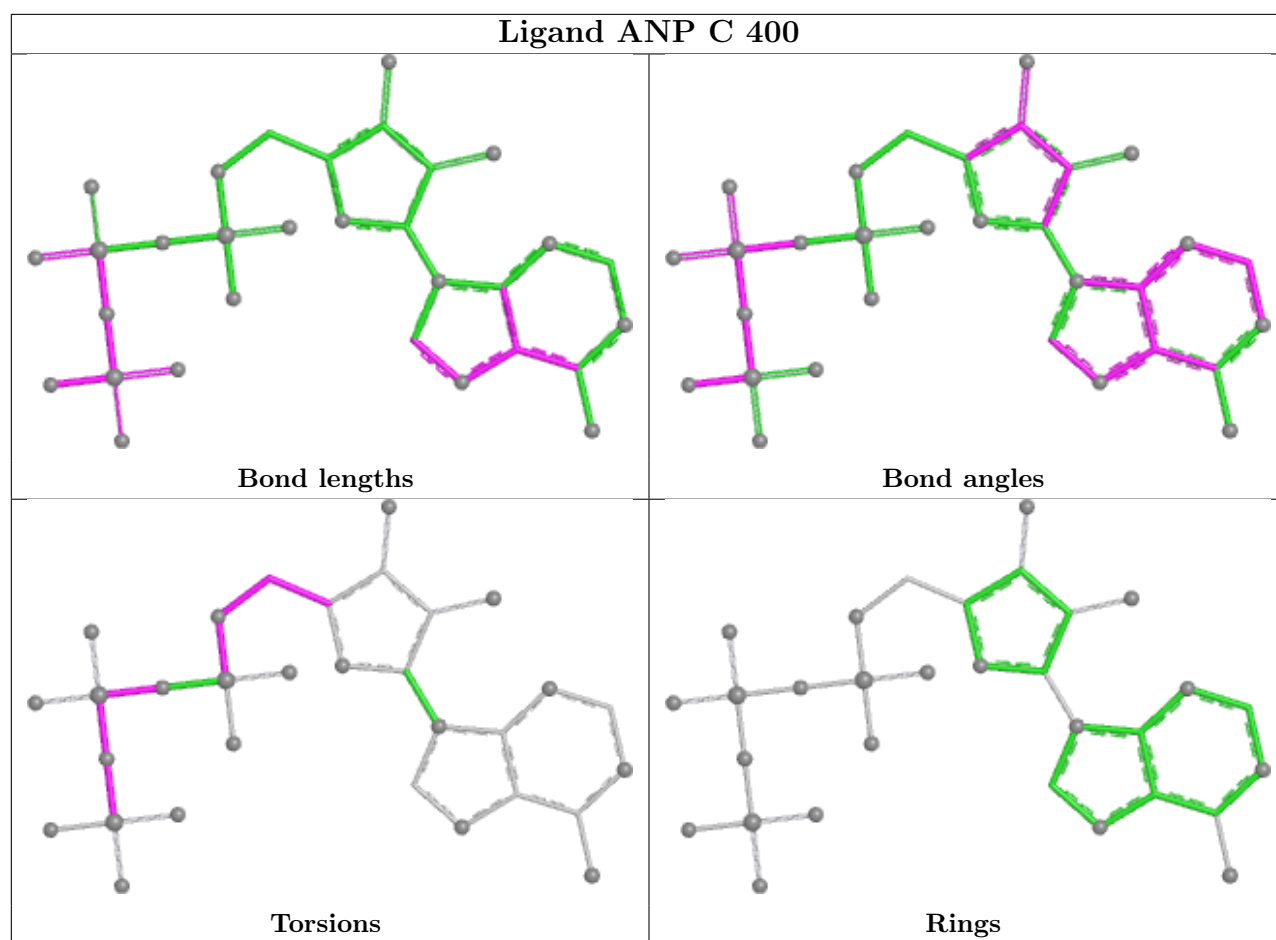


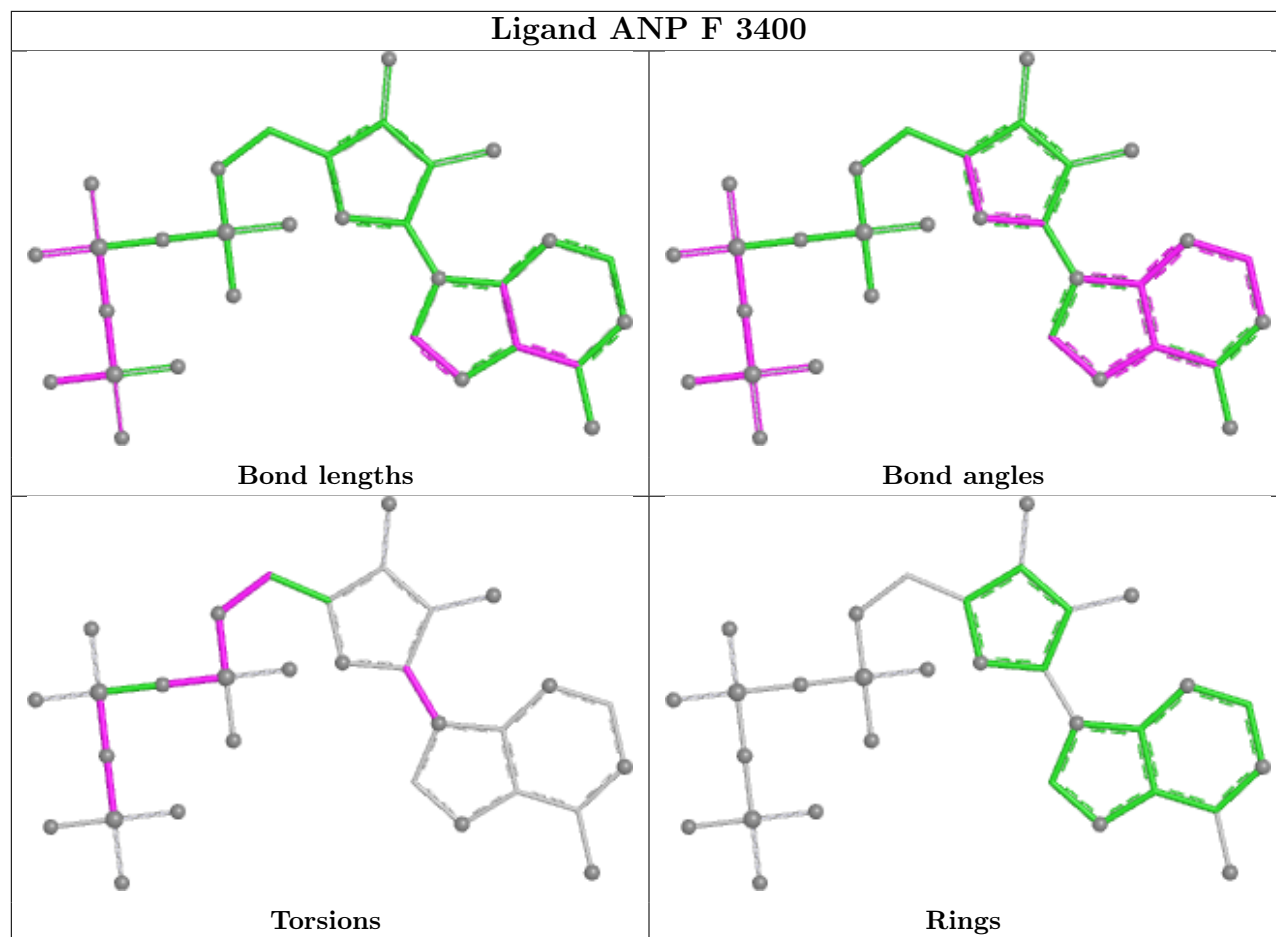


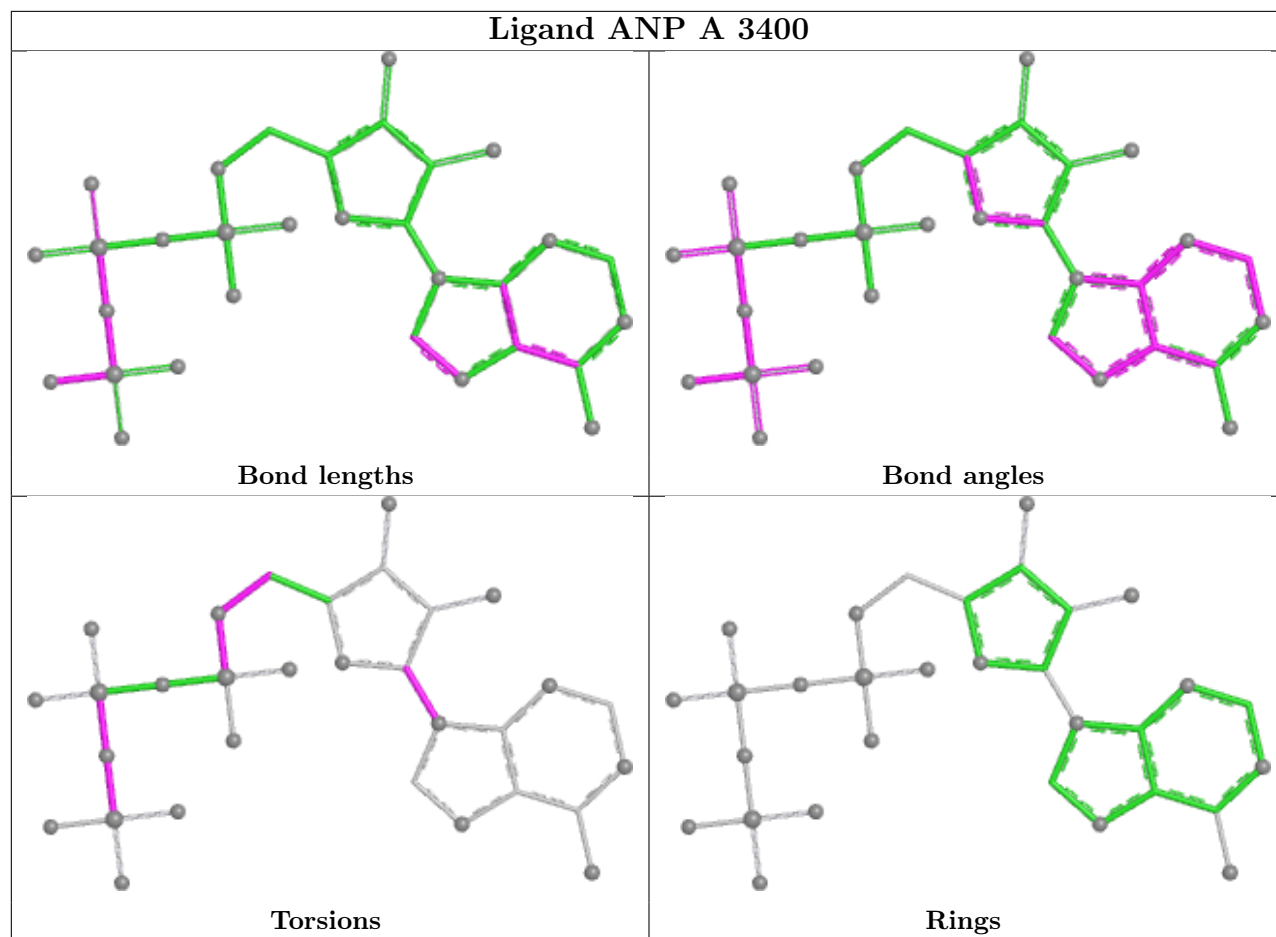


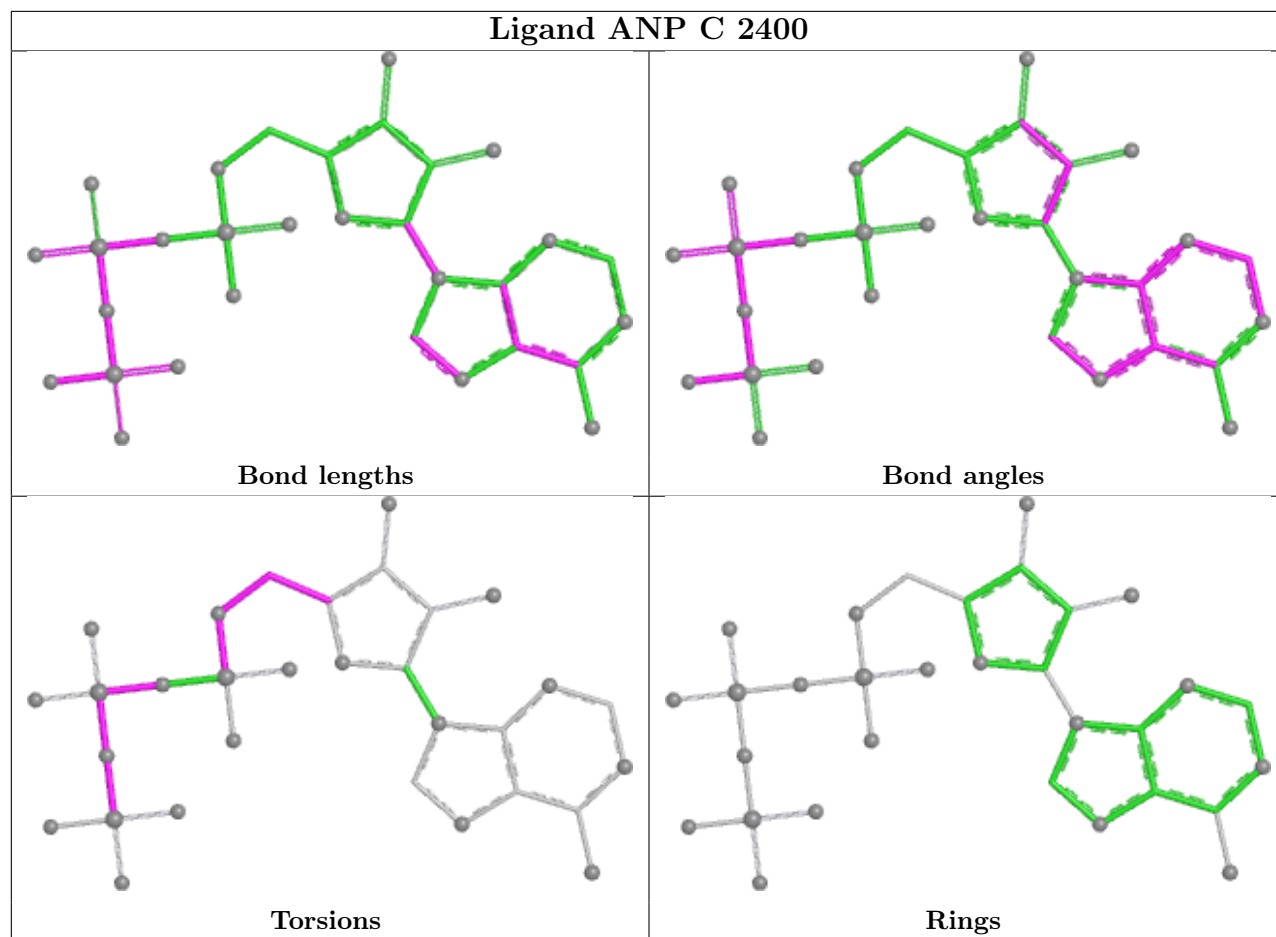


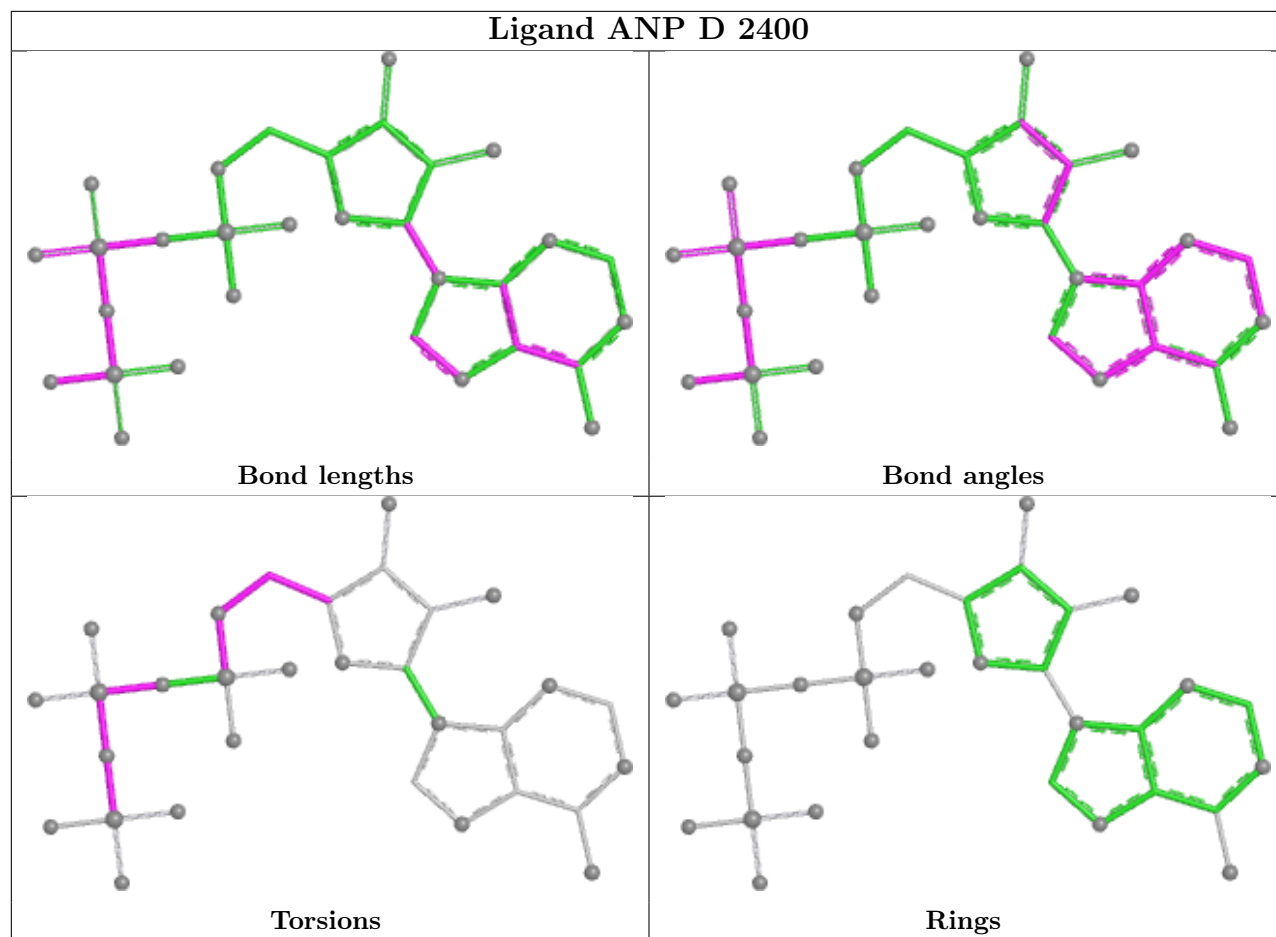




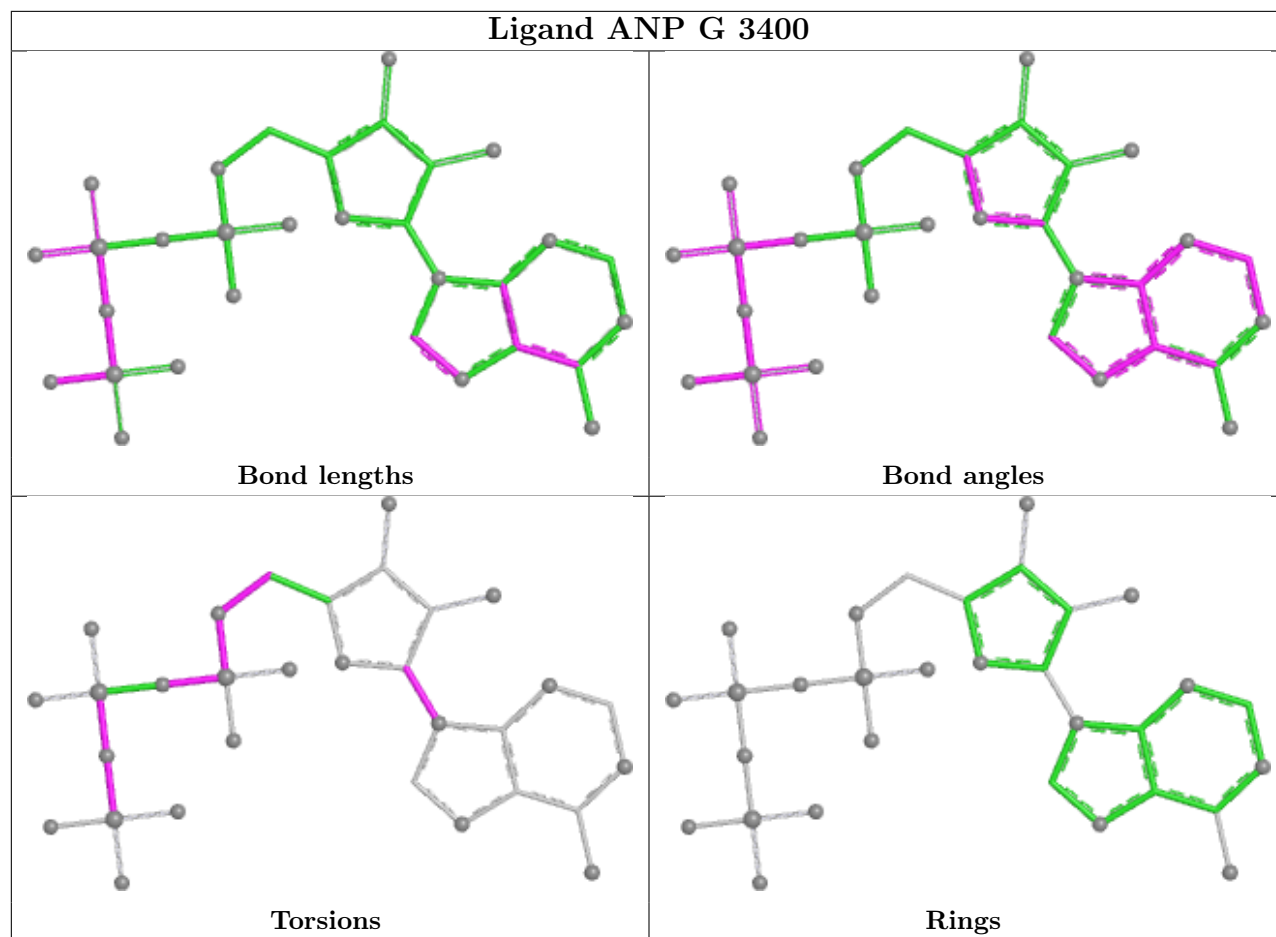


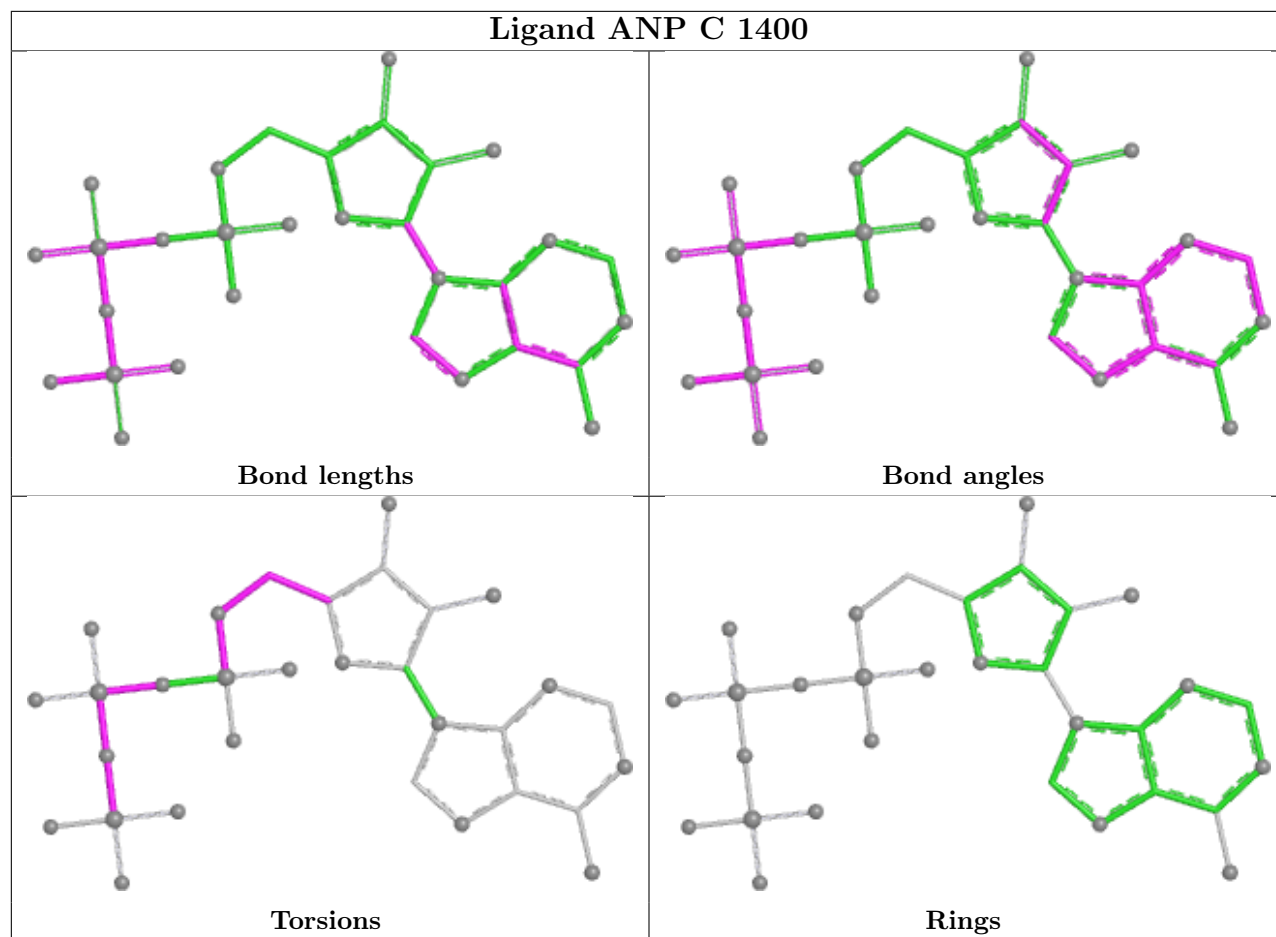


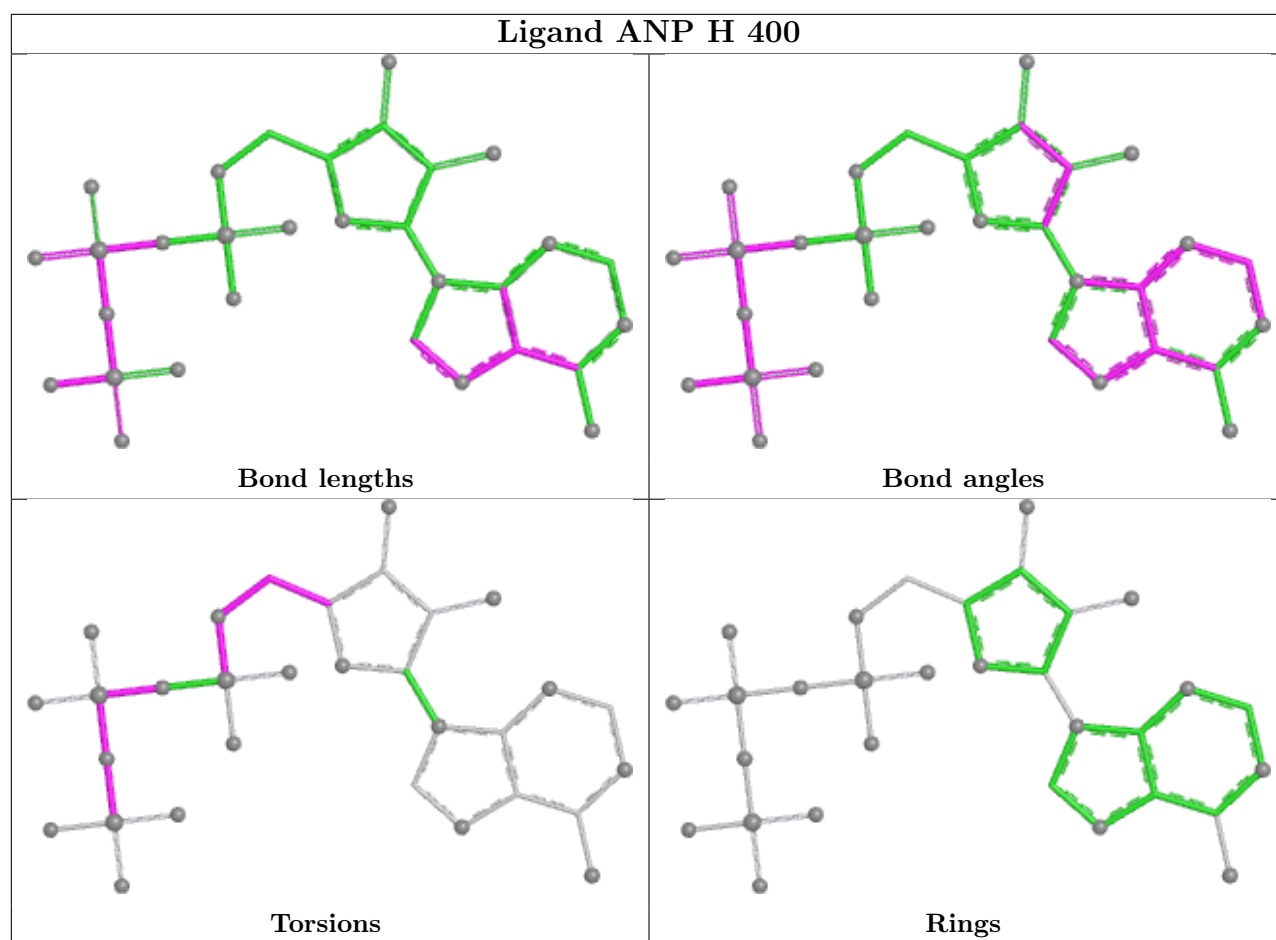


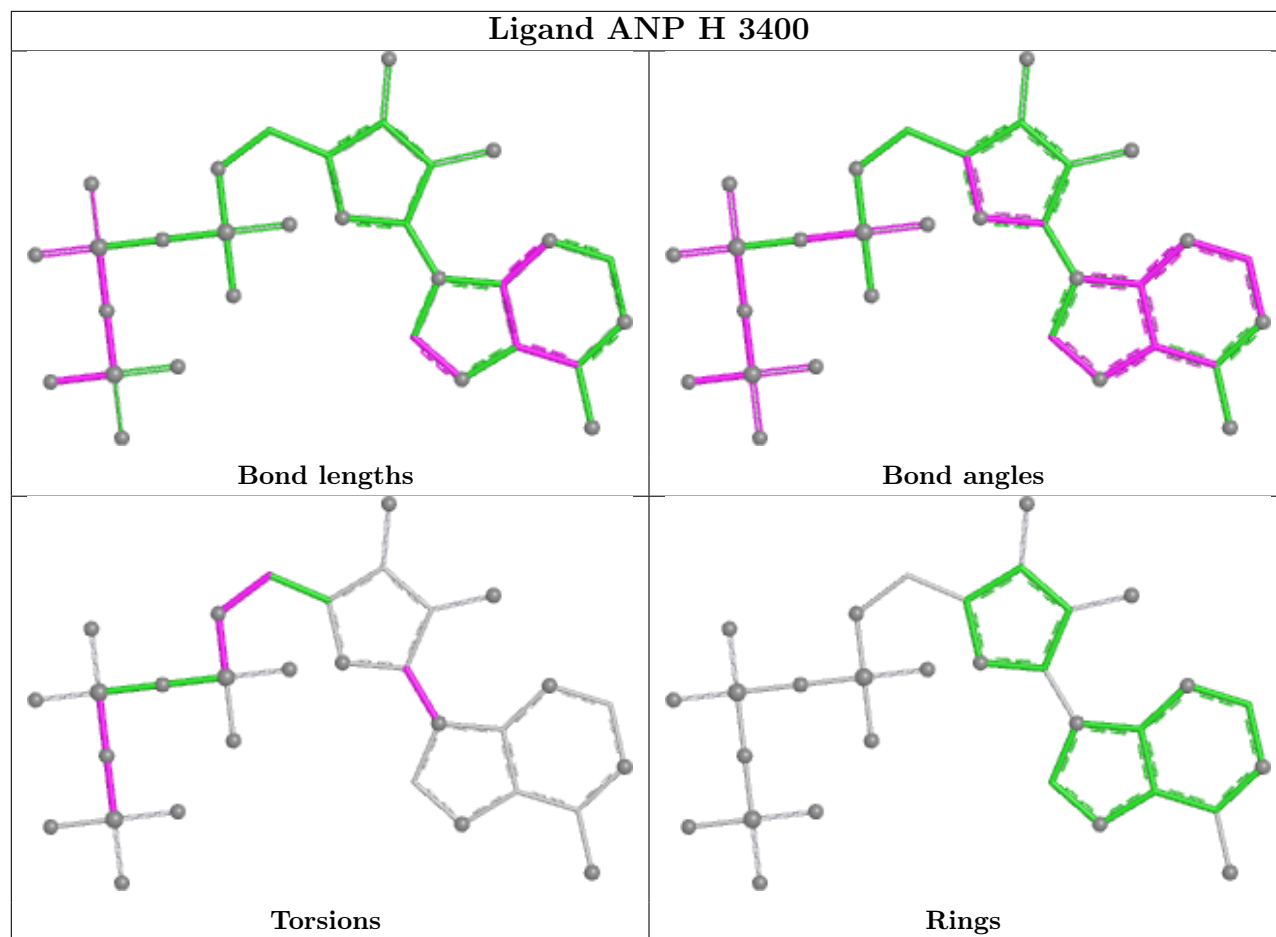


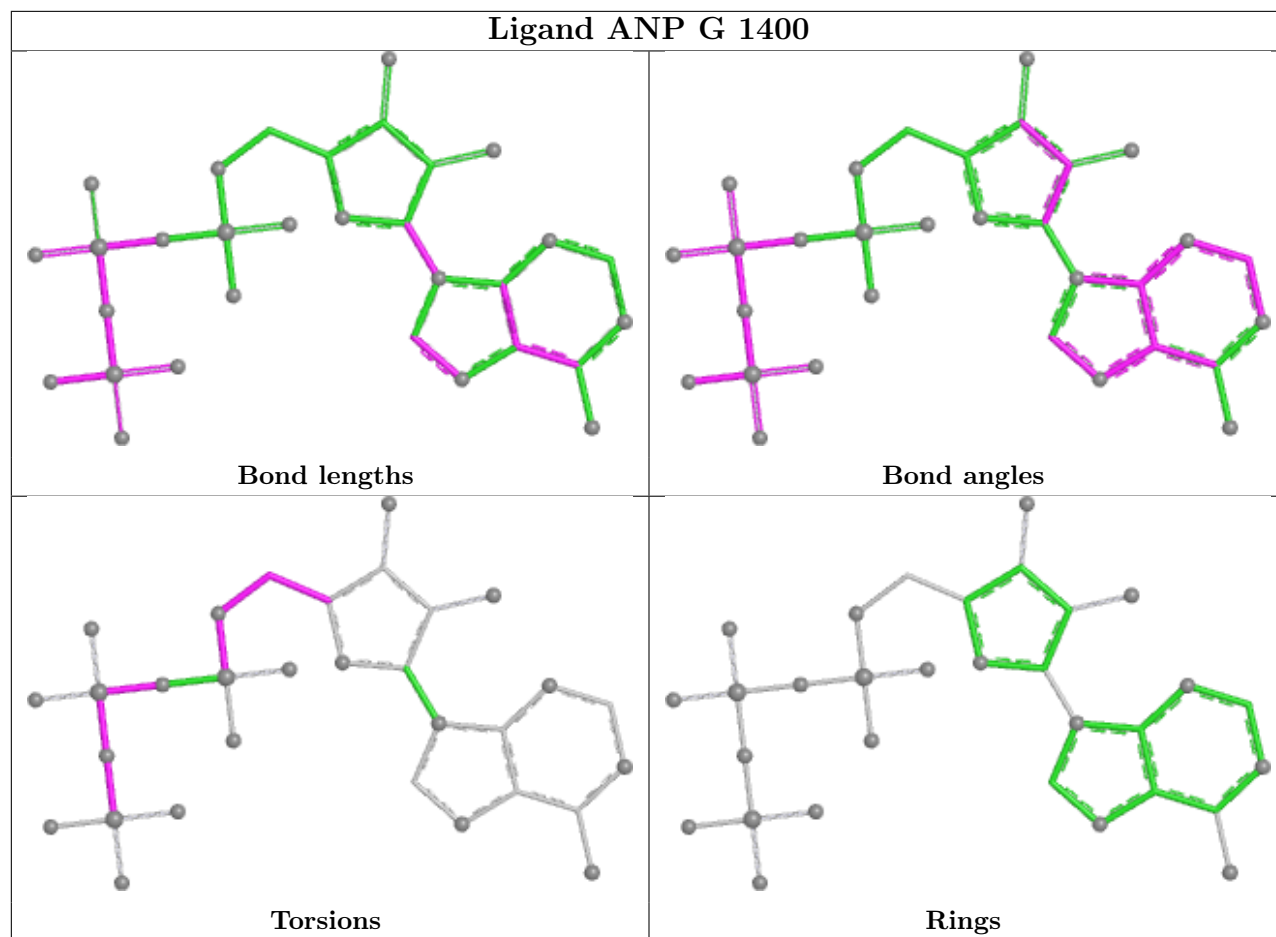
Ligand ANP G 3400

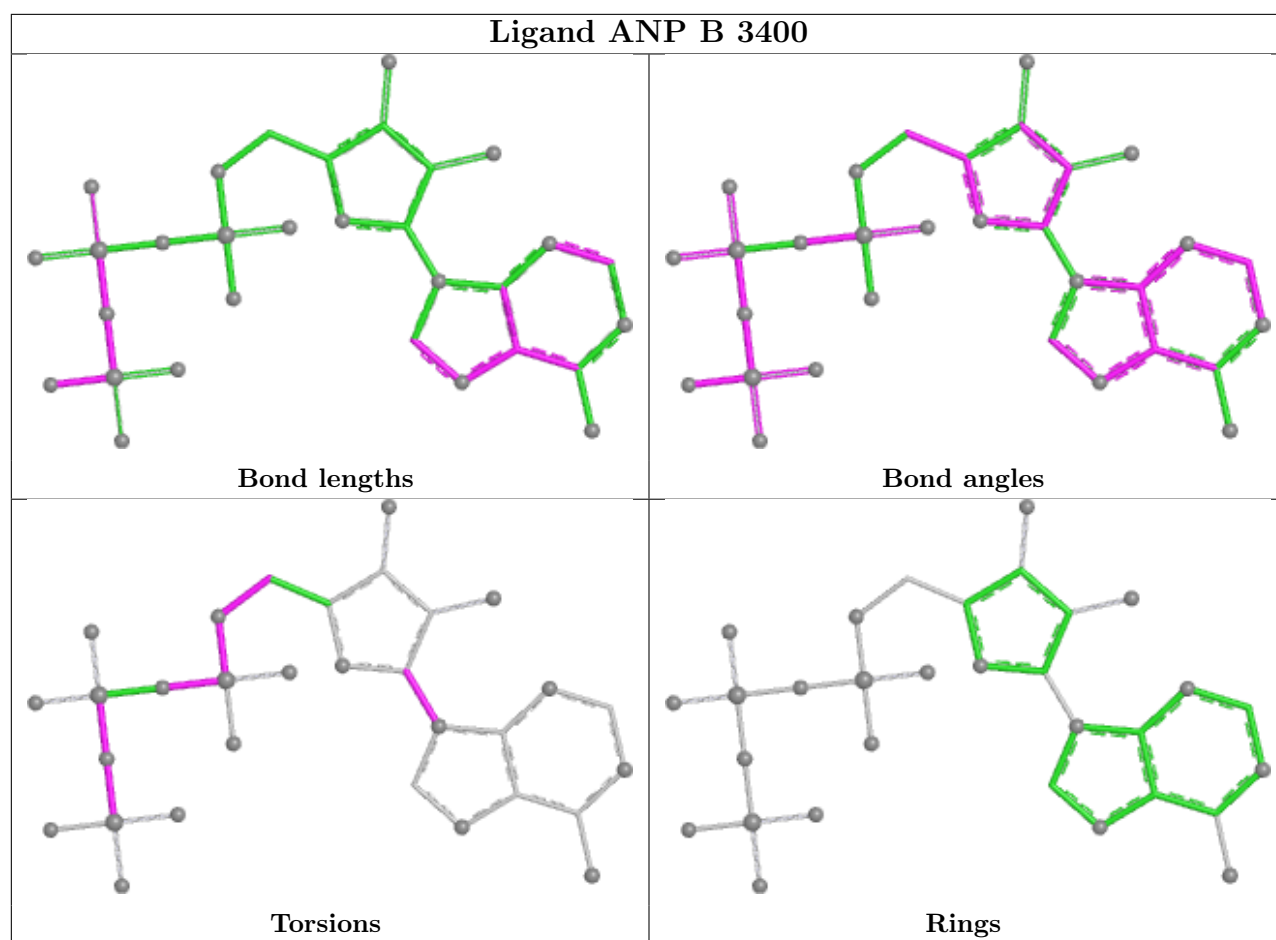


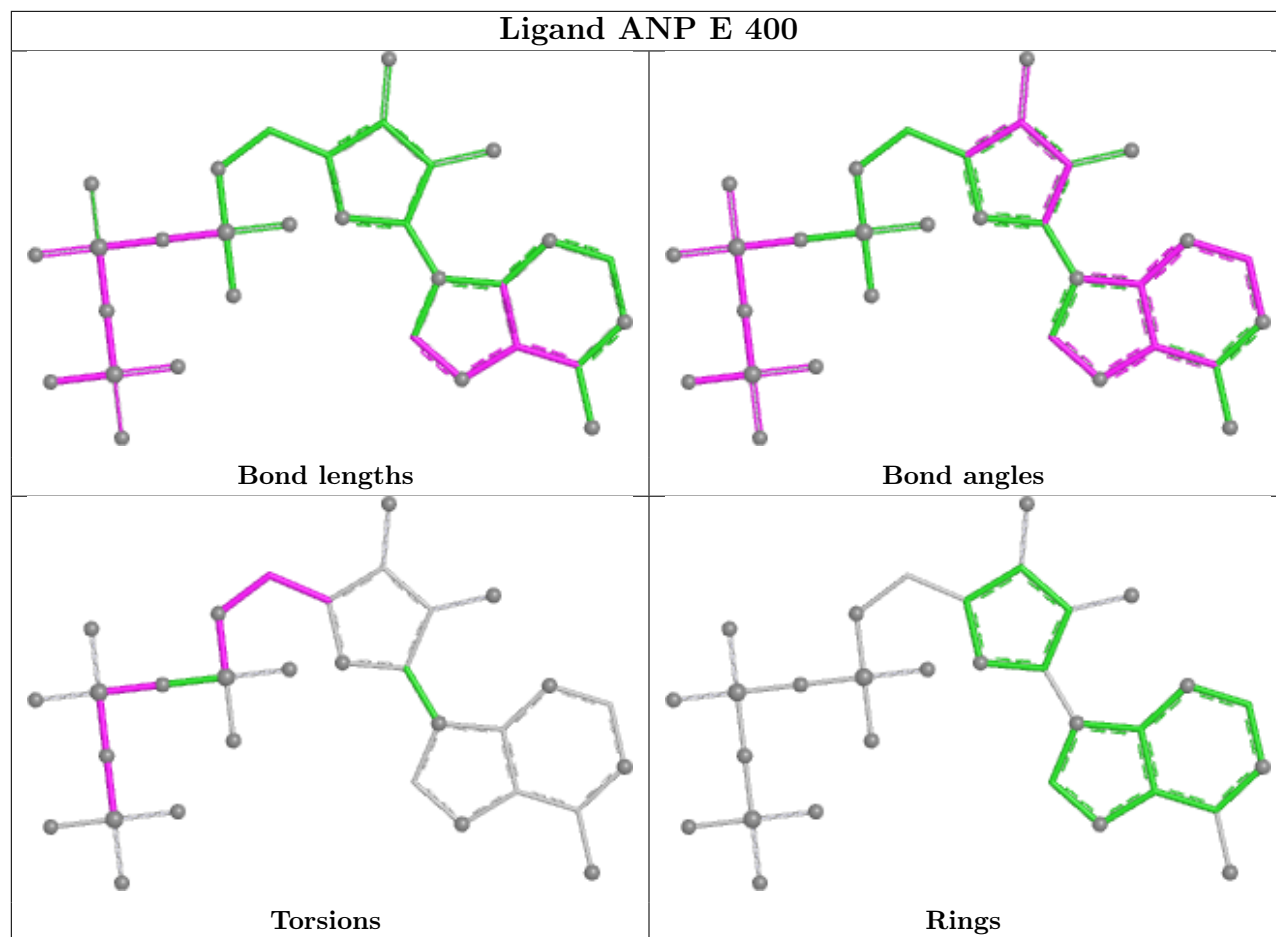


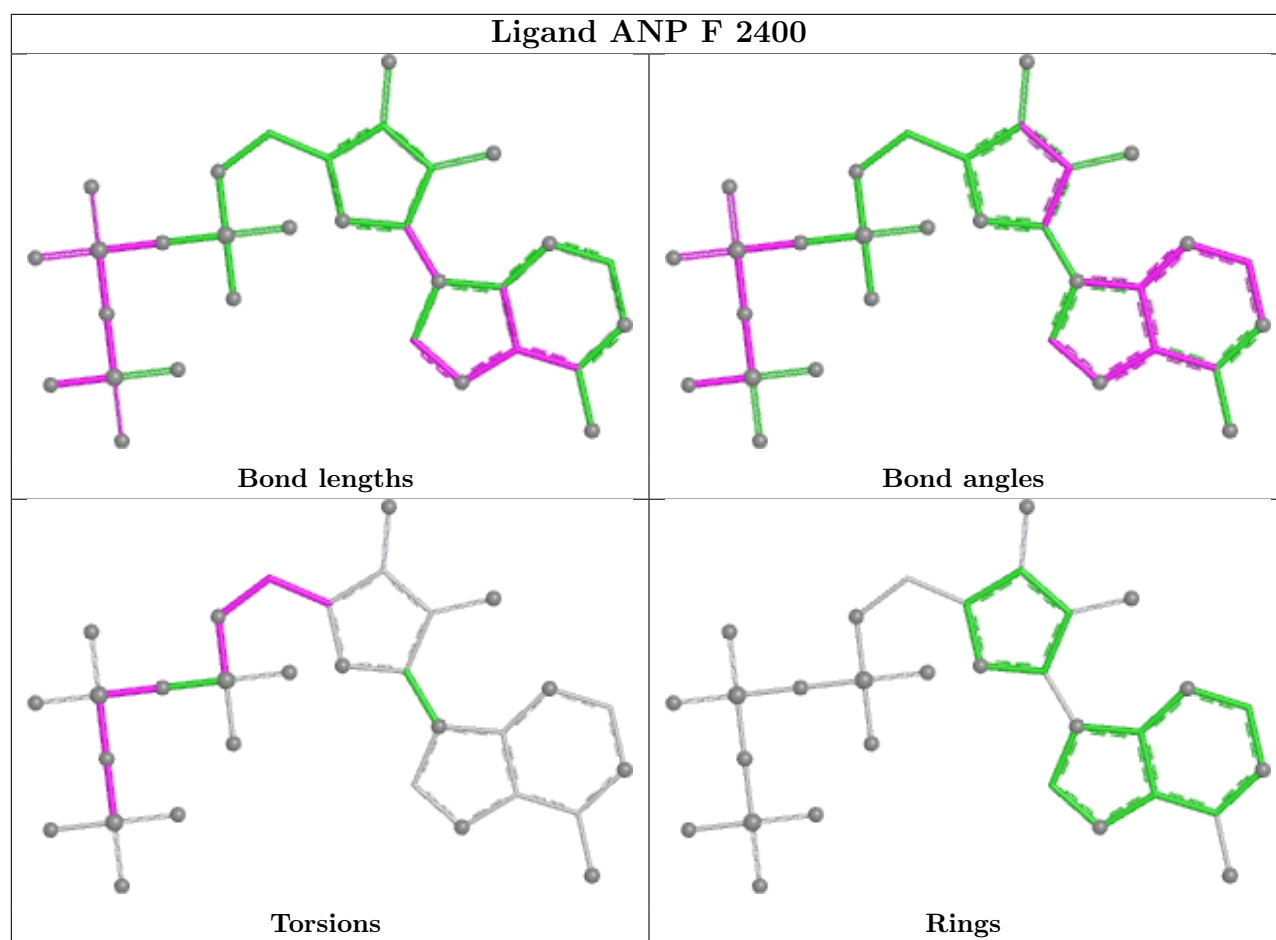


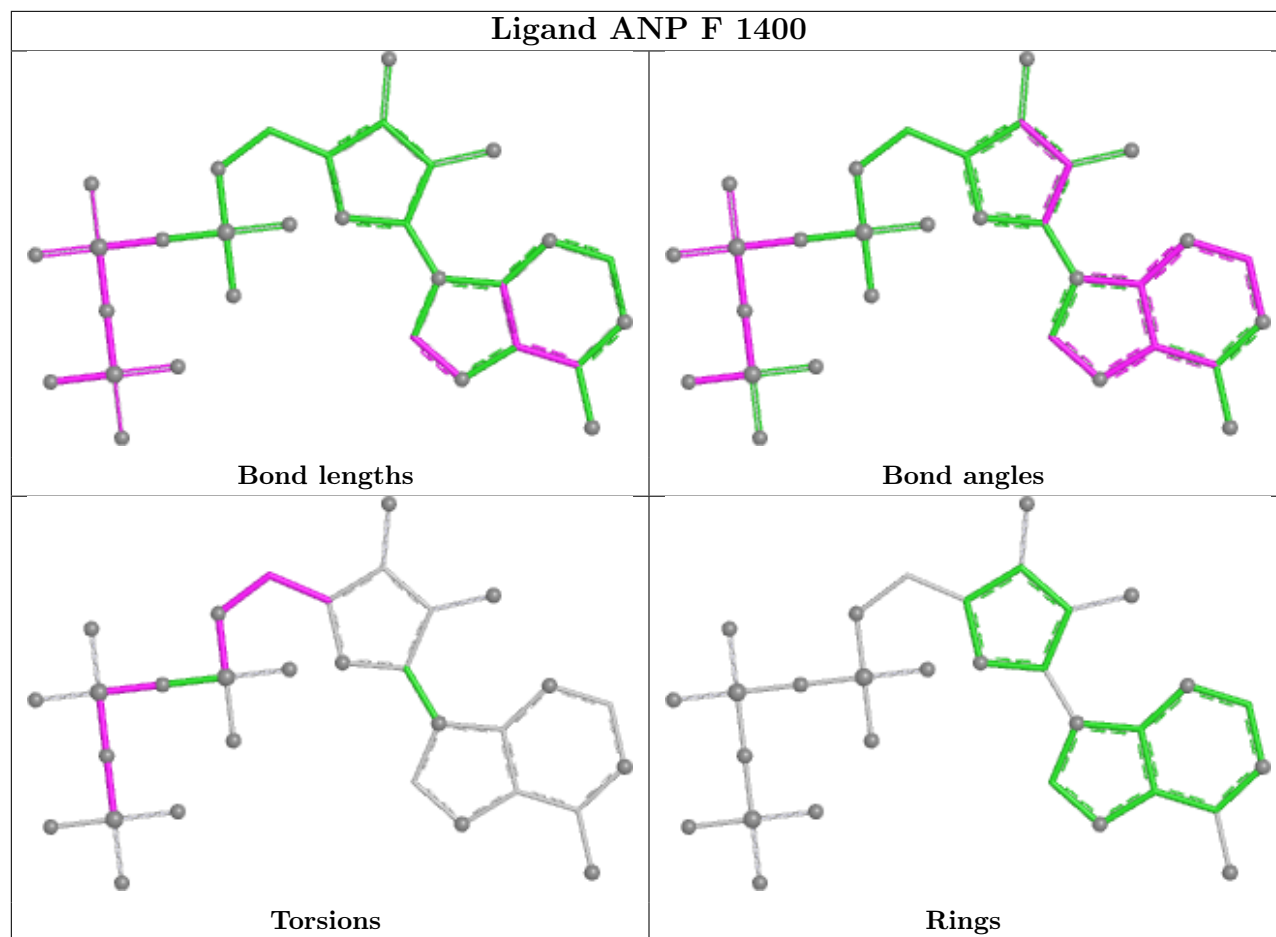


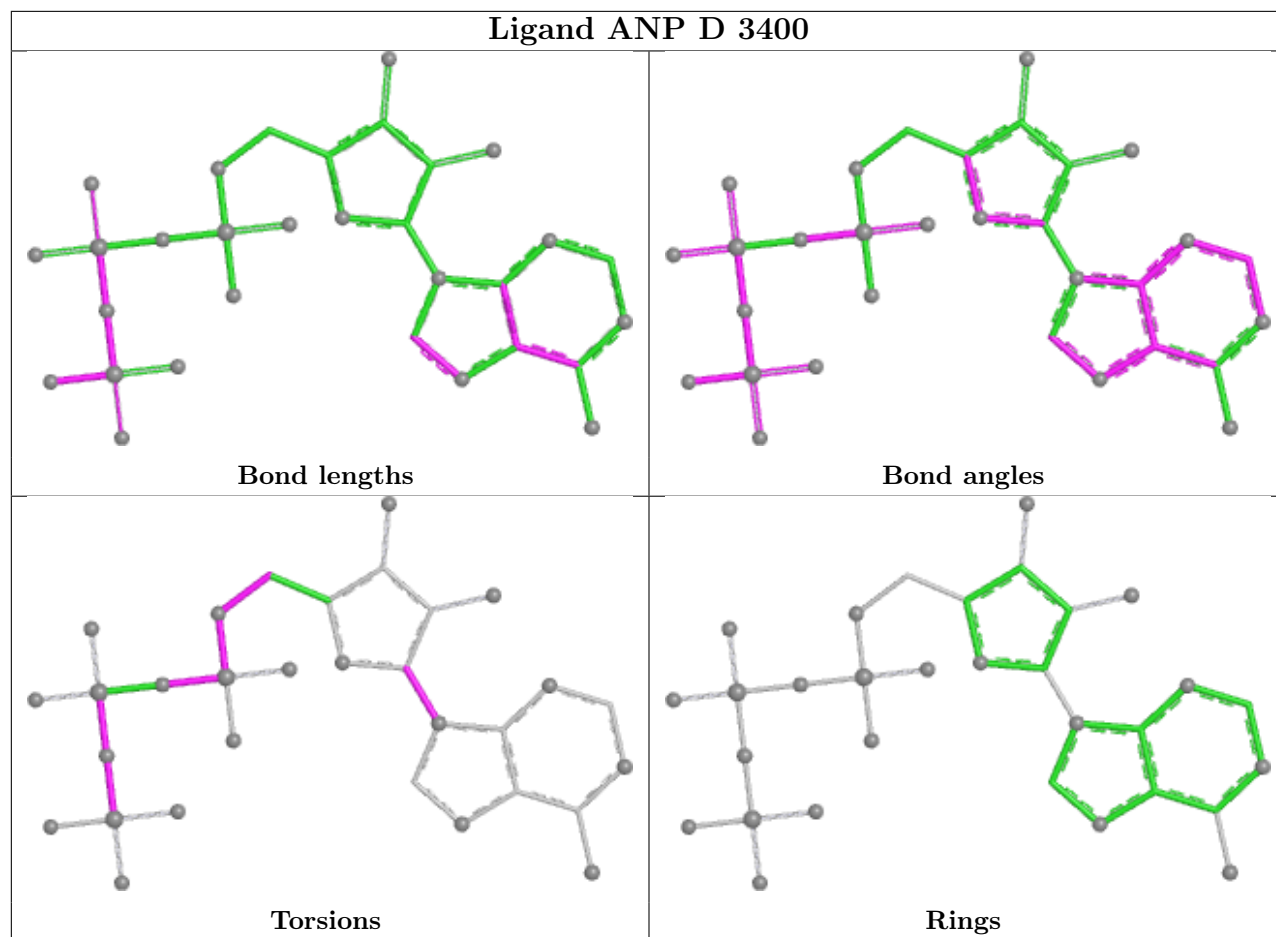


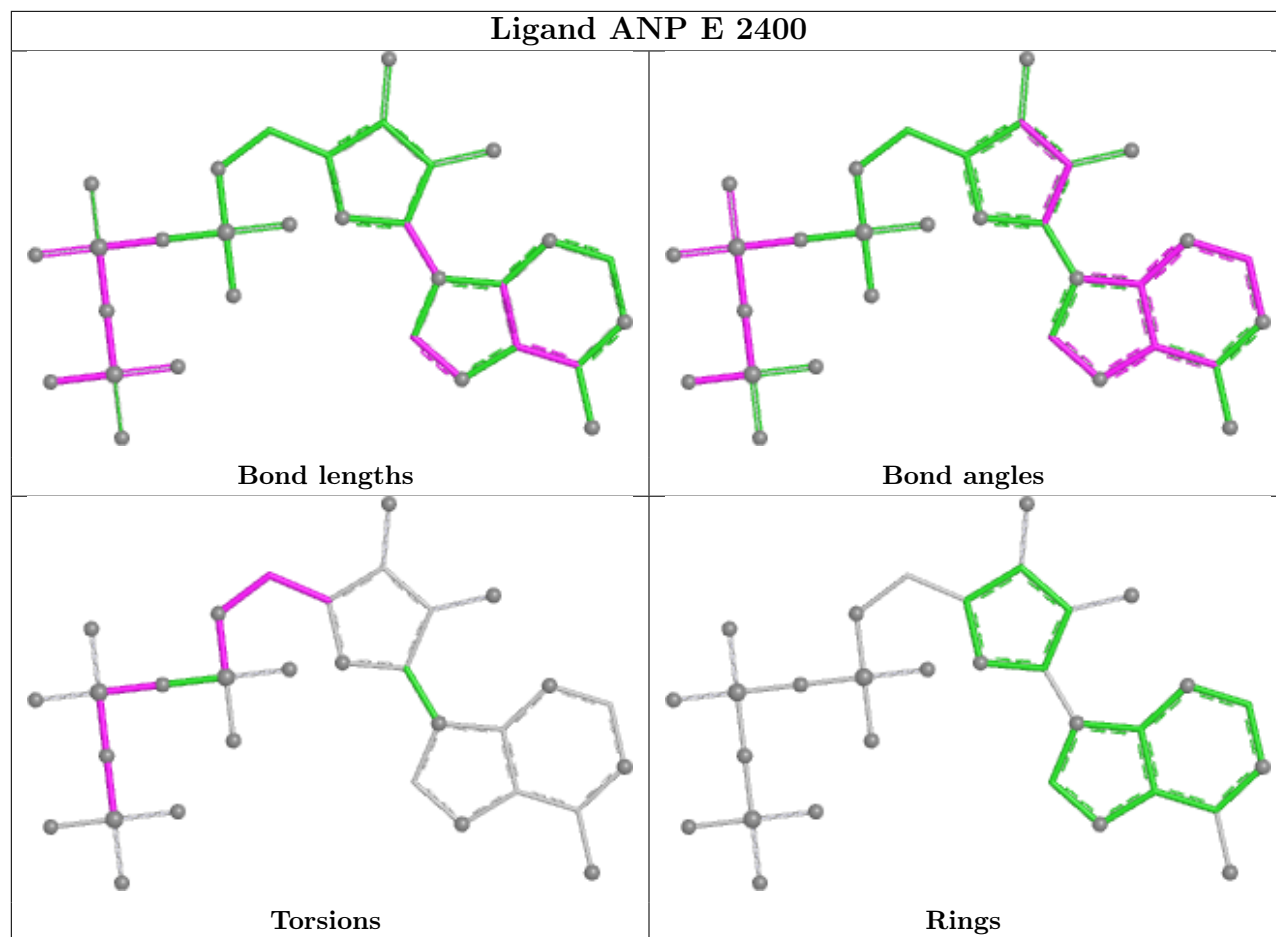


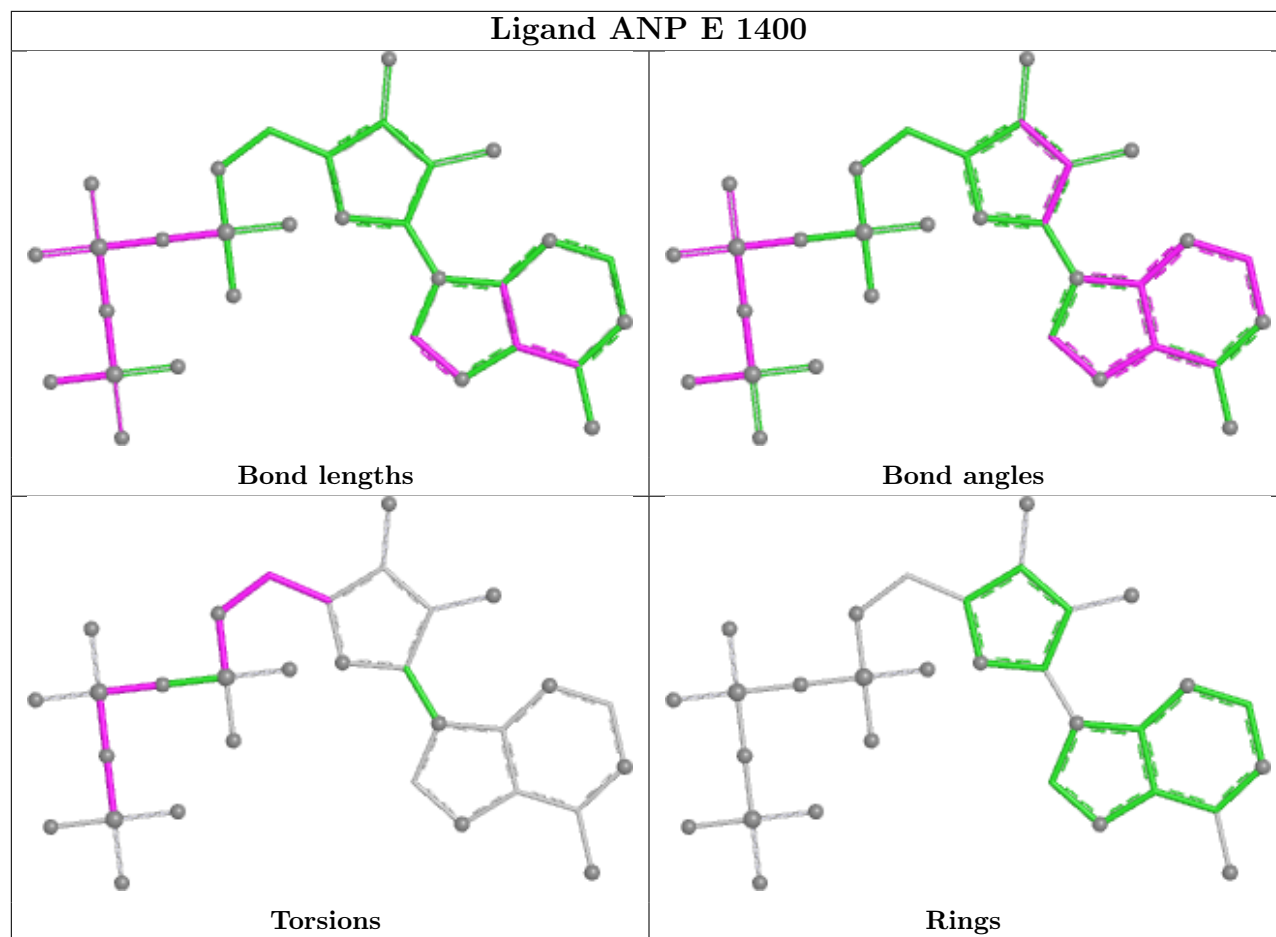


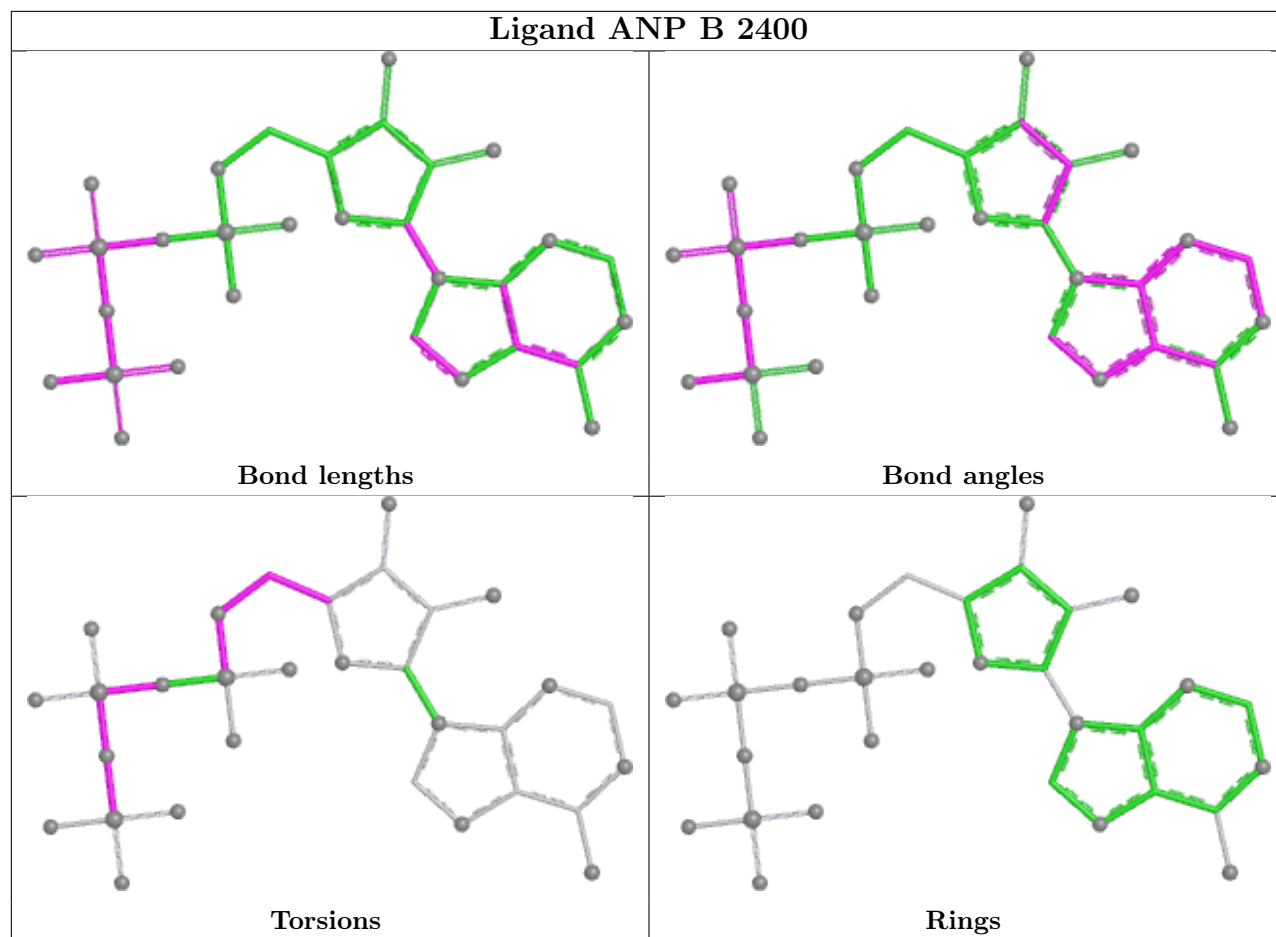


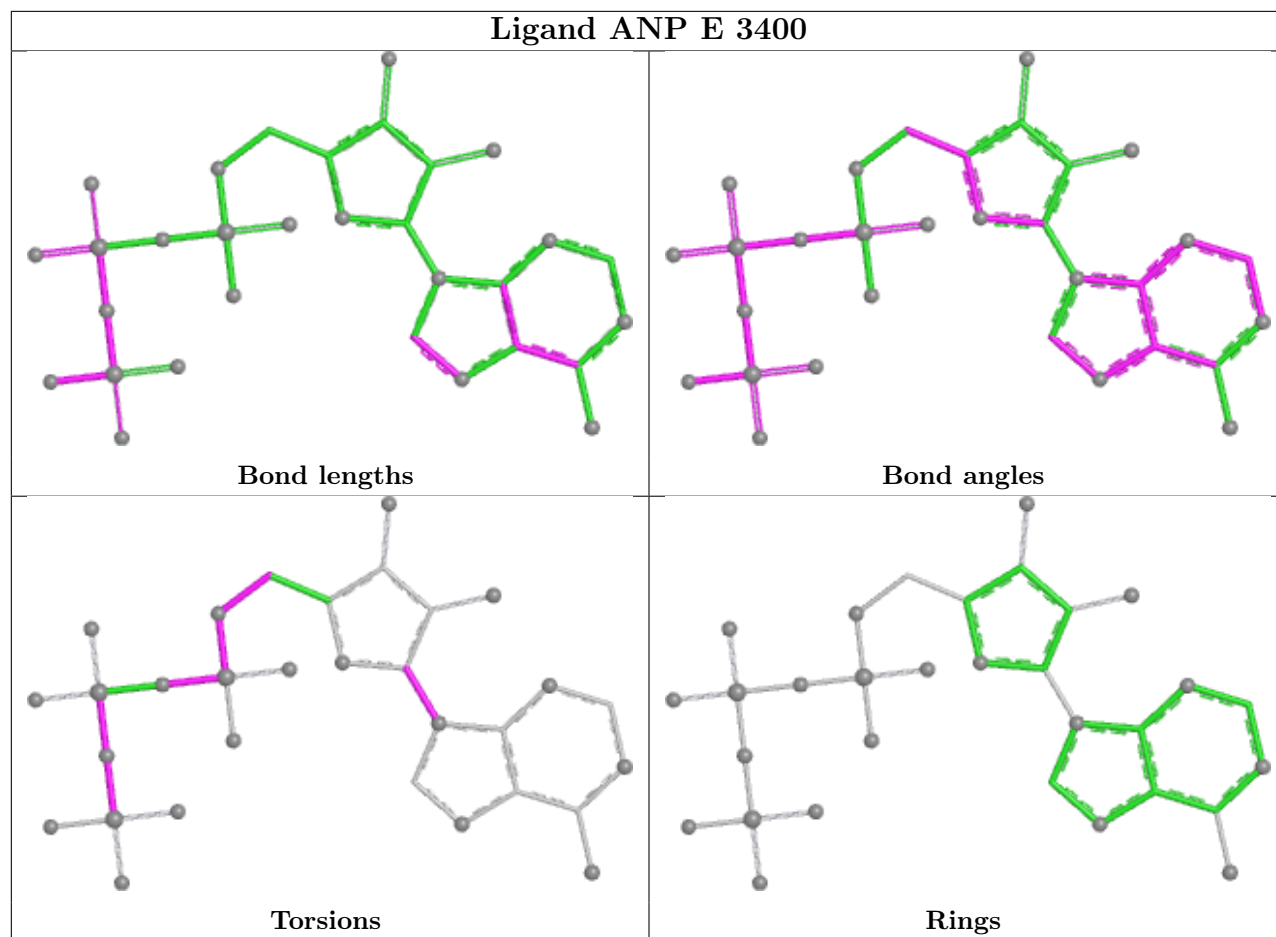


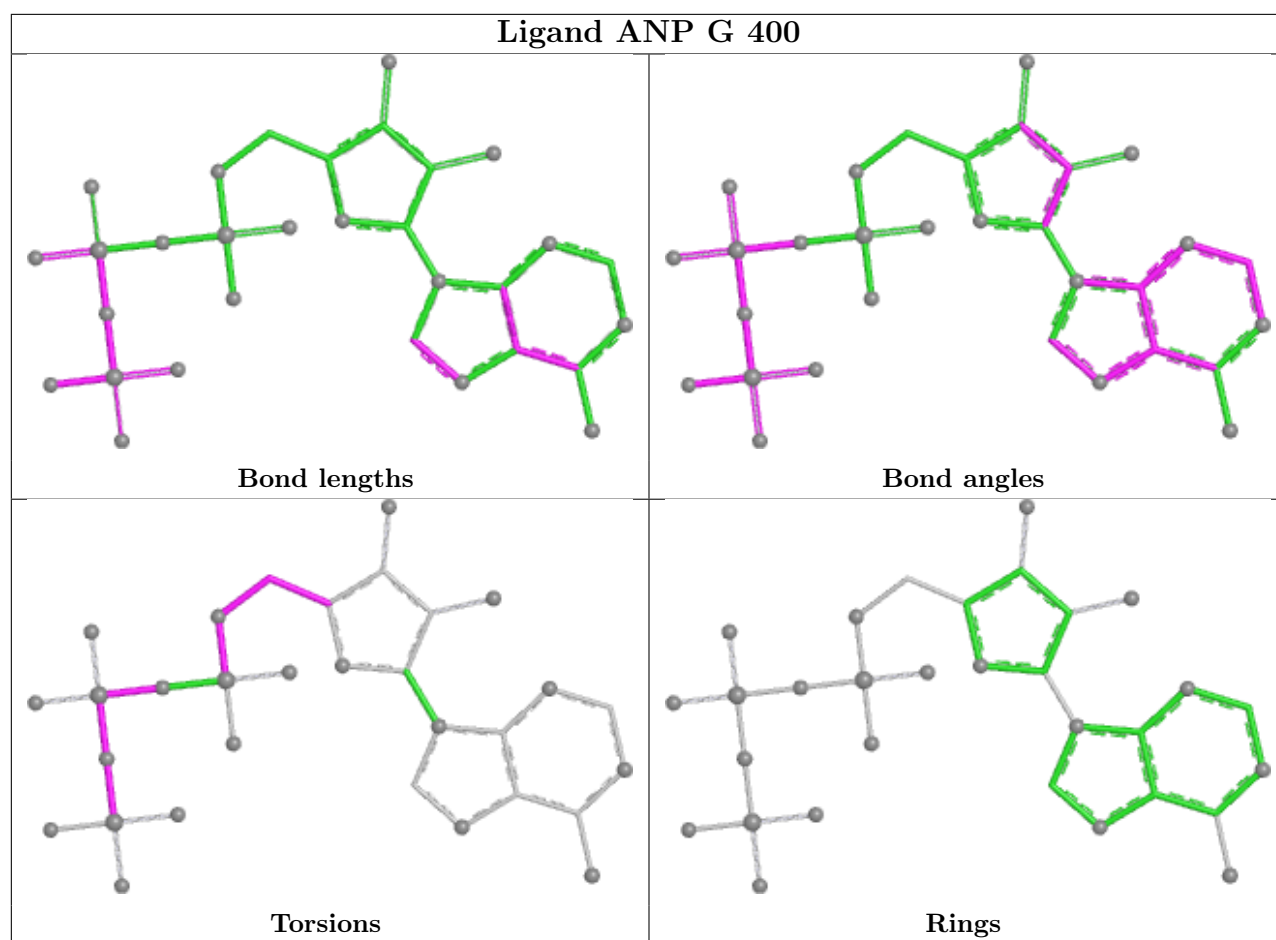


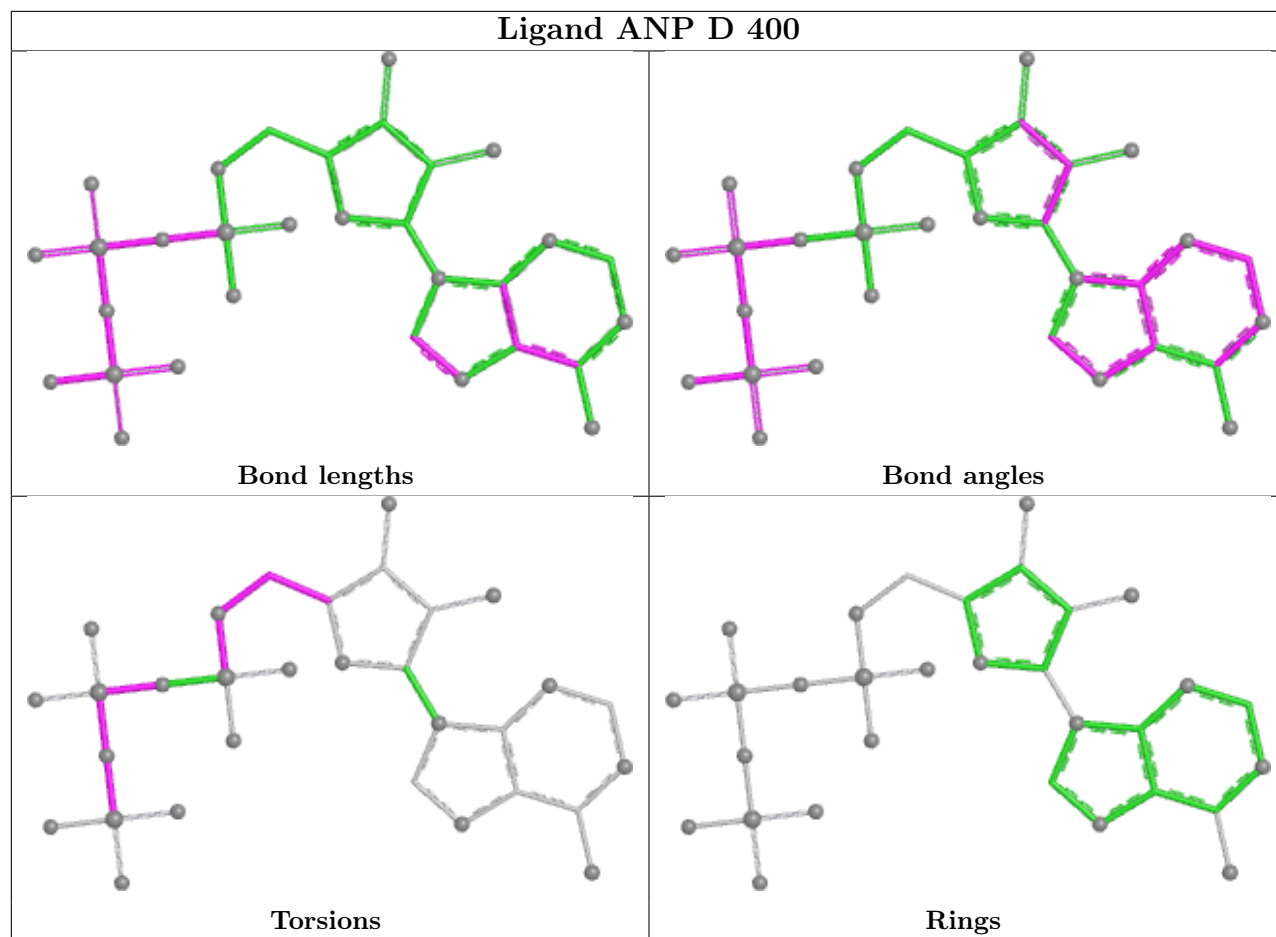


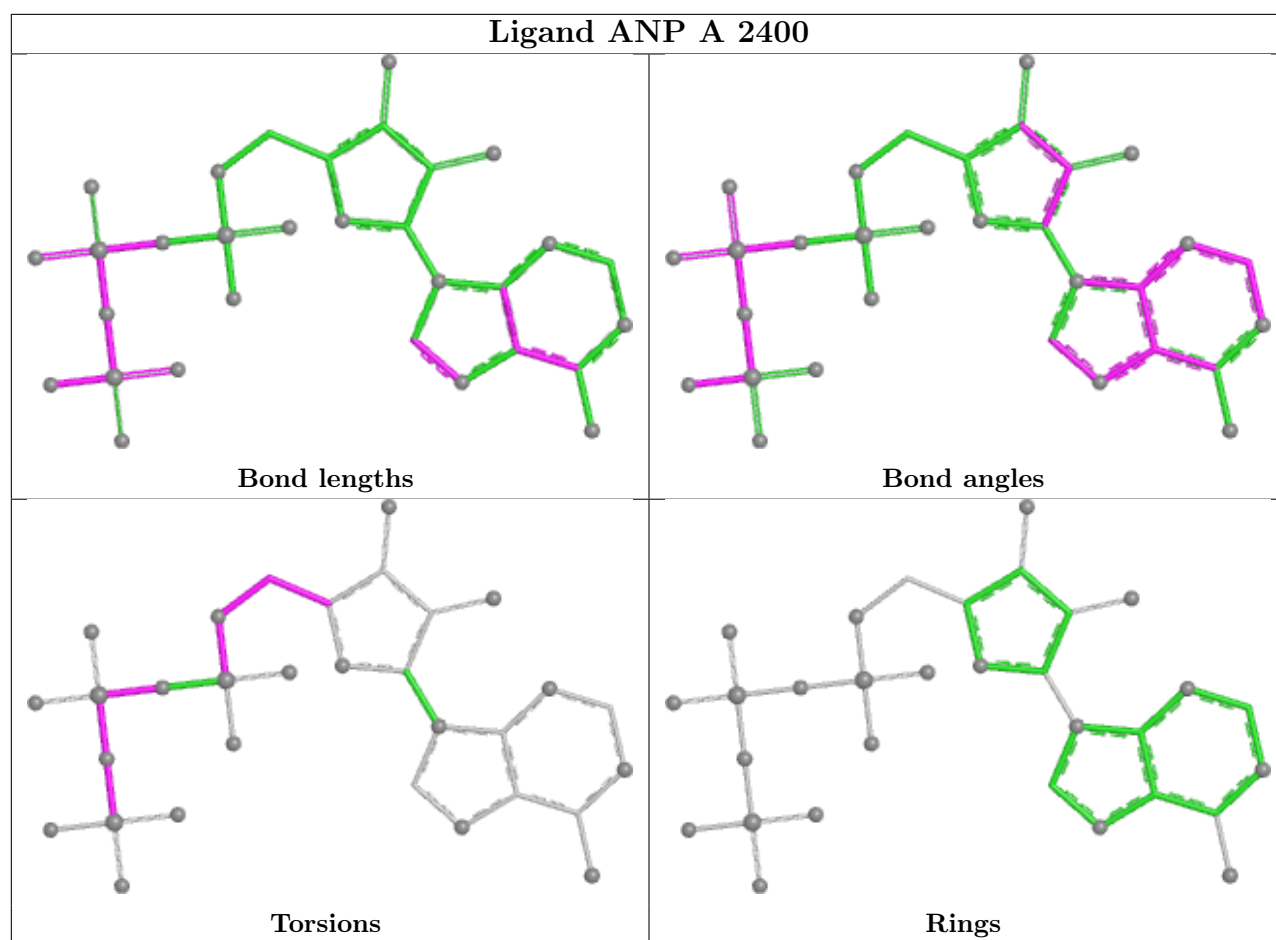


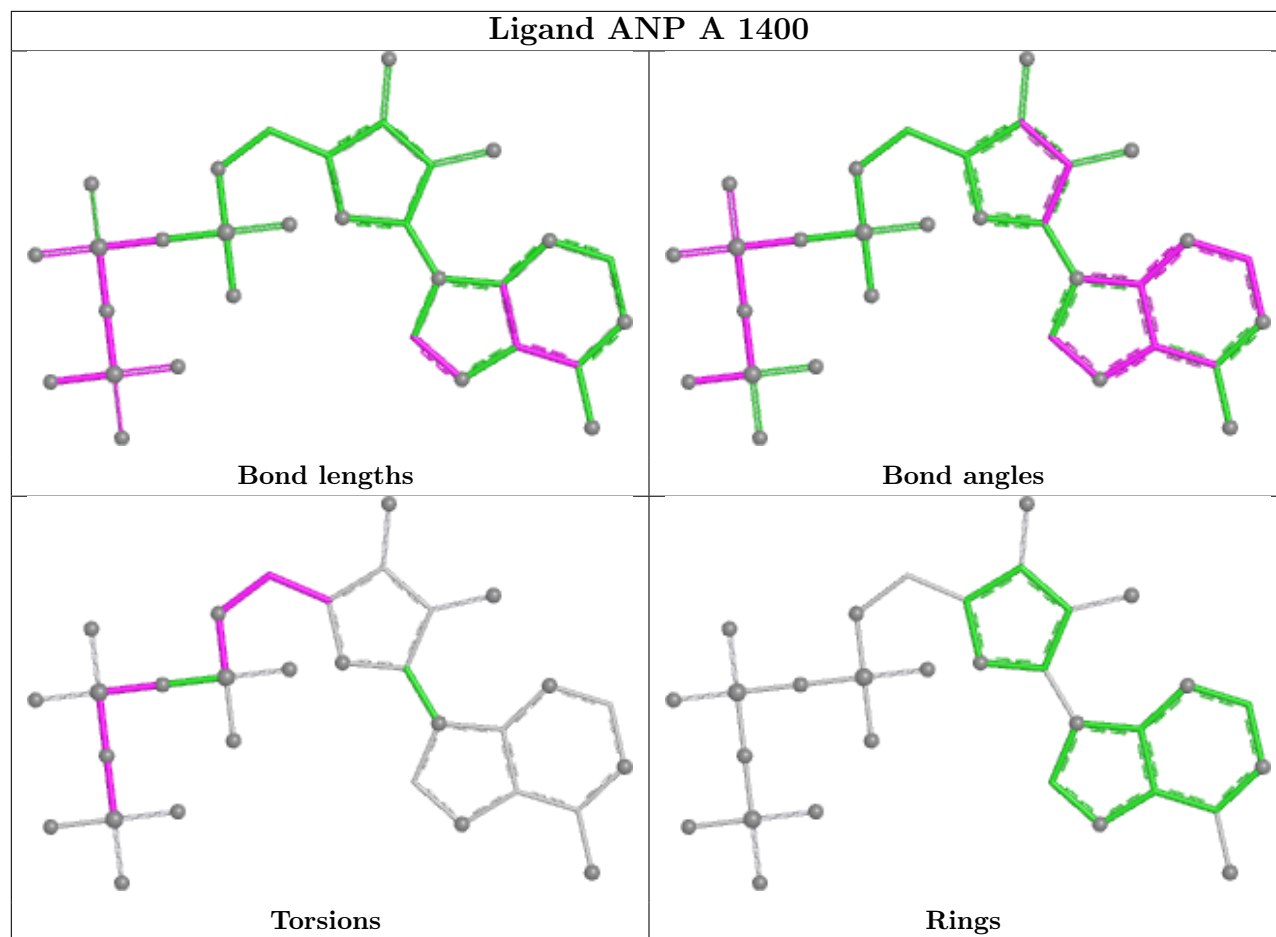


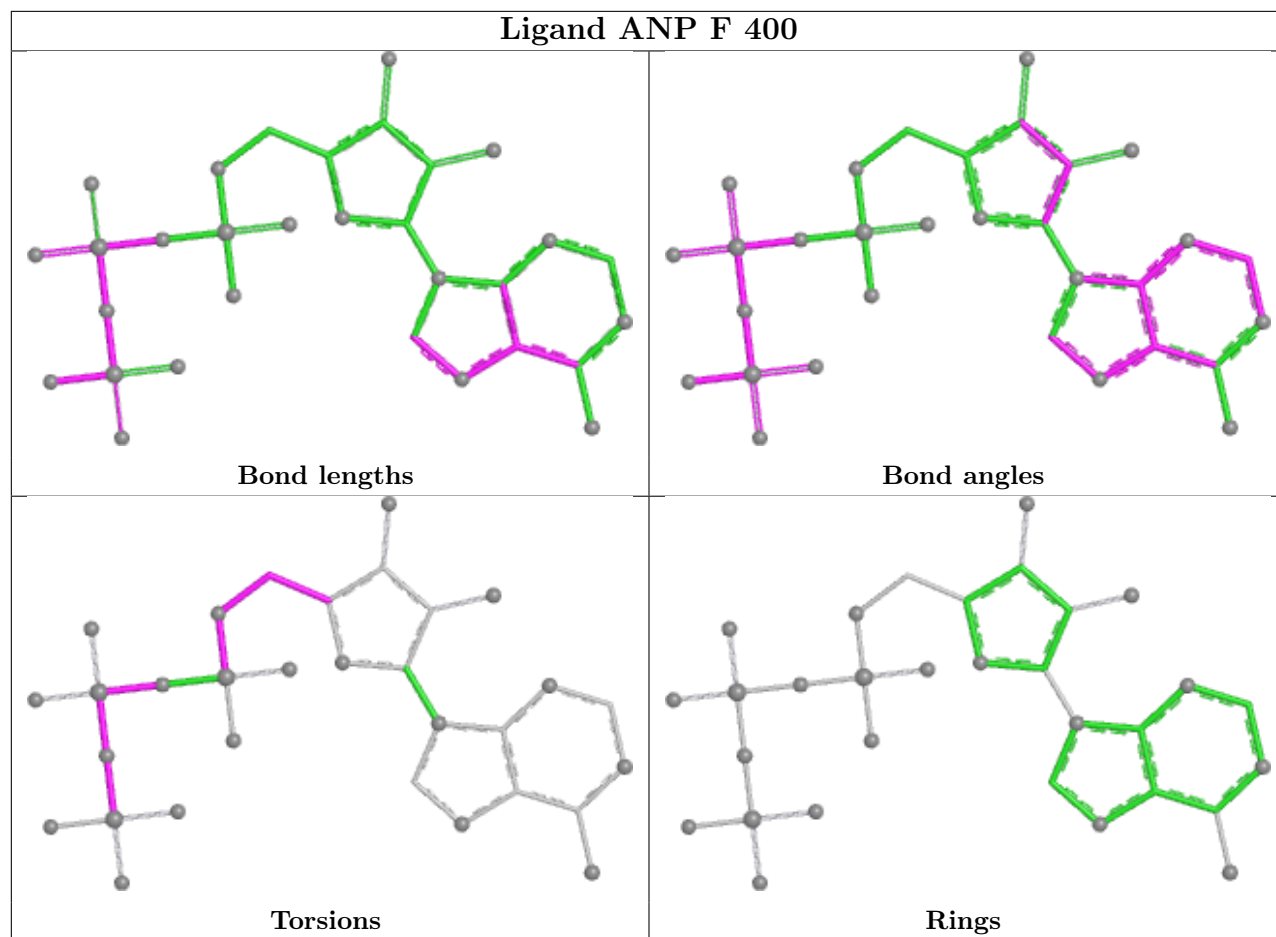


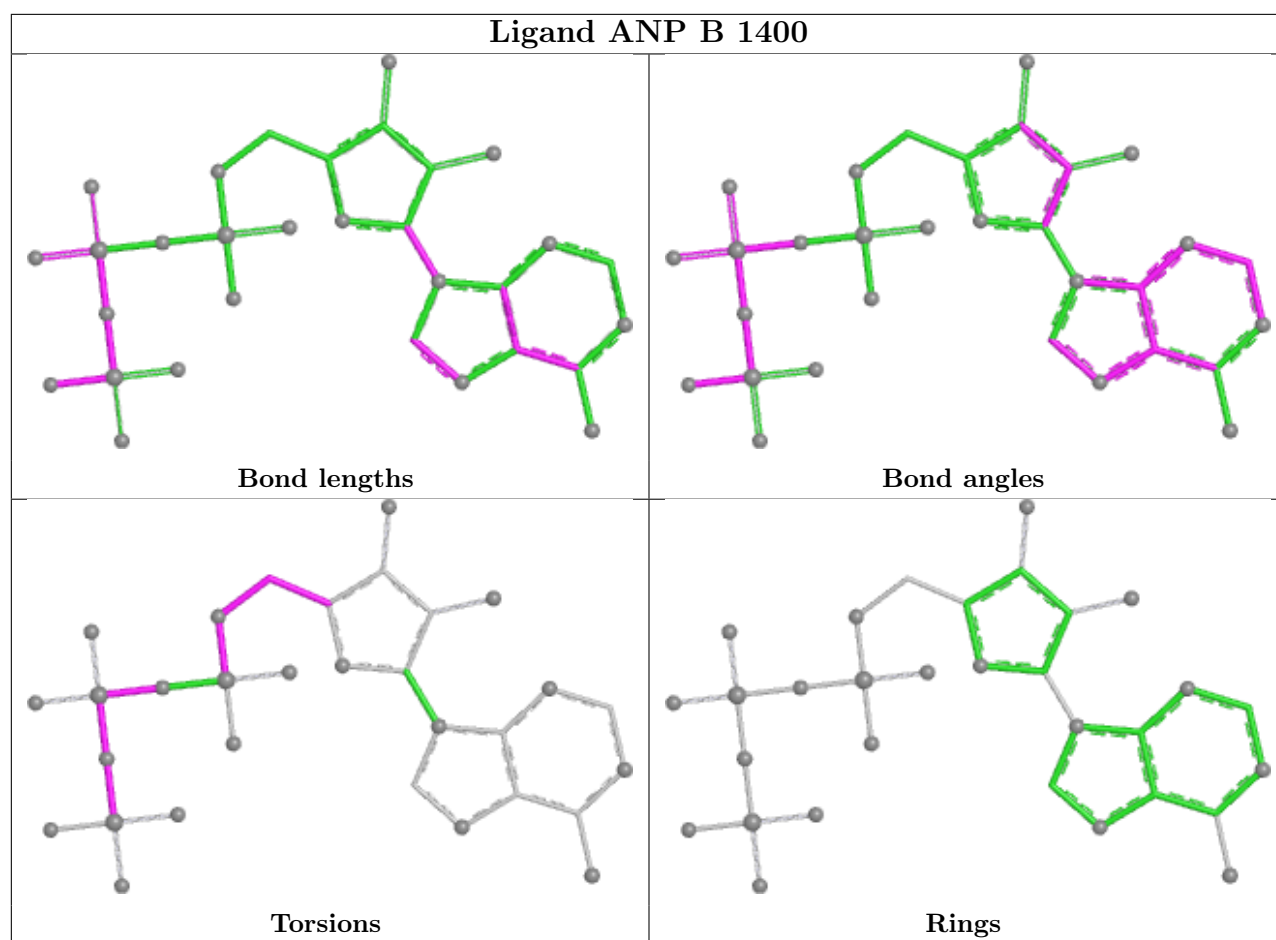












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1190/1357 (87%)	-0.14	6 (0%) 87 75	181, 217, 253, 285	0
1	B	1163/1357 (85%)	-0.22	2 (0%) 91 83	175, 217, 254, 286	0
1	C	1175/1357 (86%)	-0.09	4 (0%) 90 80	187, 216, 253, 284	0
1	D	1175/1357 (86%)	-0.21	2 (0%) 91 83	181, 218, 256, 286	0
1	E	1165/1357 (85%)	-0.16	5 (0%) 88 77	186, 218, 255, 288	0
1	F	1175/1357 (86%)	-0.15	2 (0%) 91 83	185, 217, 255, 285	0
1	G	1167/1357 (85%)	-0.13	5 (0%) 88 77	185, 216, 254, 291	0
1	H	1173/1357 (86%)	-0.18	3 (0%) 90 80	186, 218, 255, 288	0
All	All	9383/10856 (86%)	-0.16	29 (0%) 90 80	175, 217, 255, 291	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	ALA	4.1
1	H	2251	ILE	4.1
1	D	3251	ILE	3.9
1	G	2083	ALA	3.5
1	A	1053	ALA	3.2
1	E	149	LEU	2.9
1	C	2137	ALA	2.9
1	G	3151	PRO	2.8
1	G	1075	LEU	2.5
1	B	3250	LYS	2.5
1	A	3151	PRO	2.5
1	C	2305	ALA	2.5
1	G	3057	PRO	2.3
1	B	3251	ILE	2.3
1	E	167	ALA	2.3
1	E	3113	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	2244	VAL	2.3
1	D	1014	LEU	2.3
1	G	2154	GLU	2.3
1	A	1167	ALA	2.2
1	H	148	ALA	2.2
1	C	3251	ILE	2.2
1	E	1043	GLY	2.1
1	E	1129	CYS	2.1
1	C	2093	ILE	2.1
1	F	320	GLU	2.1
1	F	1284	ILE	2.1
1	A	2120	ASP	2.0
1	A	2155	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	G	701	1/1	0.27	0.20	215,215,215,215	0
2	MG	F	1701	1/1	0.62	0.33	175,175,175,175	0
2	MG	F	701	1/1	0.63	0.26	189,189,189,189	0
2	MG	D	701	1/1	0.65	0.32	261,261,261,261	0
2	MG	D	1701	1/1	0.68	0.30	212,212,212,212	0
2	MG	H	1701	1/1	0.69	0.25	188,188,188,188	0
2	MG	E	701	1/1	0.74	0.22	204,204,204,204	0
3	ANP	E	2400	31/31	0.75	0.11	307,317,320,320	0
2	MG	H	701	1/1	0.76	0.19	200,200,200,200	0
2	MG	C	701	1/1	0.78	0.17	177,177,177,177	0

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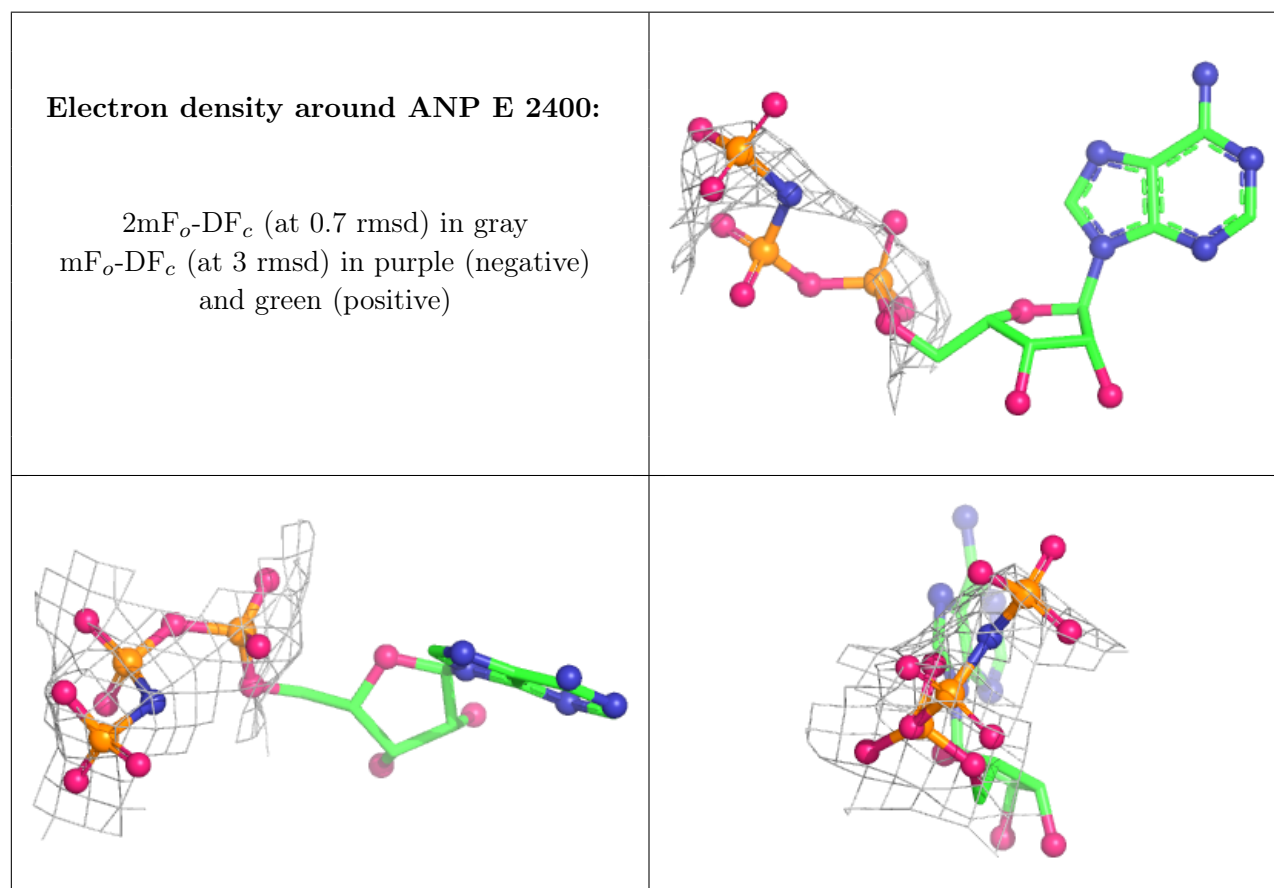
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ANP	C	1400	31/31	0.78	0.11	288,291,293,294	0
2	MG	A	701	1/1	0.78	0.14	143,143,143,143	0
2	MG	B	701	1/1	0.80	0.16	184,184,184,184	0
3	ANP	A	2400	31/31	0.80	0.13	308,311,315,315	0
3	ANP	H	1400	31/31	0.80	0.12	296,299,304,304	0
3	ANP	E	1400	31/31	0.81	0.11	287,293,296,296	0
2	MG	H	3701	1/1	0.81	0.15	121,121,121,121	0
3	ANP	F	1400	31/31	0.81	0.11	271,280,286,286	0
3	ANP	D	400	31/31	0.81	0.10	263,273,274,274	0
2	MG	E	3701	1/1	0.82	0.16	131,131,131,131	0
2	MG	E	1701	1/1	0.83	0.17	190,190,190,190	0
3	ANP	D	2400	31/31	0.83	0.10	305,310,315,315	0
2	MG	E	2701	1/1	0.84	0.20	228,228,228,228	0
3	ANP	G	1400	31/31	0.84	0.12	279,285,289,290	0
3	ANP	G	2400	31/31	0.84	0.12	303,308,315,315	0
2	MG	C	3701	1/1	0.84	0.11	140,140,140,140	0
2	MG	G	1701	1/1	0.85	0.21	191,191,191,191	0
3	ANP	A	1400	31/31	0.85	0.11	267,280,283,283	0
2	MG	B	2701	1/1	0.85	0.29	238,238,238,238	0
3	ANP	B	1400	31/31	0.85	0.10	275,286,290,290	0
2	MG	B	1701	1/1	0.85	0.21	214,214,214,214	0
2	MG	H	2701	1/1	0.85	0.28	271,271,271,271	0
3	ANP	D	1400	31/31	0.85	0.09	287,290,294,294	0
3	ANP	B	400	31/31	0.87	0.09	242,255,259,260	0
3	ANP	C	2400	31/31	0.87	0.09	296,309,314,315	0
3	ANP	F	2400	31/31	0.87	0.11	286,303,310,310	0
3	ANP	H	2400	31/31	0.87	0.10	298,312,316,316	0
3	ANP	H	400	31/31	0.88	0.08	254,263,265,265	0
3	ANP	F	400	31/31	0.89	0.09	243,257,263,263	0
3	ANP	G	400	31/31	0.90	0.09	253,262,264,265	0
2	MG	G	2701	1/1	0.90	0.24	192,192,192,192	0
3	ANP	A	400	31/31	0.90	0.09	246,250,255,256	0
3	ANP	H	3400	31/31	0.90	0.08	180,187,196,197	0
3	ANP	B	2400	31/31	0.91	0.10	306,312,314,314	0
2	MG	D	2701	1/1	0.91	0.39	237,237,237,237	0
3	ANP	E	400	31/31	0.92	0.07	256,261,264,265	0
2	MG	A	1701	1/1	0.92	0.13	181,181,181,181	0
3	ANP	D	3400	31/31	0.92	0.08	149,170,188,189	0
3	ANP	G	3400	31/31	0.92	0.08	153,176,191,192	0
3	ANP	C	3400	31/31	0.93	0.07	176,190,200,200	0
3	ANP	C	400	31/31	0.93	0.07	226,245,250,250	0
3	ANP	E	3400	31/31	0.93	0.07	163,180,187,187	0

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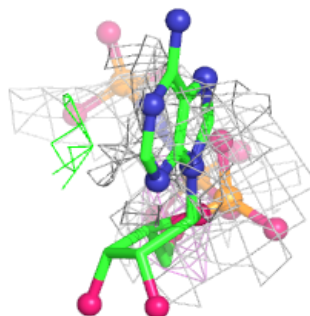
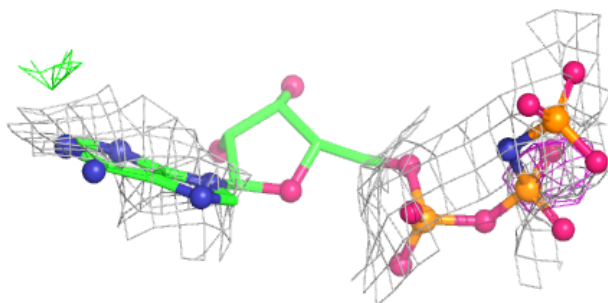
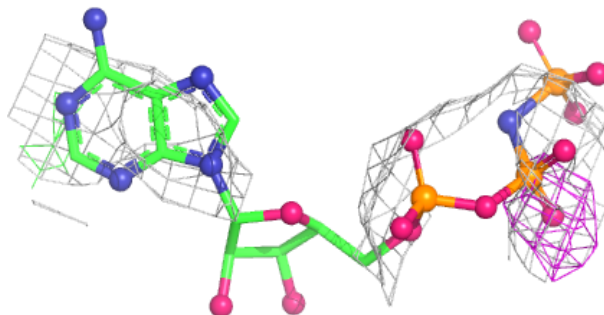
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ANP	F	3400	31/31	0.93	0.08	148,171,183,183	0
2	MG	D	3701	1/1	0.94	0.14	108,108,108,108	0
2	MG	F	2701	1/1	0.94	0.25	232,232,232,232	0
3	ANP	A	3400	31/31	0.94	0.06	152,165,180,181	0
2	MG	B	3701	1/1	0.95	0.11	69,69,69,69	0
2	MG	A	3701	1/1	0.95	0.04	116,116,116,116	0
2	MG	C	1701	1/1	0.95	0.10	132,132,132,132	0
2	MG	C	2701	1/1	0.95	0.17	211,211,211,211	0
2	MG	A	2701	1/1	0.95	0.15	247,247,247,247	0
3	ANP	B	3400	31/31	0.95	0.06	143,159,176,178	0
2	MG	G	3701	1/1	0.96	0.06	100,100,100,100	0
2	MG	F	3701	1/1	0.97	0.06	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.

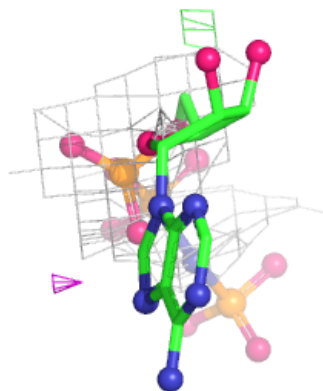
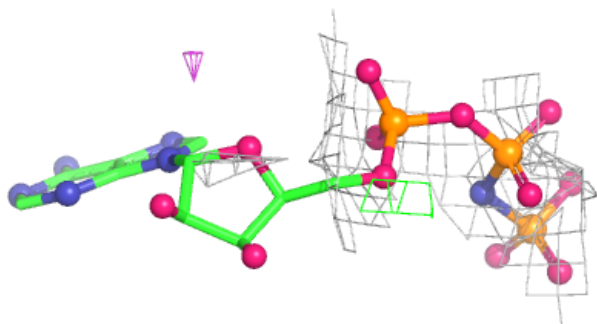
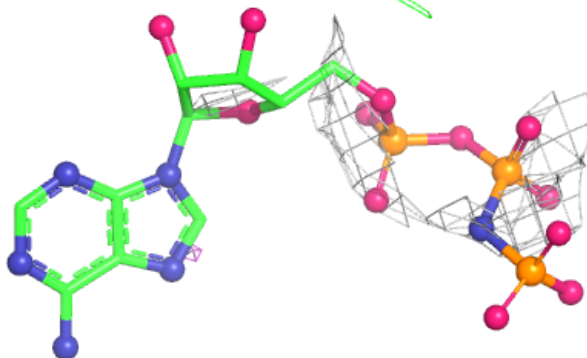


Electron density around ANP C 1400:

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

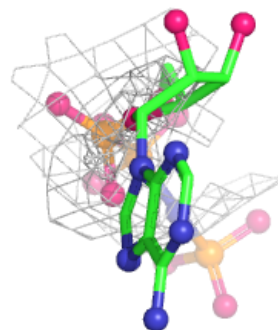
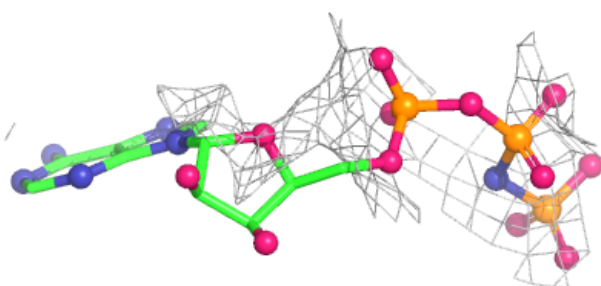
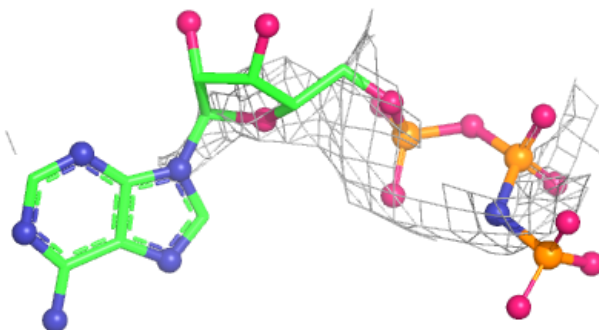
**Electron density around ANP A 2400:**

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

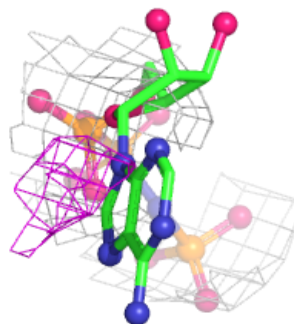
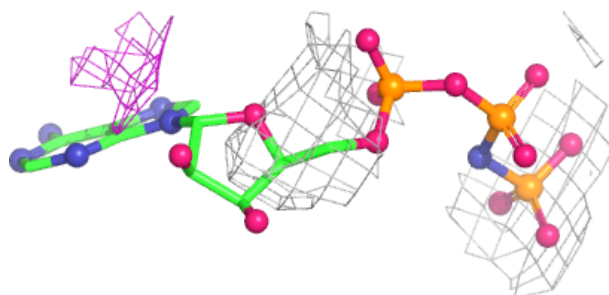
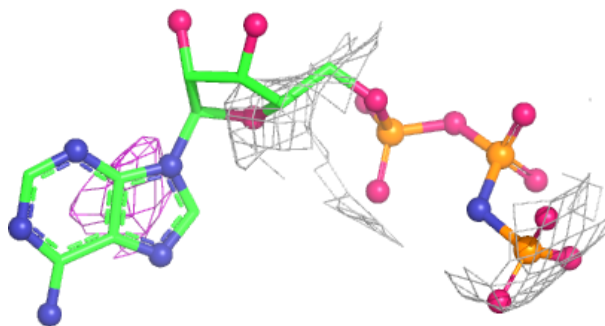


Electron density around ANP H 1400:

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

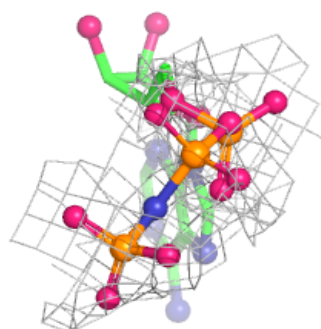
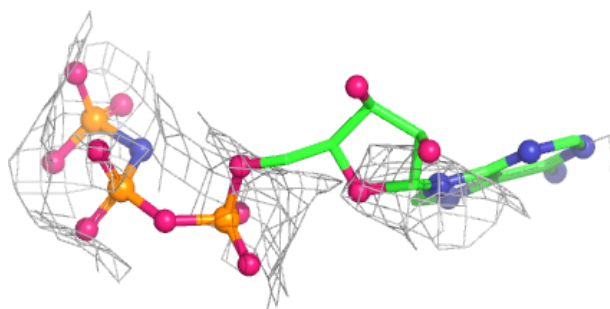
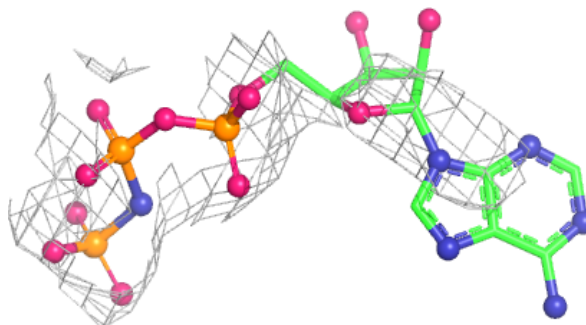
**Electron density around ANP E 1400:**

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and green (positive)

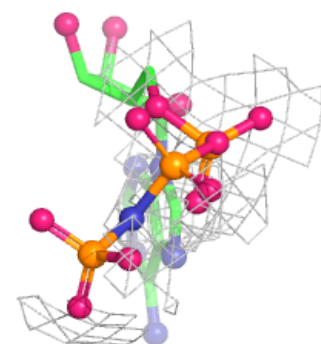
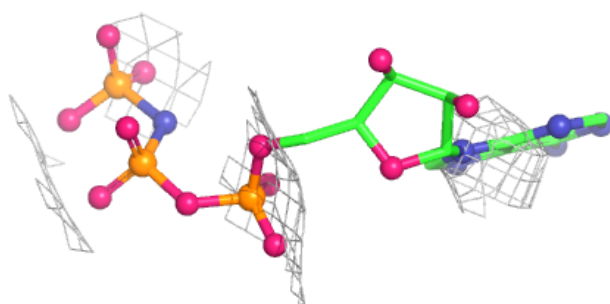
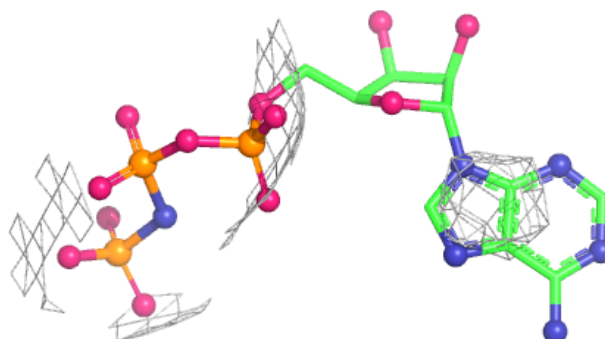


Electron density around ANP F 1400:

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

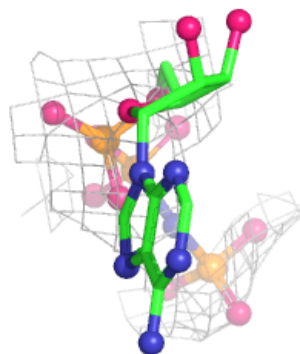
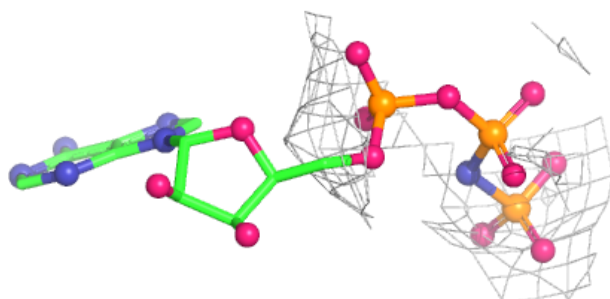
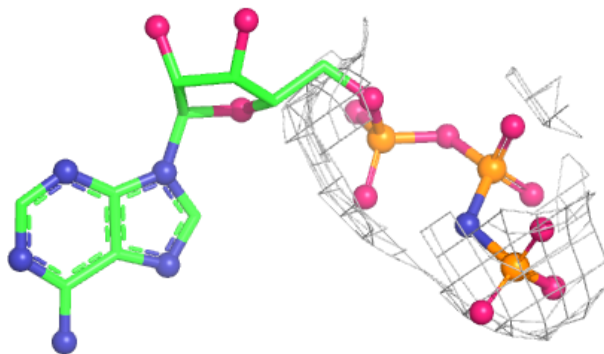
**Electron density around ANP D 400:**

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

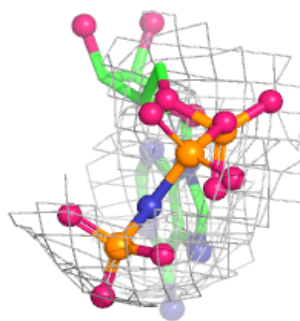
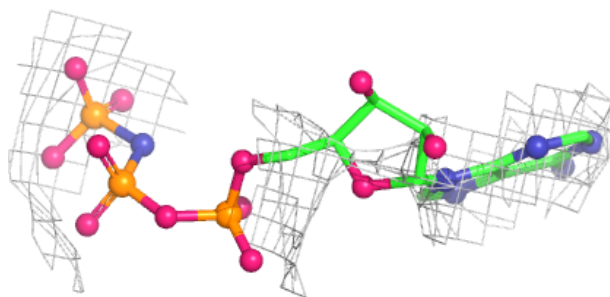
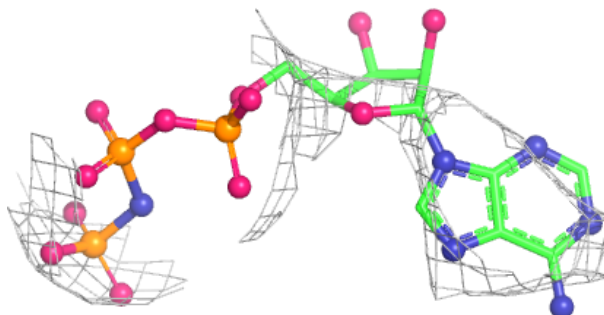


Electron density around ANP D 2400:

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

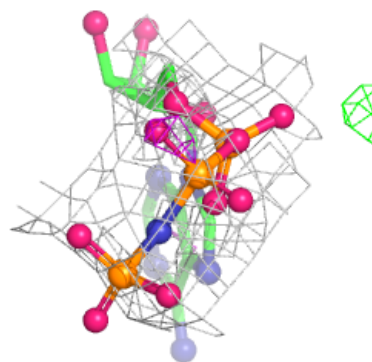
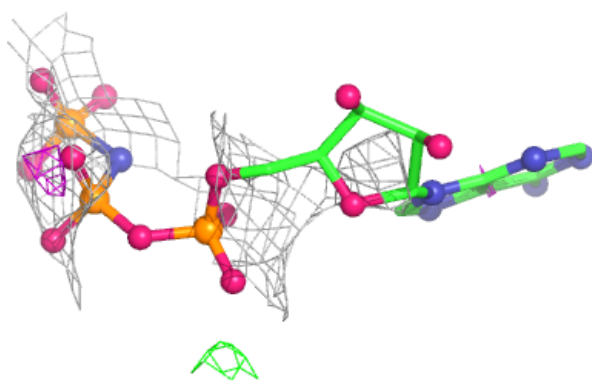
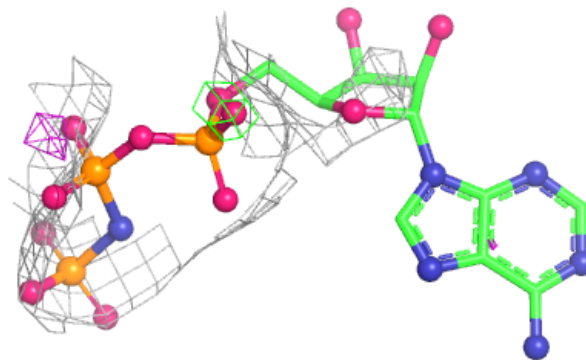
**Electron density around ANP G 1400:**

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

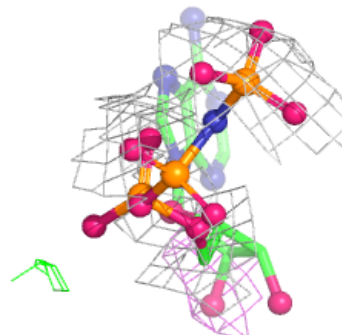
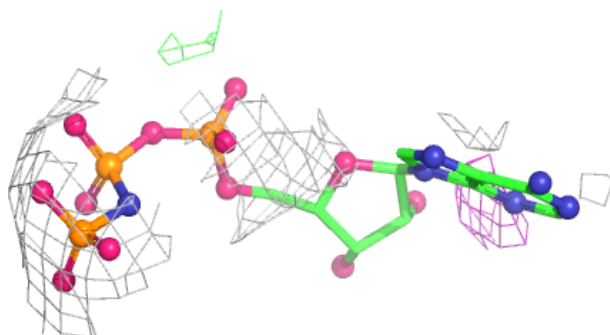
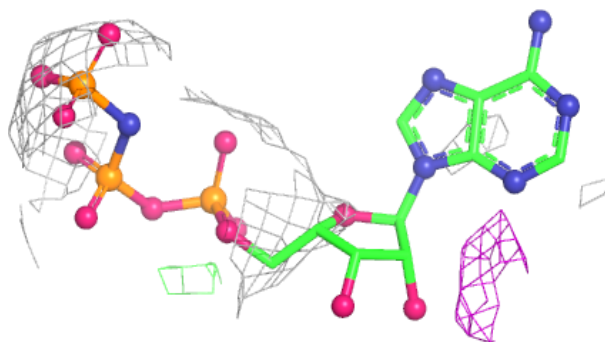


Electron density around ANP G 2400:

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

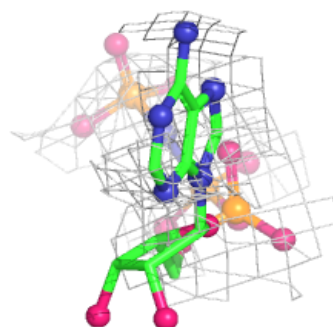
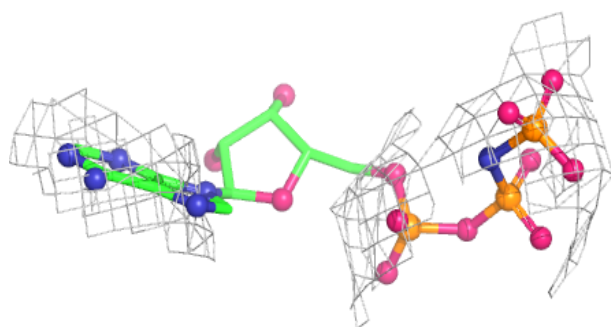
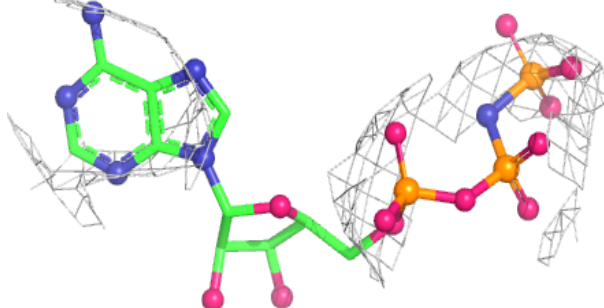
**Electron density around ANP A 1400:**

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

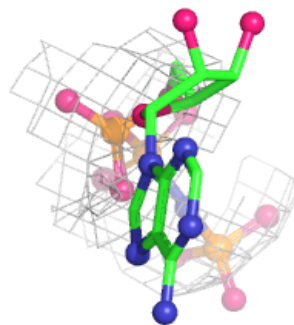
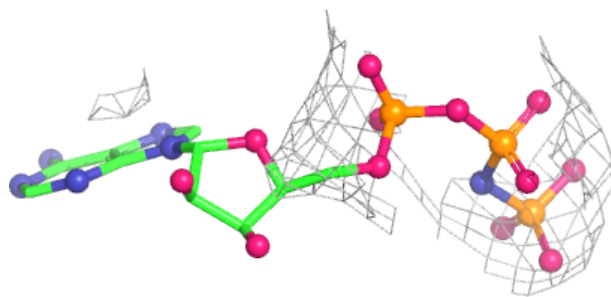
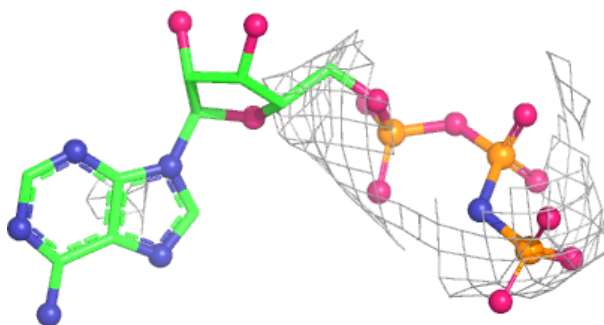


Electron density around ANP B 1400:

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

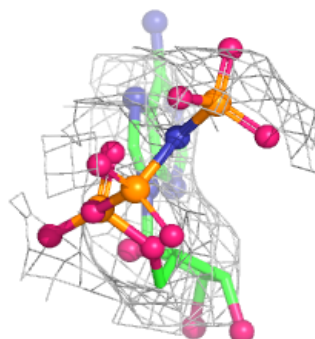
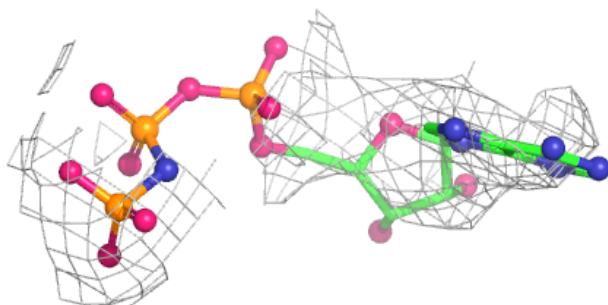
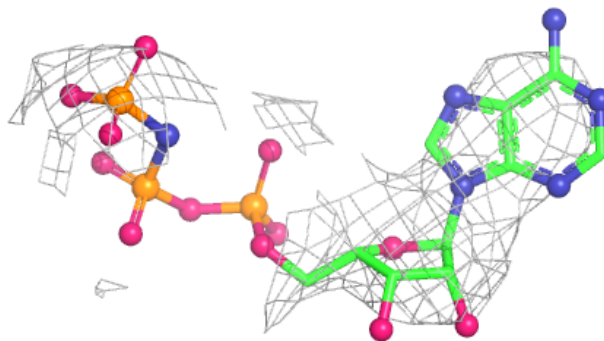
**Electron density around ANP D 1400:**

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

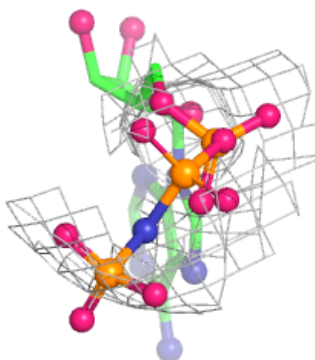
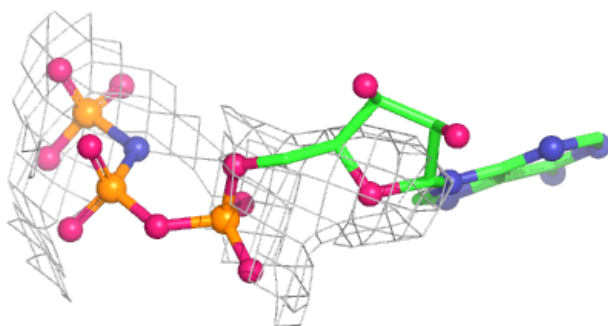
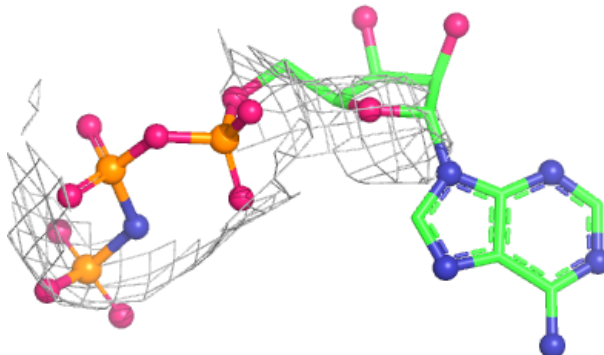


Electron density around ANP B 400:

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

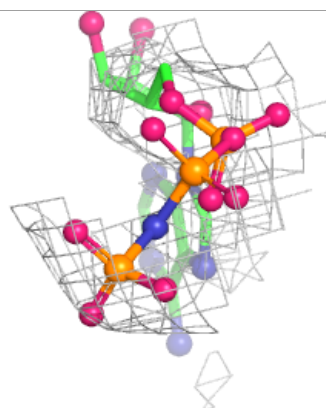
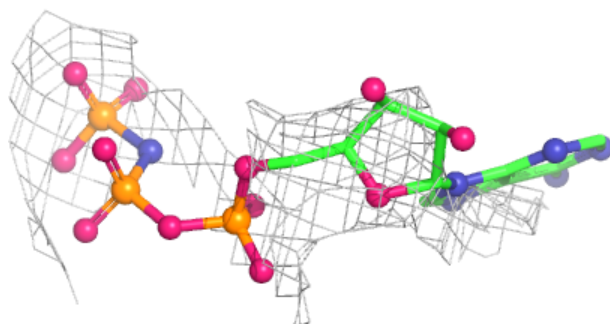
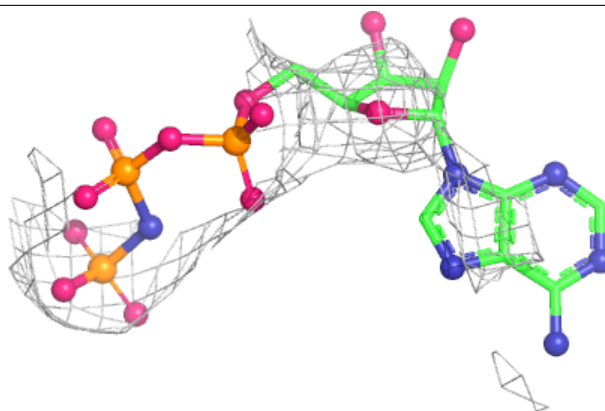
**Electron density around ANP C 2400:**

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

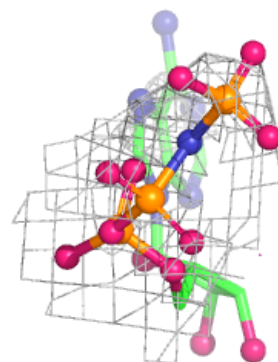
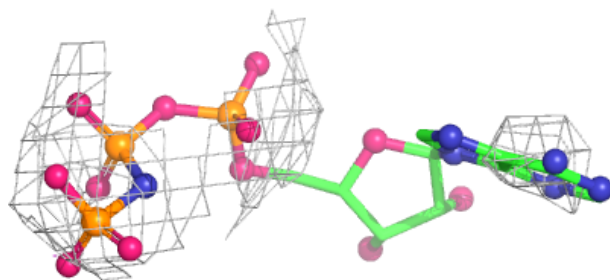
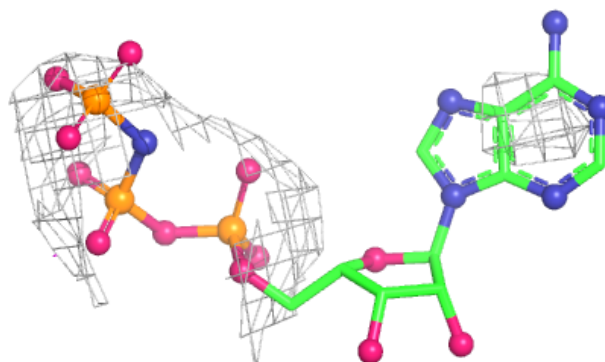


Electron density around ANP F 2400:

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

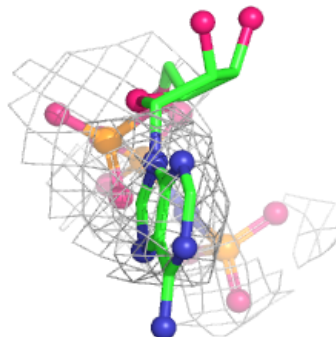
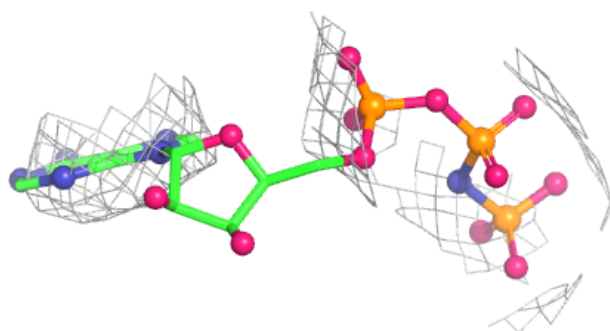
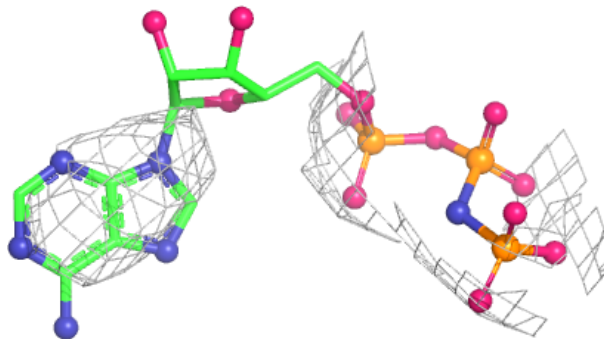
**Electron density around ANP H 2400:**

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

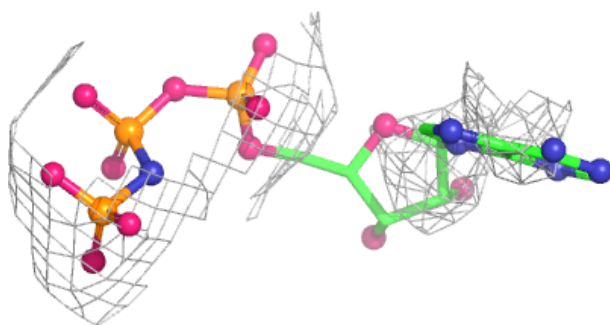
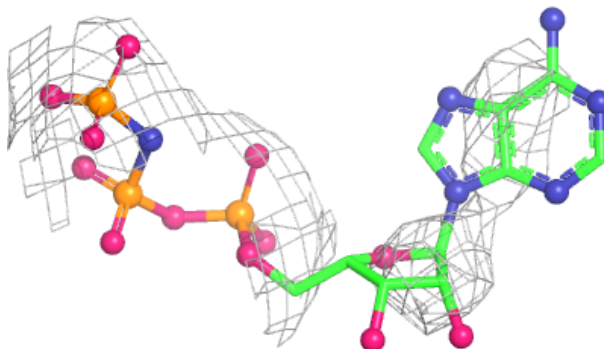


Electron density around ANP H 400:

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

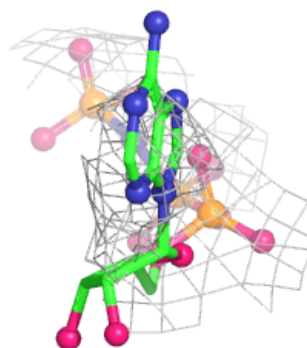
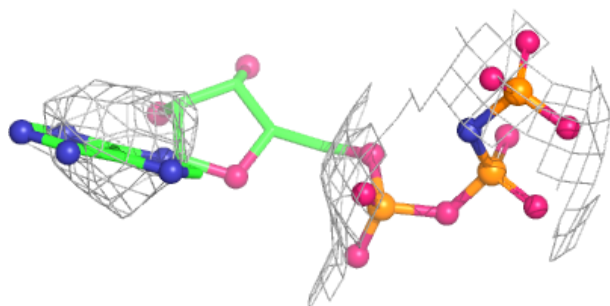
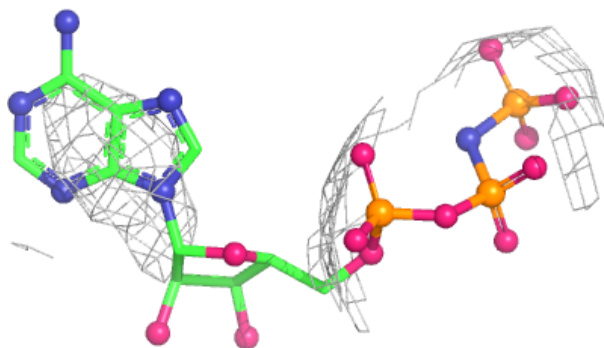
**Electron density around ANP F 400:**

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

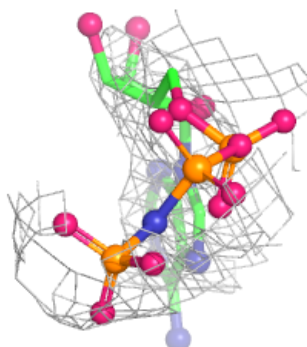
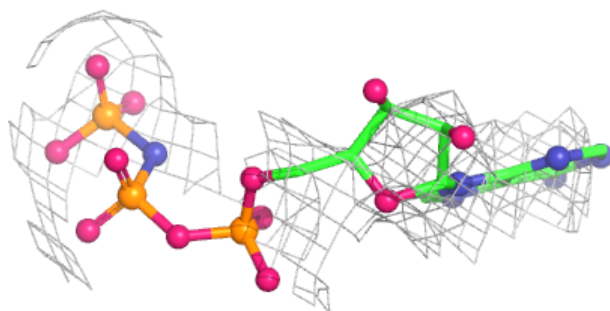
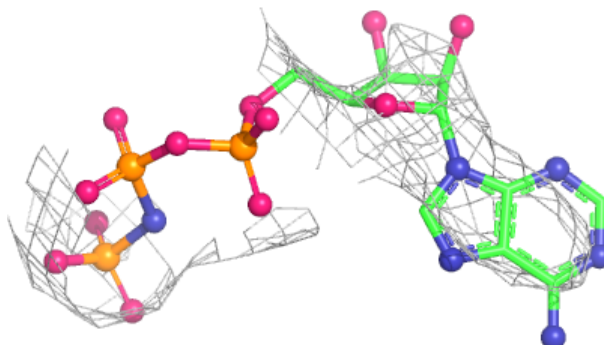


Electron density around ANP G 400:

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

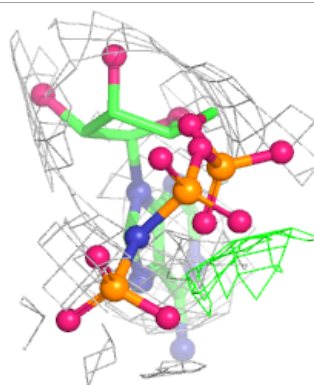
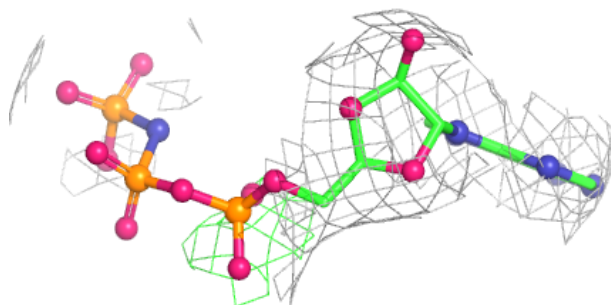
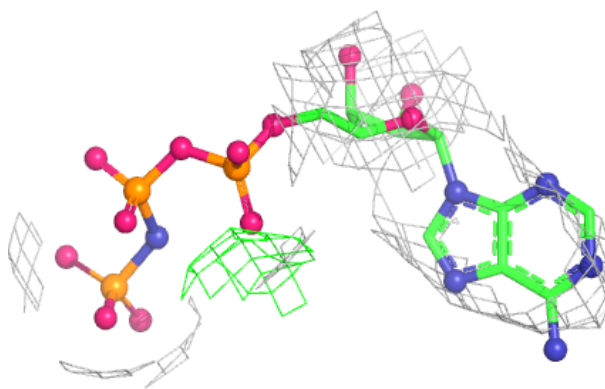
**Electron density around ANP A 400:**

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

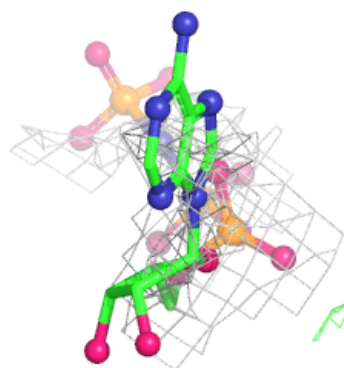
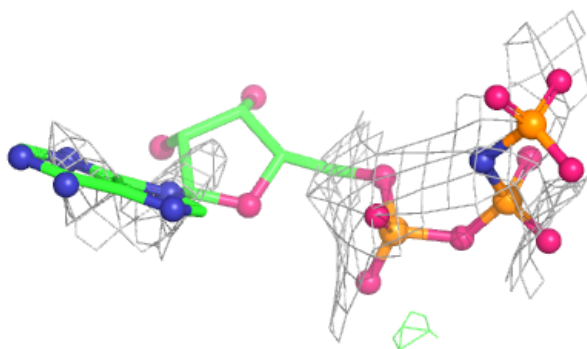
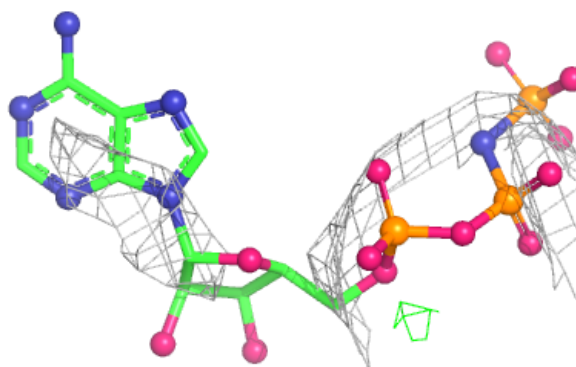


Electron density around ANP H 3400:

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

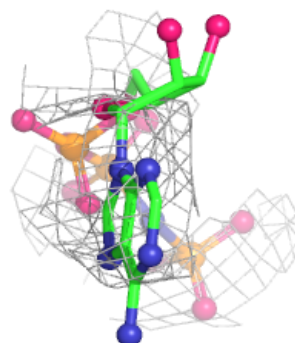
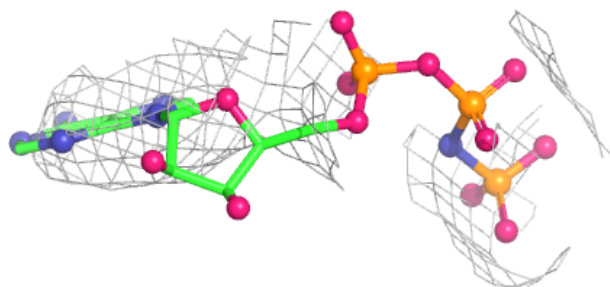
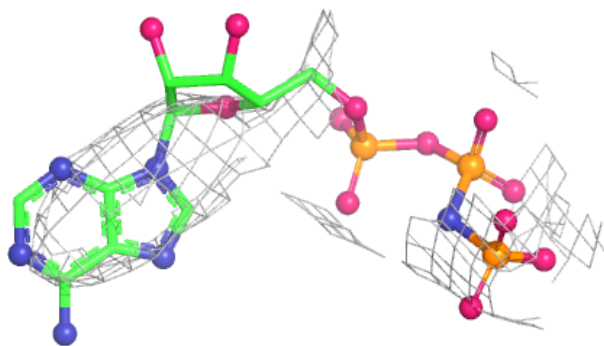
**Electron density around ANP B 2400:**

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

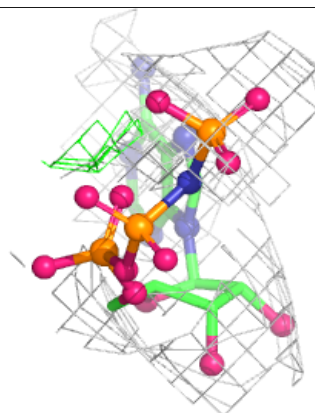
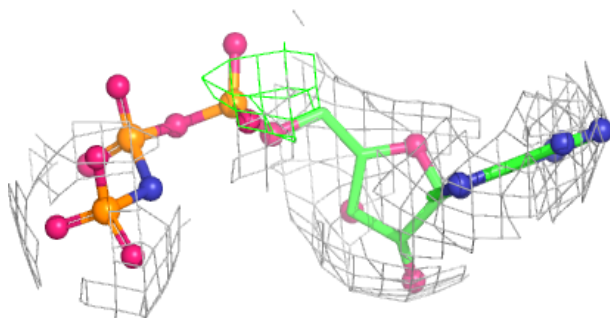
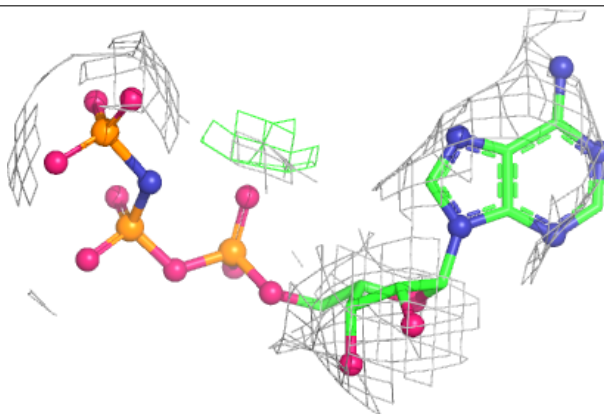


Electron density around ANP E 400:

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

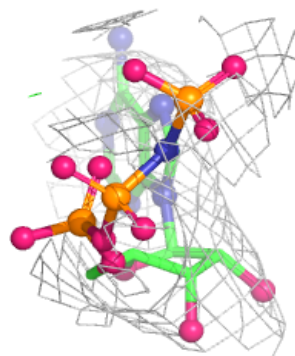
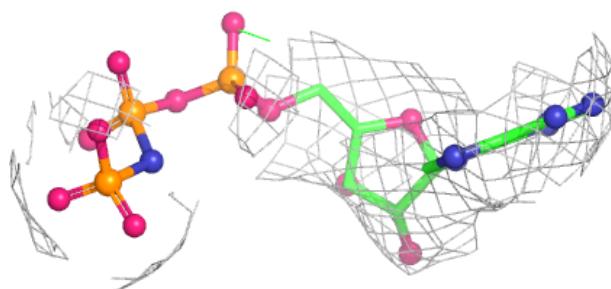
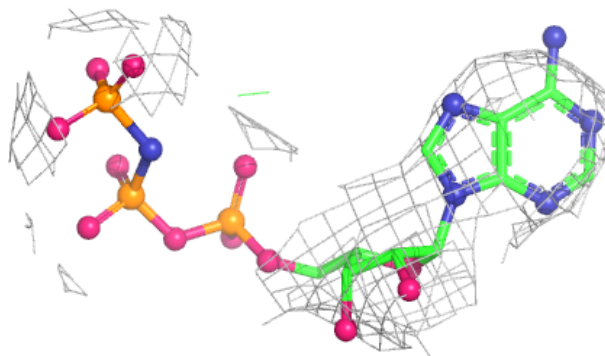
**Electron density around ANP D 3400:**

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

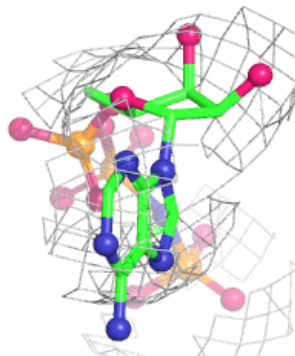
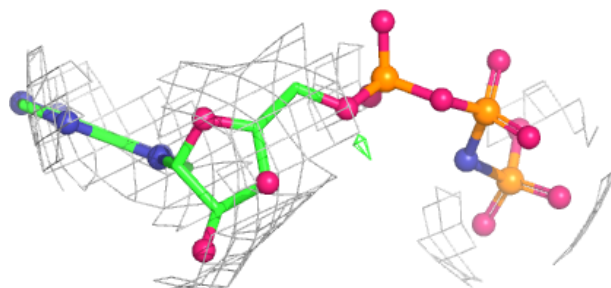
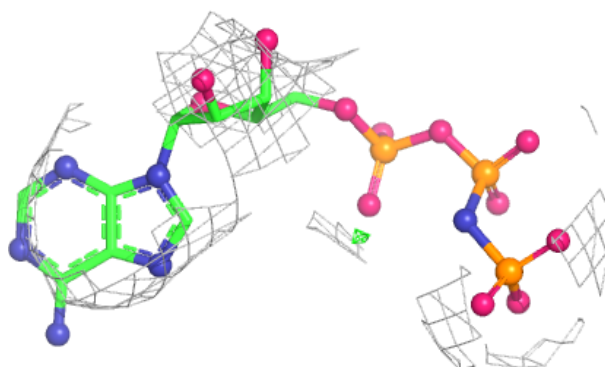


Electron density around ANP G 3400:

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

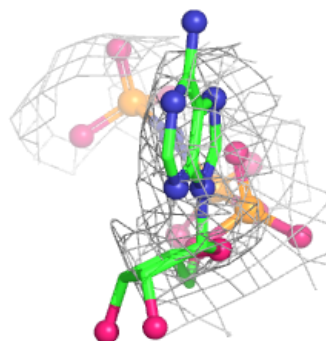
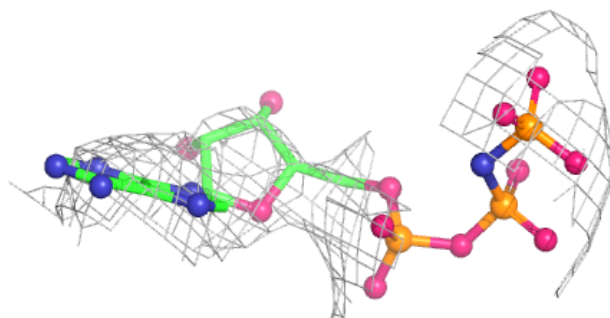
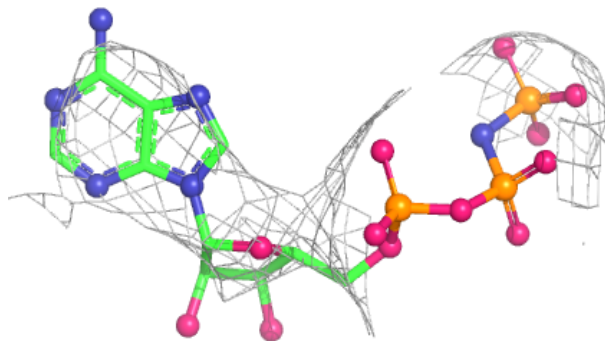
**Electron density around ANP C 3400:**

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

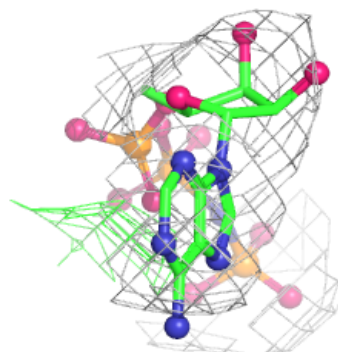
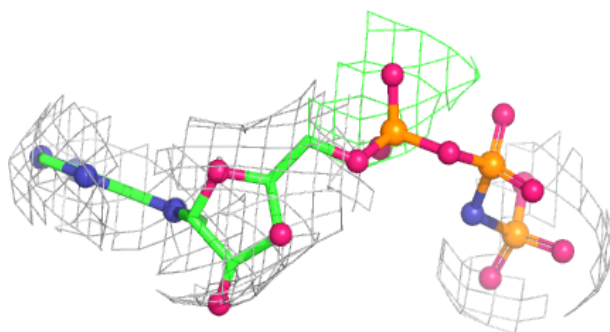
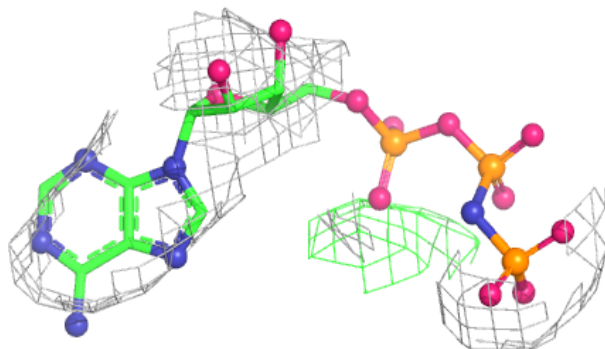


Electron density around ANP C 400:

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

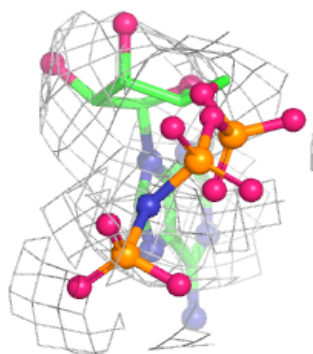
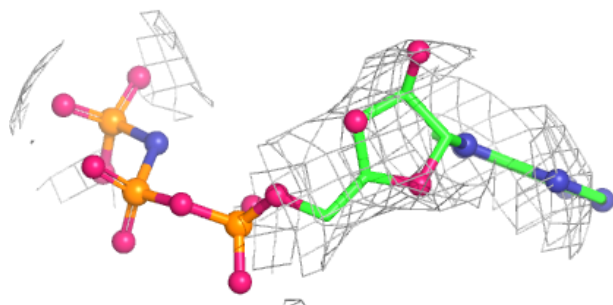
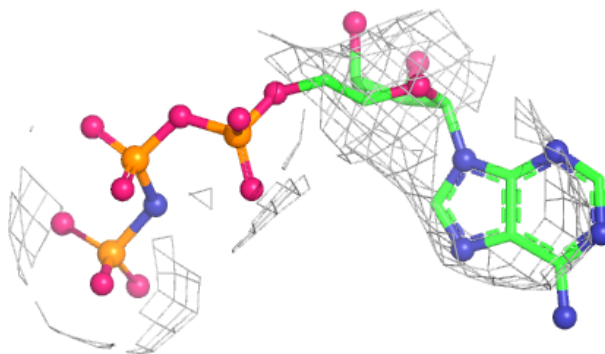
**Electron density around ANP E 3400:**

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

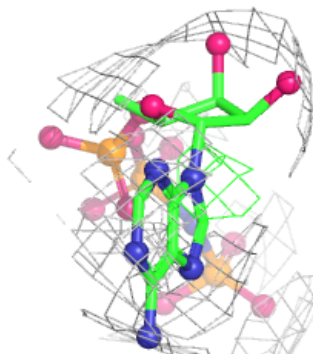
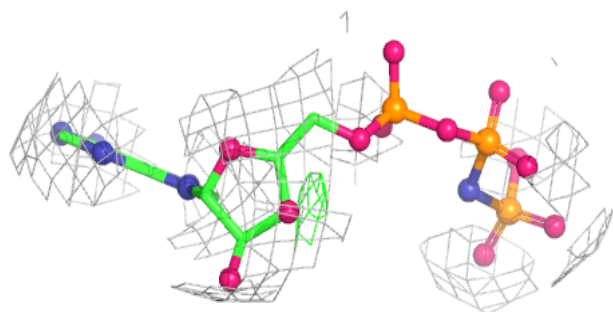
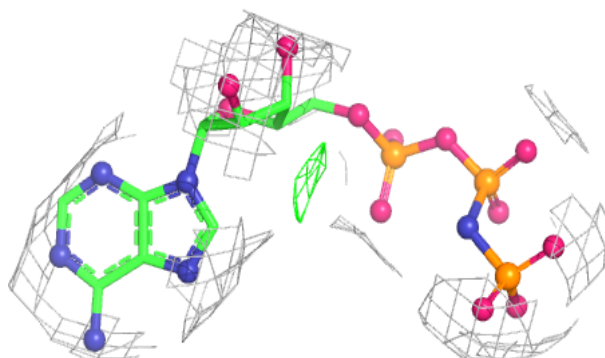


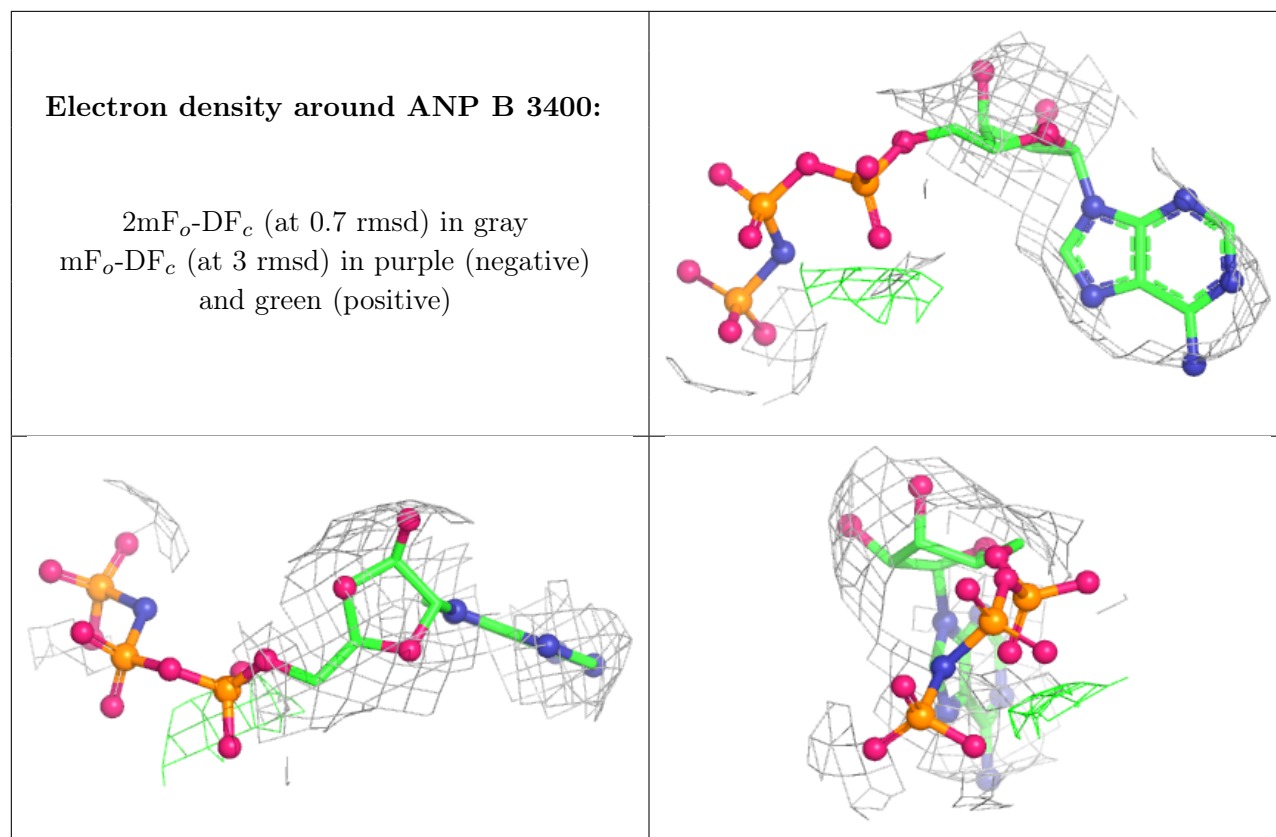
Electron density around ANP F 3400:

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

**Electron density around ANP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.