



Full wwPDB EM Validation Report ⓘ

Feb 24, 2025 – 12:18 pm GMT

PDB ID : 8RC5
EMDB ID : EMD-19048
Title : Complex between the RecA-like Sak4 SSAP and the SaPI2 Stl master regulator
Authors : Debiasi-Anders, G.; Mir-Sanchis, I.
Deposited on : 2023-12-06
Resolution : 3.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

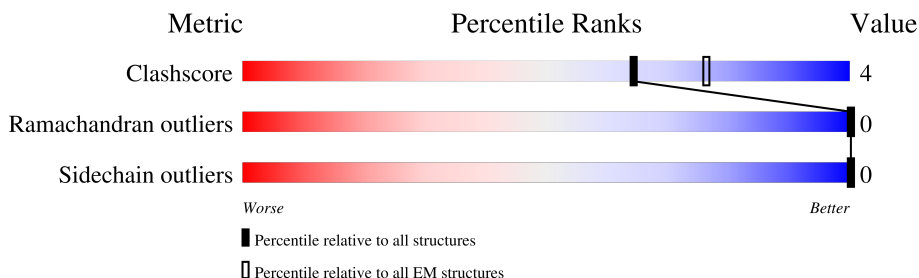
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY










The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	1A	279	
1	1B	279	
1	1C	279	
1	1D	279	
1	1E	279	
1	1F	279	
1	1G	279	
1	1H	279	
1	1I	279	



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Mol	Chain	Length	Quality of chain
1	4A	279	
1	4B	279	
1	4C	279	
1	4D	279	
1	4E	279	
1	4F	279	
1	4G	279	
1	4H	279	
1	4I	279	
2	2A	232	
2	2B	232	
2	2C	232	
2	2D	232	
2	2E	232	
2	2F	232	
2	2G	232	
2	2H	232	
2	2I	232	
2	3A	232	
2	3B	232	
2	3C	232	
2	3D	232	
2	3E	232	
2	3F	232	
2	3G	232	

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Mol	Chain	Length	Quality of chain
2	3H	232	 87%7%6%
2	3I	232	 89%5%6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 64360 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ORF016.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	4A	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	1B	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	4B	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	1C	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	4C	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	1D	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	4D	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	1E	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	4E	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	1F	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	4F	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	1G	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	4G	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	1H	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	4H	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		
1	1I	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	4I	219	Total	C	N	O	S	0	0
			1758	1113	303	337	5		

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	-19	MET	-	initiating methionine	UNP Q4ZAS5
1A	-18	GLY	-	expression tag	UNP Q4ZAS5
1A	-17	SER	-	expression tag	UNP Q4ZAS5
1A	-16	SER	-	expression tag	UNP Q4ZAS5
1A	-15	HIS	-	expression tag	UNP Q4ZAS5
1A	-14	HIS	-	expression tag	UNP Q4ZAS5
1A	-13	HIS	-	expression tag	UNP Q4ZAS5
1A	-12	HIS	-	expression tag	UNP Q4ZAS5
1A	-11	HIS	-	expression tag	UNP Q4ZAS5
1A	-10	HIS	-	expression tag	UNP Q4ZAS5
1A	-9	SER	-	expression tag	UNP Q4ZAS5
1A	-8	SER	-	expression tag	UNP Q4ZAS5
1A	-7	GLY	-	expression tag	UNP Q4ZAS5
1A	-6	LEU	-	expression tag	UNP Q4ZAS5
1A	-5	VAL	-	expression tag	UNP Q4ZAS5
1A	-4	PRO	-	expression tag	UNP Q4ZAS5
1A	-3	ARG	-	expression tag	UNP Q4ZAS5
1A	-2	GLY	-	expression tag	UNP Q4ZAS5
1A	-1	SER	-	expression tag	UNP Q4ZAS5
1A	0	HIS	-	expression tag	UNP Q4ZAS5
4A	-19	MET	-	initiating methionine	UNP Q4ZAS5
4A	-18	GLY	-	expression tag	UNP Q4ZAS5
4A	-17	SER	-	expression tag	UNP Q4ZAS5
4A	-16	SER	-	expression tag	UNP Q4ZAS5
4A	-15	HIS	-	expression tag	UNP Q4ZAS5
4A	-14	HIS	-	expression tag	UNP Q4ZAS5
4A	-13	HIS	-	expression tag	UNP Q4ZAS5
4A	-12	HIS	-	expression tag	UNP Q4ZAS5
4A	-11	HIS	-	expression tag	UNP Q4ZAS5
4A	-10	HIS	-	expression tag	UNP Q4ZAS5
4A	-9	SER	-	expression tag	UNP Q4ZAS5
4A	-8	SER	-	expression tag	UNP Q4ZAS5
4A	-7	GLY	-	expression tag	UNP Q4ZAS5
4A	-6	LEU	-	expression tag	UNP Q4ZAS5
4A	-5	VAL	-	expression tag	UNP Q4ZAS5
4A	-4	PRO	-	expression tag	UNP Q4ZAS5

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Chain	Residue	Modelled	Actual	Comment	Reference
4A	-3	ARG	-	expression tag	UNP Q4ZAS5
4A	-2	GLY	-	expression tag	UNP Q4ZAS5
4A	-1	SER	-	expression tag	UNP Q4ZAS5
4A	0	HIS	-	expression tag	UNP Q4ZAS5
1B	-19	MET	-	initiating methionine	UNP Q4ZAS5
1B	-18	GLY	-	expression tag	UNP Q4ZAS5
1B	-17	SER	-	expression tag	UNP Q4ZAS5
1B	-16	SER	-	expression tag	UNP Q4ZAS5
1B	-15	HIS	-	expression tag	UNP Q4ZAS5
1B	-14	HIS	-	expression tag	UNP Q4ZAS5
1B	-13	HIS	-	expression tag	UNP Q4ZAS5
1B	-12	HIS	-	expression tag	UNP Q4ZAS5
1B	-11	HIS	-	expression tag	UNP Q4ZAS5
1B	-10	HIS	-	expression tag	UNP Q4ZAS5
1B	-9	SER	-	expression tag	UNP Q4ZAS5
1B	-8	SER	-	expression tag	UNP Q4ZAS5
1B	-7	GLY	-	expression tag	UNP Q4ZAS5
1B	-6	LEU	-	expression tag	UNP Q4ZAS5
1B	-5	VAL	-	expression tag	UNP Q4ZAS5
1B	-4	PRO	-	expression tag	UNP Q4ZAS5
1B	-3	ARG	-	expression tag	UNP Q4ZAS5
1B	-2	GLY	-	expression tag	UNP Q4ZAS5
1B	-1	SER	-	expression tag	UNP Q4ZAS5
1B	0	HIS	-	expression tag	UNP Q4ZAS5
4B	-19	MET	-	initiating methionine	UNP Q4ZAS5
4B	-18	GLY	-	expression tag	UNP Q4ZAS5
4B	-17	SER	-	expression tag	UNP Q4ZAS5
4B	-16	SER	-	expression tag	UNP Q4ZAS5
4B	-15	HIS	-	expression tag	UNP Q4ZAS5
4B	-14	HIS	-	expression tag	UNP Q4ZAS5
4B	-13	HIS	-	expression tag	UNP Q4ZAS5
4B	-12	HIS	-	expression tag	UNP Q4ZAS5
4B	-11	HIS	-	expression tag	UNP Q4ZAS5
4B	-10	HIS	-	expression tag	UNP Q4ZAS5
4B	-9	SER	-	expression tag	UNP Q4ZAS5
4B	-8	SER	-	expression tag	UNP Q4ZAS5
4B	-7	GLY	-	expression tag	UNP Q4ZAS5
4B	-6	LEU	-	expression tag	UNP Q4ZAS5
4B	-5	VAL	-	expression tag	UNP Q4ZAS5
4B	-4	PRO	-	expression tag	UNP Q4ZAS5
4B	-3	ARG	-	expression tag	UNP Q4ZAS5
4B	-2	GLY	-	expression tag	UNP Q4ZAS5

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Chain	Residue	Modelled	Actual	Comment	Reference
4B	-1	SER	-	expression tag	UNP Q4ZAS5
4B	0	HIS	-	expression tag	UNP Q4ZAS5
1C	-19	MET	-	initiating methionine	UNP Q4ZAS5
1C	-18	GLY	-	expression tag	UNP Q4ZAS5
1C	-17	SER	-	expression tag	UNP Q4ZAS5
1C	-16	SER	-	expression tag	UNP Q4ZAS5
1C	-15	HIS	-	expression tag	UNP Q4ZAS5
1C	-14	HIS	-	expression tag	UNP Q4ZAS5
1C	-13	HIS	-	expression tag	UNP Q4ZAS5
1C	-12	HIS	-	expression tag	UNP Q4ZAS5
1C	-11	HIS	-	expression tag	UNP Q4ZAS5
1C	-10	HIS	-	expression tag	UNP Q4ZAS5
1C	-9	SER	-	expression tag	UNP Q4ZAS5
1C	-8	SER	-	expression tag	UNP Q4ZAS5
1C	-7	GLY	-	expression tag	UNP Q4ZAS5
1C	-6	LEU	-	expression tag	UNP Q4ZAS5
1C	-5	VAL	-	expression tag	UNP Q4ZAS5
1C	-4	PRO	-	expression tag	UNP Q4ZAS5
1C	-3	ARG	-	expression tag	UNP Q4ZAS5
1C	-2	GLY	-	expression tag	UNP Q4ZAS5
1C	-1	SER	-	expression tag	UNP Q4ZAS5
1C	0	HIS	-	expression tag	UNP Q4ZAS5
4C	-19	MET	-	initiating methionine	UNP Q4ZAS5
4C	-18	GLY	-	expression tag	UNP Q4ZAS5
4C	-17	SER	-	expression tag	UNP Q4ZAS5
4C	-16	SER	-	expression tag	UNP Q4ZAS5
4C	-15	HIS	-	expression tag	UNP Q4ZAS5
4C	-14	HIS	-	expression tag	UNP Q4ZAS5
4C	-13	HIS	-	expression tag	UNP Q4ZAS5
4C	-12	HIS	-	expression tag	UNP Q4ZAS5
4C	-11	HIS	-	expression tag	UNP Q4ZAS5
4C	-10	HIS	-	expression tag	UNP Q4ZAS5
4C	-9	SER	-	expression tag	UNP Q4ZAS5
4C	-8	SER	-	expression tag	UNP Q4ZAS5
4C	-7	GLY	-	expression tag	UNP Q4ZAS5
4C	-6	LEU	-	expression tag	UNP Q4ZAS5
4C	-5	VAL	-	expression tag	UNP Q4ZAS5
4C	-4	PRO	-	expression tag	UNP Q4ZAS5
4C	-3	ARG	-	expression tag	UNP Q4ZAS5
4C	-2	GLY	-	expression tag	UNP Q4ZAS5
4C	-1	SER	-	expression tag	UNP Q4ZAS5
4C	0	HIS	-	expression tag	UNP Q4ZAS5

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Chain	Residue	Modelled	Actual	Comment	Reference
1D	-19	MET	-	initiating methionine	UNP Q4ZAS5
1D	-18	GLY	-	expression tag	UNP Q4ZAS5
1D	-17	SER	-	expression tag	UNP Q4ZAS5
1D	-16	SER	-	expression tag	UNP Q4ZAS5
1D	-15	HIS	-	expression tag	UNP Q4ZAS5
1D	-14	HIS	-	expression tag	UNP Q4ZAS5
1D	-13	HIS	-	expression tag	UNP Q4ZAS5
1D	-12	HIS	-	expression tag	UNP Q4ZAS5
1D	-11	HIS	-	expression tag	UNP Q4ZAS5
1D	-10	HIS	-	expression tag	UNP Q4ZAS5
1D	-9	SER	-	expression tag	UNP Q4ZAS5
1D	-8	SER	-	expression tag	UNP Q4ZAS5
1D	-7	GLY	-	expression tag	UNP Q4ZAS5
1D	-6	LEU	-	expression tag	UNP Q4ZAS5
1D	-5	VAL	-	expression tag	UNP Q4ZAS5
1D	-4	PRO	-	expression tag	UNP Q4ZAS5
1D	-3	ARG	-	expression tag	UNP Q4ZAS5
1D	-2	GLY	-	expression tag	UNP Q4ZAS5
1D	-1	SER	-	expression tag	UNP Q4ZAS5
1D	0	HIS	-	expression tag	UNP Q4ZAS5
4D	-19	MET	-	initiating methionine	UNP Q4ZAS5
4D	-18	GLY	-	expression tag	UNP Q4ZAS5
4D	-17	SER	-	expression tag	UNP Q4ZAS5
4D	-16	SER	-	expression tag	UNP Q4ZAS5
4D	-15	HIS	-	expression tag	UNP Q4ZAS5
4D	-14	HIS	-	expression tag	UNP Q4ZAS5
4D	-13	HIS	-	expression tag	UNP Q4ZAS5
4D	-12	HIS	-	expression tag	UNP Q4ZAS5
4D	-11	HIS	-	expression tag	UNP Q4ZAS5
4D	-10	HIS	-	expression tag	UNP Q4ZAS5
4D	-9	SER	-	expression tag	UNP Q4ZAS5
4D	-8	SER	-	expression tag	UNP Q4ZAS5
4D	-7	GLY	-	expression tag	UNP Q4ZAS5
4D	-6	LEU	-	expression tag	UNP Q4ZAS5
4D	-5	VAL	-	expression tag	UNP Q4ZAS5
4D	-4	PRO	-	expression tag	UNP Q4ZAS5
4D	-3	ARG	-	expression tag	UNP Q4ZAS5
4D	-2	GLY	-	expression tag	UNP Q4ZAS5
4D	-1	SER	-	expression tag	UNP Q4ZAS5
4D	0	HIS	-	expression tag	UNP Q4ZAS5
1E	-19	MET	-	initiating methionine	UNP Q4ZAS5
1E	-18	GLY	-	expression tag	UNP Q4ZAS5

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Chain	Residue	Modelled	Actual	Comment	Reference
1E	-17	SER	-	expression tag	UNP Q4ZAS5
1E	-16	SER	-	expression tag	UNP Q4ZAS5
1E	-15	HIS	-	expression tag	UNP Q4ZAS5
1E	-14	HIS	-	expression tag	UNP Q4ZAS5
1E	-13	HIS	-	expression tag	UNP Q4ZAS5
1E	-12	HIS	-	expression tag	UNP Q4ZAS5
1E	-11	HIS	-	expression tag	UNP Q4ZAS5
1E	-10	HIS	-	expression tag	UNP Q4ZAS5
1E	-9	SER	-	expression tag	UNP Q4ZAS5
1E	-8	SER	-	expression tag	UNP Q4ZAS5
1E	-7	GLY	-	expression tag	UNP Q4ZAS5
1E	-6	LEU	-	expression tag	UNP Q4ZAS5
1E	-5	VAL	-	expression tag	UNP Q4ZAS5
1E	-4	PRO	-	expression tag	UNP Q4ZAS5
1E	-3	ARG	-	expression tag	UNP Q4ZAS5
1E	-2	GLY	-	expression tag	UNP Q4ZAS5
1E	-1	SER	-	expression tag	UNP Q4ZAS5
1E	0	HIS	-	expression tag	UNP Q4ZAS5
4E	-19	MET	-	initiating methionine	UNP Q4ZAS5
4E	-18	GLY	-	expression tag	UNP Q4ZAS5
4E	-17	SER	-	expression tag	UNP Q4ZAS5
4E	-16	SER	-	expression tag	UNP Q4ZAS5
4E	-15	HIS	-	expression tag	UNP Q4ZAS5
4E	-14	HIS	-	expression tag	UNP Q4ZAS5
4E	-13	HIS	-	expression tag	UNP Q4ZAS5
4E	-12	HIS	-	expression tag	UNP Q4ZAS5
4E	-11	HIS	-	expression tag	UNP Q4ZAS5
4E	-10	HIS	-	expression tag	UNP Q4ZAS5
4E	-9	SER	-	expression tag	UNP Q4ZAS5
4E	-8	SER	-	expression tag	UNP Q4ZAS5
4E	-7	GLY	-	expression tag	UNP Q4ZAS5
4E	-6	LEU	-	expression tag	UNP Q4ZAS5
4E	-5	VAL	-	expression tag	UNP Q4ZAS5
4E	-4	PRO	-	expression tag	UNP Q4ZAS5
4E	-3	ARG	-	expression tag	UNP Q4ZAS5
4E	-2	GLY	-	expression tag	UNP Q4ZAS5
4E	-1	SER	-	expression tag	UNP Q4ZAS5
4E	0	HIS	-	expression tag	UNP Q4ZAS5
1F	-19	MET	-	initiating methionine	UNP Q4ZAS5
1F	-18	GLY	-	expression tag	UNP Q4ZAS5
1F	-17	SER	-	expression tag	UNP Q4ZAS5
1F	-16	SER	-	expression tag	UNP Q4ZAS5

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Chain	Residue	Modelled	Actual	Comment	Reference
1F	-15	HIS	-	expression tag	UNP Q4ZAS5
1F	-14	HIS	-	expression tag	UNP Q4ZAS5
1F	-13	HIS	-	expression tag	UNP Q4ZAS5
1F	-12	HIS	-	expression tag	UNP Q4ZAS5
1F	-11	HIS	-	expression tag	UNP Q4ZAS5
1F	-10	HIS	-	expression tag	UNP Q4ZAS5
1F	-9	SER	-	expression tag	UNP Q4ZAS5
1F	-8	SER	-	expression tag	UNP Q4ZAS5
1F	-7	GLY	-	expression tag	UNP Q4ZAS5
1F	-6	LEU	-	expression tag	UNP Q4ZAS5
1F	-5	VAL	-	expression tag	UNP Q4ZAS5
1F	-4	PRO	-	expression tag	UNP Q4ZAS5
1F	-3	ARG	-	expression tag	UNP Q4ZAS5
1F	-2	GLY	-	expression tag	UNP Q4ZAS5
1F	-1	SER	-	expression tag	UNP Q4ZAS5
1F	0	HIS	-	expression tag	UNP Q4ZAS5
4F	-19	MET	-	initiating methionine	UNP Q4ZAS5
4F	-18	GLY	-	expression tag	UNP Q4ZAS5
4F	-17	SER	-	expression tag	UNP Q4ZAS5
4F	-16	SER	-	expression tag	UNP Q4ZAS5
4F	-15	HIS	-	expression tag	UNP Q4ZAS5
4F	-14	HIS	-	expression tag	UNP Q4ZAS5
4F	-13	HIS	-	expression tag	UNP Q4ZAS5
4F	-12	HIS	-	expression tag	UNP Q4ZAS5
4F	-11	HIS	-	expression tag	UNP Q4ZAS5
4F	-10	HIS	-	expression tag	UNP Q4ZAS5
4F	-9	SER	-	expression tag	UNP Q4ZAS5
4F	-8	SER	-	expression tag	UNP Q4ZAS5
4F	-7	GLY	-	expression tag	UNP Q4ZAS5
4F	-6	LEU	-	expression tag	UNP Q4ZAS5
4F	-5	VAL	-	expression tag	UNP Q4ZAS5
4F	-4	PRO	-	expression tag	UNP Q4ZAS5
4F	-3	ARG	-	expression tag	UNP Q4ZAS5
4F	-2	GLY	-	expression tag	UNP Q4ZAS5
4F	-1	SER	-	expression tag	UNP Q4ZAS5
4F	0	HIS	-	expression tag	UNP Q4ZAS5
1G	-19	MET	-	initiating methionine	UNP Q4ZAS5
1G	-18	GLY	-	expression tag	UNP Q4ZAS5
1G	-17	SER	-	expression tag	UNP Q4ZAS5
1G	-16	SER	-	expression tag	UNP Q4ZAS5
1G	-15	HIS	-	expression tag	UNP Q4ZAS5
1G	-14	HIS	-	expression tag	UNP Q4ZAS5

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Chain	Residue	Modelled	Actual	Comment	Reference
1G	-13	HIS	-	expression tag	UNP Q4ZAS5
1G	-12	HIS	-	expression tag	UNP Q4ZAS5
1G	-11	HIS	-	expression tag	UNP Q4ZAS5
1G	-10	HIS	-	expression tag	UNP Q4ZAS5
1G	-9	SER	-	expression tag	UNP Q4ZAS5
1G	-8	SER	-	expression tag	UNP Q4ZAS5
1G	-7	GLY	-	expression tag	UNP Q4ZAS5
1G	-6	LEU	-	expression tag	UNP Q4ZAS5
1G	-5	VAL	-	expression tag	UNP Q4ZAS5
1G	-4	PRO	-	expression tag	UNP Q4ZAS5
1G	-3	ARG	-	expression tag	UNP Q4ZAS5
1G	-2	GLY	-	expression tag	UNP Q4ZAS5
1G	-1	SER	-	expression tag	UNP Q4ZAS5
1G	0	HIS	-	expression tag	UNP Q4ZAS5
4G	-19	MET	-	initiating methionine	UNP Q4ZAS5
4G	-18	GLY	-	expression tag	UNP Q4ZAS5
4G	-17	SER	-	expression tag	UNP Q4ZAS5
4G	-16	SER	-	expression tag	UNP Q4ZAS5
4G	-15	HIS	-	expression tag	UNP Q4ZAS5
4G	-14	HIS	-	expression tag	UNP Q4ZAS5
4G	-13	HIS	-	expression tag	UNP Q4ZAS5
4G	-12	HIS	-	expression tag	UNP Q4ZAS5
4G	-11	HIS	-	expression tag	UNP Q4ZAS5
4G	-10	HIS	-	expression tag	UNP Q4ZAS5
4G	-9	SER	-	expression tag	UNP Q4ZAS5
4G	-8	SER	-	expression tag	UNP Q4ZAS5
4G	-7	GLY	-	expression tag	UNP Q4ZAS5
4G	-6	LEU	-	expression tag	UNP Q4ZAS5
4G	-5	VAL	-	expression tag	UNP Q4ZAS5
4G	-4	PRO	-	expression tag	UNP Q4ZAS5
4G	-3	ARG	-	expression tag	UNP Q4ZAS5
4G	-2	GLY	-	expression tag	UNP Q4ZAS5
4G	-1	SER	-	expression tag	UNP Q4ZAS5
4G	0	HIS	-	expression tag	UNP Q4ZAS5
1H	-19	MET	-	initiating methionine	UNP Q4ZAS5
1H	-18	GLY	-	expression tag	UNP Q4ZAS5
1H	-17	SER	-	expression tag	UNP Q4ZAS5
1H	-16	SER	-	expression tag	UNP Q4ZAS5
1H	-15	HIS	-	expression tag	UNP Q4ZAS5
1H	-14	HIS	-	expression tag	UNP Q4ZAS5
1H	-13	HIS	-	expression tag	UNP Q4ZAS5
1H	-12	HIS	-	expression tag	UNP Q4ZAS5

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Chain	Residue	Modelled	Actual	Comment	Reference
1H	-11	HIS	-	expression tag	UNP Q4ZAS5
1H	-10	HIS	-	expression tag	UNP Q4ZAS5
1H	-9	SER	-	expression tag	UNP Q4ZAS5
1H	-8	SER	-	expression tag	UNP Q4ZAS5
1H	-7	GLY	-	expression tag	UNP Q4ZAS5
1H	-6	LEU	-	expression tag	UNP Q4ZAS5
1H	-5	VAL	-	expression tag	UNP Q4ZAS5
1H	-4	PRO	-	expression tag	UNP Q4ZAS5
1H	-3	ARG	-	expression tag	UNP Q4ZAS5
1H	-2	GLY	-	expression tag	UNP Q4ZAS5
1H	-1	SER	-	expression tag	UNP Q4ZAS5
1H	0	HIS	-	expression tag	UNP Q4ZAS5
4H	-19	MET	-	initiating methionine	UNP Q4ZAS5
4H	-18	GLY	-	expression tag	UNP Q4ZAS5
4H	-17	SER	-	expression tag	UNP Q4ZAS5
4H	-16	SER	-	expression tag	UNP Q4ZAS5
4H	-15	HIS	-	expression tag	UNP Q4ZAS5
4H	-14	HIS	-	expression tag	UNP Q4ZAS5
4H	-13	HIS	-	expression tag	UNP Q4ZAS5
4H	-12	HIS	-	expression tag	UNP Q4ZAS5
4H	-11	HIS	-	expression tag	UNP Q4ZAS5
4H	-10	HIS	-	expression tag	UNP Q4ZAS5
4H	-9	SER	-	expression tag	UNP Q4ZAS5
4H	-8	SER	-	expression tag	UNP Q4ZAS5
4H	-7	GLY	-	expression tag	UNP Q4ZAS5
4H	-6	LEU	-	expression tag	UNP Q4ZAS5
4H	-5	VAL	-	expression tag	UNP Q4ZAS5
4H	-4	PRO	-	expression tag	UNP Q4ZAS5
4H	-3	ARG	-	expression tag	UNP Q4ZAS5
4H	-2	GLY	-	expression tag	UNP Q4ZAS5
4H	-1	SER	-	expression tag	UNP Q4ZAS5
4H	0	HIS	-	expression tag	UNP Q4ZAS5
1I	-19	MET	-	initiating methionine	UNP Q4ZAS5
1I	-18	GLY	-	expression tag	UNP Q4ZAS5
1I	-17	SER	-	expression tag	UNP Q4ZAS5
1I	-16	SER	-	expression tag	UNP Q4ZAS5
1I	-15	HIS	-	expression tag	UNP Q4ZAS5
1I	-14	HIS	-	expression tag	UNP Q4ZAS5
1I	-13	HIS	-	expression tag	UNP Q4ZAS5
1I	-12	HIS	-	expression tag	UNP Q4ZAS5
1I	-11	HIS	-	expression tag	UNP Q4ZAS5
1I	-10	HIS	-	expression tag	UNP Q4ZAS5

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Chain	Residue	Modelled	Actual	Comment	Reference
1I	-9	SER	-	expression tag	UNP Q4ZAS5
1I	-8	SER	-	expression tag	UNP Q4ZAS5
1I	-7	GLY	-	expression tag	UNP Q4ZAS5
1I	-6	LEU	-	expression tag	UNP Q4ZAS5
1I	-5	VAL	-	expression tag	UNP Q4ZAS5
1I	-4	PRO	-	expression tag	UNP Q4ZAS5
1I	-3	ARG	-	expression tag	UNP Q4ZAS5
1I	-2	GLY	-	expression tag	UNP Q4ZAS5
1I	-1	SER	-	expression tag	UNP Q4ZAS5
1I	0	HIS	-	expression tag	UNP Q4ZAS5
4I	-19	MET	-	initiating methionine	UNP Q4ZAS5
4I	-18	GLY	-	expression tag	UNP Q4ZAS5
4I	-17	SER	-	expression tag	UNP Q4ZAS5
4I	-16	SER	-	expression tag	UNP Q4ZAS5
4I	-15	HIS	-	expression tag	UNP Q4ZAS5
4I	-14	HIS	-	expression tag	UNP Q4ZAS5
4I	-13	HIS	-	expression tag	UNP Q4ZAS5
4I	-12	HIS	-	expression tag	UNP Q4ZAS5
4I	-11	HIS	-	expression tag	UNP Q4ZAS5
4I	-10	HIS	-	expression tag	UNP Q4ZAS5
4I	-9	SER	-	expression tag	UNP Q4ZAS5
4I	-8	SER	-	expression tag	UNP Q4ZAS5
4I	-7	GLY	-	expression tag	UNP Q4ZAS5
4I	-6	LEU	-	expression tag	UNP Q4ZAS5
4I	-5	VAL	-	expression tag	UNP Q4ZAS5
4I	-4	PRO	-	expression tag	UNP Q4ZAS5
4I	-3	ARG	-	expression tag	UNP Q4ZAS5
4I	-2	GLY	-	expression tag	UNP Q4ZAS5
4I	-1	SER	-	expression tag	UNP Q4ZAS5
4I	0	HIS	-	expression tag	UNP Q4ZAS5

- Molecule 2 is a protein called Helix-turn-helix XRE family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2A	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	3A	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	2B	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	3B	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	2C	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	3C	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	2D	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	3D	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	2E	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	3E	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	2F	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	3F	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	2G	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	3G	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	2H	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	3H	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	2I	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		
2	3I	218	Total	C	N	O	S	0	0
			1790	1137	295	354	4		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2A	225	LEU	-	expression tag	UNP A0FIL5
2A	226	GLU	-	expression tag	UNP A0FIL5
2A	227	HIS	-	expression tag	UNP A0FIL5
2A	228	HIS	-	expression tag	UNP A0FIL5
2A	229	HIS	-	expression tag	UNP A0FIL5
2A	230	HIS	-	expression tag	UNP A0FIL5
2A	231	HIS	-	expression tag	UNP A0FIL5
2A	232	HIS	-	expression tag	UNP A0FIL5
3A	225	LEU	-	expression tag	UNP A0FIL5
3A	226	GLU	-	expression tag	UNP A0FIL5
3A	227	HIS	-	expression tag	UNP A0FIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
3A	228	HIS	-	expression tag	UNP A0FIL5
3A	229	HIS	-	expression tag	UNP A0FIL5
3A	230	HIS	-	expression tag	UNP A0FIL5
3A	231	HIS	-	expression tag	UNP A0FIL5
3A	232	HIS	-	expression tag	UNP A0FIL5
2B	225	LEU	-	expression tag	UNP A0FIL5
2B	226	GLU	-	expression tag	UNP A0FIL5
2B	227	HIS	-	expression tag	UNP A0FIL5
2B	228	HIS	-	expression tag	UNP A0FIL5
2B	229	HIS	-	expression tag	UNP A0FIL5
2B	230	HIS	-	expression tag	UNP A0FIL5
2B	231	HIS	-	expression tag	UNP A0FIL5
2B	232	HIS	-	expression tag	UNP A0FIL5
3B	225	LEU	-	expression tag	UNP A0FIL5
3B	226	GLU	-	expression tag	UNP A0FIL5
3B	227	HIS	-	expression tag	UNP A0FIL5
3B	228	HIS	-	expression tag	UNP A0FIL5
3B	229	HIS	-	expression tag	UNP A0FIL5
3B	230	HIS	-	expression tag	UNP A0FIL5
3B	231	HIS	-	expression tag	UNP A0FIL5
3B	232	HIS	-	expression tag	UNP A0FIL5
2C	225	LEU	-	expression tag	UNP A0FIL5
2C	226	GLU	-	expression tag	UNP A0FIL5
2C	227	HIS	-	expression tag	UNP A0FIL5
2C	228	HIS	-	expression tag	UNP A0FIL5
2C	229	HIS	-	expression tag	UNP A0FIL5
2C	230	HIS	-	expression tag	UNP A0FIL5
2C	231	HIS	-	expression tag	UNP A0FIL5
2C	232	HIS	-	expression tag	UNP A0FIL5
3C	225	LEU	-	expression tag	UNP A0FIL5
3C	226	GLU	-	expression tag	UNP A0FIL5
3C	227	HIS	-	expression tag	UNP A0FIL5
3C	228	HIS	-	expression tag	UNP A0FIL5
3C	229	HIS	-	expression tag	UNP A0FIL5
3C	230	HIS	-	expression tag	UNP A0FIL5
3C	231	HIS	-	expression tag	UNP A0FIL5
3C	232	HIS	-	expression tag	UNP A0FIL5
2D	225	LEU	-	expression tag	UNP A0FIL5
2D	226	GLU	-	expression tag	UNP A0FIL5
2D	227	HIS	-	expression tag	UNP A0FIL5
2D	228	HIS	-	expression tag	UNP A0FIL5
2D	229	HIS	-	expression tag	UNP A0FIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
2D	230	HIS	-	expression tag	UNP A0FIL5
2D	231	HIS	-	expression tag	UNP A0FIL5
2D	232	HIS	-	expression tag	UNP A0FIL5
3D	225	LEU	-	expression tag	UNP A0FIL5
3D	226	GLU	-	expression tag	UNP A0FIL5
3D	227	HIS	-	expression tag	UNP A0FIL5
3D	228	HIS	-	expression tag	UNP A0FIL5
3D	229	HIS	-	expression tag	UNP A0FIL5
3D	230	HIS	-	expression tag	UNP A0FIL5
3D	231	HIS	-	expression tag	UNP A0FIL5
3D	232	HIS	-	expression tag	UNP A0FIL5
2E	225	LEU	-	expression tag	UNP A0FIL5
2E	226	GLU	-	expression tag	UNP A0FIL5
2E	227	HIS	-	expression tag	UNP A0FIL5
2E	228	HIS	-	expression tag	UNP A0FIL5
2E	229	HIS	-	expression tag	UNP A0FIL5
2E	230	HIS	-	expression tag	UNP A0FIL5
2E	231	HIS	-	expression tag	UNP A0FIL5
2E	232	HIS	-	expression tag	UNP A0FIL5
3E	225	LEU	-	expression tag	UNP A0FIL5
3E	226	GLU	-	expression tag	UNP A0FIL5
3E	227	HIS	-	expression tag	UNP A0FIL5
3E	228	HIS	-	expression tag	UNP A0FIL5
3E	229	HIS	-	expression tag	UNP A0FIL5
3E	230	HIS	-	expression tag	UNP A0FIL5
3E	231	HIS	-	expression tag	UNP A0FIL5
3E	232	HIS	-	expression tag	UNP A0FIL5
2F	225	LEU	-	expression tag	UNP A0FIL5
2F	226	GLU	-	expression tag	UNP A0FIL5
2F	227	HIS	-	expression tag	UNP A0FIL5
2F	228	HIS	-	expression tag	UNP A0FIL5
2F	229	HIS	-	expression tag	UNP A0FIL5
2F	230	HIS	-	expression tag	UNP A0FIL5
2F	231	HIS	-	expression tag	UNP A0FIL5
2F	232	HIS	-	expression tag	UNP A0FIL5
3F	225	LEU	-	expression tag	UNP A0FIL5
3F	226	GLU	-	expression tag	UNP A0FIL5
3F	227	HIS	-	expression tag	UNP A0FIL5
3F	228	HIS	-	expression tag	UNP A0FIL5
3F	229	HIS	-	expression tag	UNP A0FIL5
3F	230	HIS	-	expression tag	UNP A0FIL5
3F	231	HIS	-	expression tag	UNP A0FIL5

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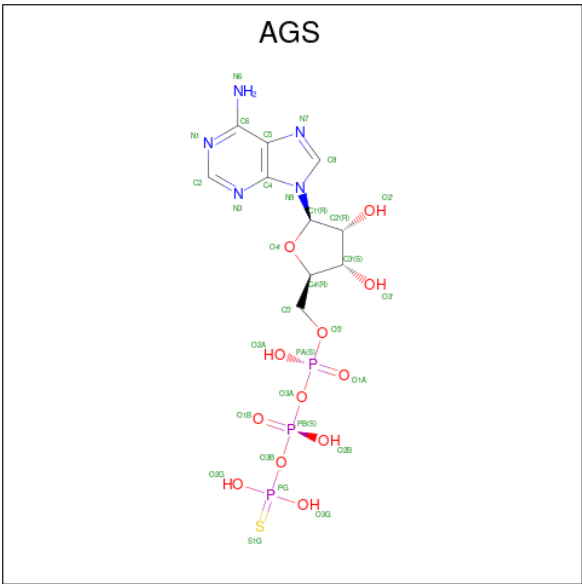
Chain	Residue	Modelled	Actual	Comment	Reference
3F	232	HIS	-	expression tag	UNP A0FIL5
2G	225	LEU	-	expression tag	UNP A0FIL5
2G	226	GLU	-	expression tag	UNP A0FIL5
2G	227	HIS	-	expression tag	UNP A0FIL5
2G	228	HIS	-	expression tag	UNP A0FIL5
2G	229	HIS	-	expression tag	UNP A0FIL5
2G	230	HIS	-	expression tag	UNP A0FIL5
2G	231	HIS	-	expression tag	UNP A0FIL5
2G	232	HIS	-	expression tag	UNP A0FIL5
3G	225	LEU	-	expression tag	UNP A0FIL5
3G	226	GLU	-	expression tag	UNP A0FIL5
3G	227	HIS	-	expression tag	UNP A0FIL5
3G	228	HIS	-	expression tag	UNP A0FIL5
3G	229	HIS	-	expression tag	UNP A0FIL5
3G	230	HIS	-	expression tag	UNP A0FIL5
3G	231	HIS	-	expression tag	UNP A0FIL5
3G	232	HIS	-	expression tag	UNP A0FIL5
2H	225	LEU	-	expression tag	UNP A0FIL5
2H	226	GLU	-	expression tag	UNP A0FIL5
2H	227	HIS	-	expression tag	UNP A0FIL5
2H	228	HIS	-	expression tag	UNP A0FIL5
2H	229	HIS	-	expression tag	UNP A0FIL5
2H	230	HIS	-	expression tag	UNP A0FIL5
2H	231	HIS	-	expression tag	UNP A0FIL5
2H	232	HIS	-	expression tag	UNP A0FIL5
3H	225	LEU	-	expression tag	UNP A0FIL5
3H	226	GLU	-	expression tag	UNP A0FIL5
3H	227	HIS	-	expression tag	UNP A0FIL5
3H	228	HIS	-	expression tag	UNP A0FIL5
3H	229	HIS	-	expression tag	UNP A0FIL5
3H	230	HIS	-	expression tag	UNP A0FIL5
3H	231	HIS	-	expression tag	UNP A0FIL5
3H	232	HIS	-	expression tag	UNP A0FIL5
2I	225	LEU	-	expression tag	UNP A0FIL5
2I	226	GLU	-	expression tag	UNP A0FIL5
2I	227	HIS	-	expression tag	UNP A0FIL5
2I	228	HIS	-	expression tag	UNP A0FIL5
2I	229	HIS	-	expression tag	UNP A0FIL5
2I	230	HIS	-	expression tag	UNP A0FIL5
2I	231	HIS	-	expression tag	UNP A0FIL5
2I	232	HIS	-	expression tag	UNP A0FIL5
3I	225	LEU	-	expression tag	UNP A0FIL5

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Chain	Residue	Modelled	Actual	Comment	Reference
3I	226	GLU	-	expression tag	UNP A0FIL5
3I	227	HIS	-	expression tag	UNP A0FIL5
3I	228	HIS	-	expression tag	UNP A0FIL5
3I	229	HIS	-	expression tag	UNP A0FIL5
3I	230	HIS	-	expression tag	UNP A0FIL5
3I	231	HIS	-	expression tag	UNP A0FIL5
3I	232	HIS	-	expression tag	UNP A0FIL5

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

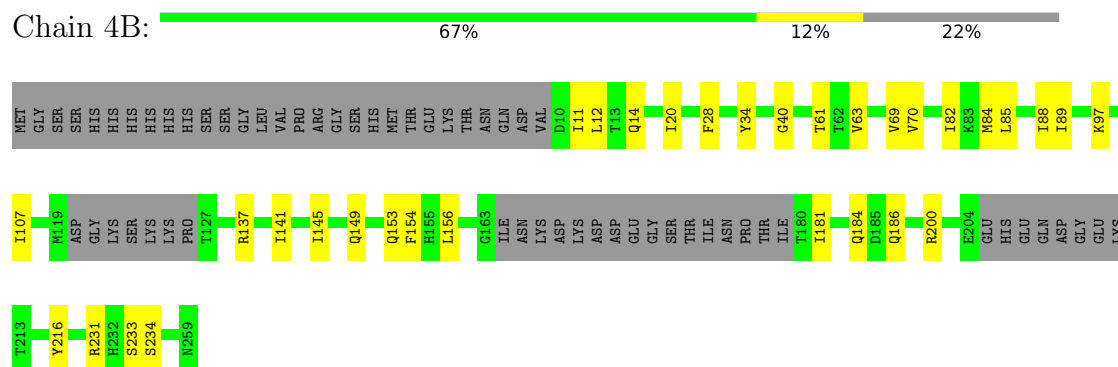


Mol	Chain	Residues	Atoms						AltConf
3	4A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	1B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	4B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	1C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	4C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	1D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
3	4D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

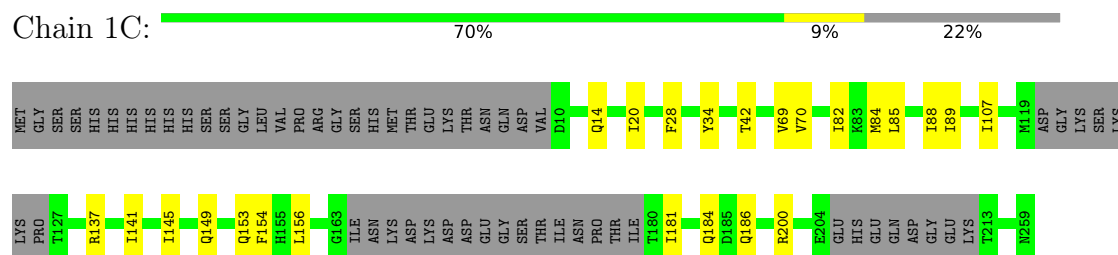
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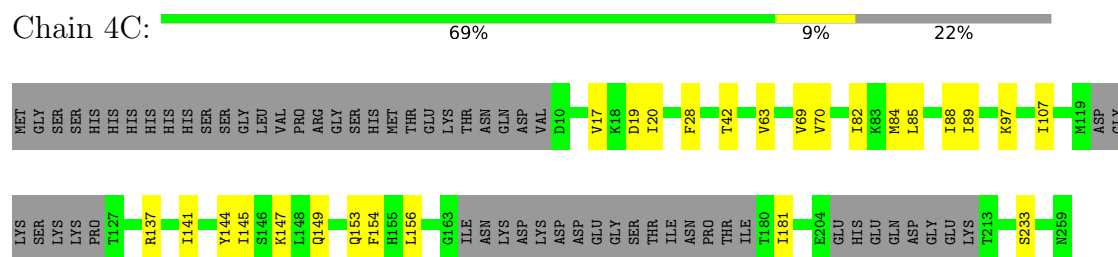
Mol	Chain	Residues	Atoms						AltConf
3	1E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	4E	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	1F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	4F	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	1G	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	4G	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	1H	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	4H	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
3	1I	1	Total 31	C 10	N 5	O 12	P 3	S 1	0



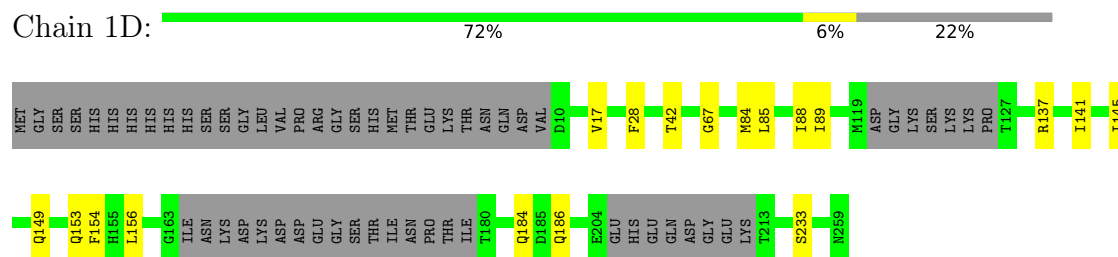
• Molecule 1: ORF016



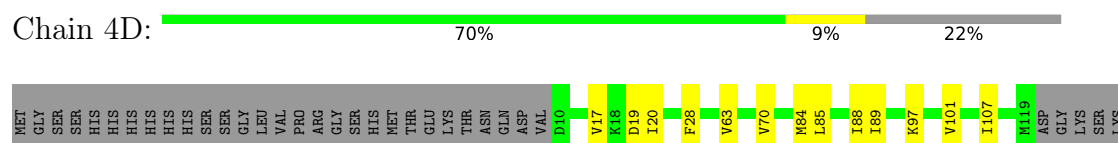
• Molecule 1: ORF016



• Molecule 1: ORF016



• Molecule 1: ORF016



[illegible]

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | V20 | V24 | F61 | F62 | N78 | V84 | F85 | E86 | G87 | H96 | D104 | F195 | PRO | ASN | LYS | GLY | GLU | K201 | L205 | I209 | E223 | TYR | LEU | GLU | LEU | HIS | HIS | HIS | HIS | HIS | HIS | HIS |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- [illegible]

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|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | L10 | G14 | I17 | S18 | R19 | V20 | A21 | K22 | D23 | V24 | L31 | F61 | F62 | N78 | V84 | F85 | E86 | H96 | D104 | D122 | F195 | P201 | L205 | L209 | E223 | Tyr | Leu | GLU | HIS | HIS | HIS | HIS | HIS |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|

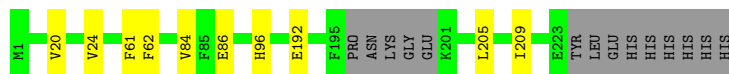
- | |
|-------------|
| F61 |
| V20 |
| V24 |
| F61
F62 |
| N82 |
| D83
V84 |
| F85
E86 |
| H96 |
| F195
PRO |
| ASN |
| LVS |
| GLY |
| GLU |
| K201 |
| L205 |
| I209 |
| E223 |
| TVR |
| LEU |
| GLU |
| HIS |
| HIS |
| HIS |
| HIS |
| HIS |
| HIS |

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| #1 | K16 | V20 | V24 | F61 | F62 | N82 | Dc3 | H84 | F85 | E86 | H96 | E192 | F195 | PRO | ASN | LYS | GLY | GLU | X201 | L205 | I209 | E223 | TVR | LEU | GLU | HIS | HIS | HIS | HIS | HIS | HIS |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|-----|-----|-----|-----|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- [illegible]

- Molecule 2: Helix-turn-helix XRE family protein

Chain 2D:  90% 5% 6%




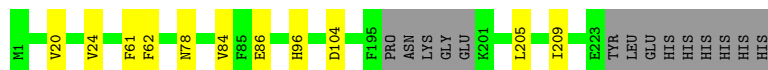
- Molecule 2: Helix-turn-helix XRE family protein

Chain 3D:  89% 5% 6%



- Molecule 2: Helix-turn-helix XRE family protein

Chain 2E:  89% 5% 6%



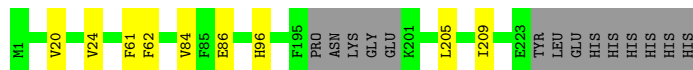
- Molecule 2: Helix-turn-helix XRE family protein

Chain 3E:  89% 5% 6%



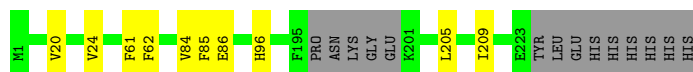
- Molecule 2: Helix-turn-helix XRE family protein

Chain 2F:  90% 5% 6%




- Molecule 2: Helix-turn-helix XRE family protein

Chain 3F:  90% 5% 6%




- Molecule 2: Helix-turn-helix XRE family protein

Chain 2G:  88% 6% 6%



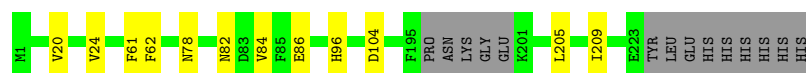
- Molecule 2: Helix-turn-helix XRE family protein

Chain 3G:  88% 6% 6%




- Molecule 2: Helix-turn-helix XRE family protein

Chain 2H:  89% 5% 6%




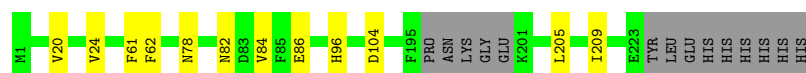
- Molecule 2: Helix-turn-helix XRE family protein

Chain 3H:  87% 7% 6%




- Molecule 2: Helix-turn-helix XRE family protein

Chain 2I:  89% 5% 6%



- Molecule 2: Helix-turn-helix XRE family protein

Chain 3I:  89% 5% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	141863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was applied on-the-fly during data collection with CryoSPARC Live.	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	190000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	1A	0.60	0/1781	0.64	0/2397
1	1B	0.60	0/1781	0.67	0/2397
1	1C	0.60	0/1781	0.64	0/2397
1	1D	0.60	0/1781	0.64	0/2397
1	1E	0.60	0/1781	0.64	0/2397
1	1F	0.60	0/1781	0.64	0/2397
1	1G	0.60	0/1781	0.64	0/2397
1	1H	0.60	0/1781	0.64	0/2397
1	1I	0.60	0/1781	0.64	0/2397
1	4A	0.60	0/1781	0.64	0/2397
1	4B	0.60	0/1781	0.64	0/2397
1	4C	0.60	0/1781	0.64	0/2397
1	4D	0.61	0/1781	0.64	0/2397
1	4E	0.60	0/1781	0.64	0/2397
1	4F	0.60	0/1781	0.64	0/2397
1	4G	0.60	0/1781	0.64	0/2397
1	4H	0.60	0/1781	0.66	0/2397
1	4I	0.61	0/1781	0.65	0/2397
2	2A	0.61	0/1818	0.62	0/2443
2	2B	0.61	0/1818	0.62	0/2443
2	2C	0.61	0/1818	0.62	0/2443
2	2D	0.61	0/1818	0.62	0/2443
2	2E	0.61	0/1818	0.62	0/2443
2	2F	0.61	0/1818	0.62	0/2443
2	2G	0.61	0/1818	0.62	0/2443
2	2H	0.61	0/1818	0.62	0/2443
2	2I	0.61	0/1818	0.62	0/2443
2	3A	0.61	0/1818	0.62	0/2443
2	3B	0.61	0/1818	0.62	0/2443
2	3C	0.61	0/1818	0.62	0/2443
2	3D	0.61	0/1818	0.62	0/2443
2	3E	0.61	0/1818	0.62	0/2443

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	3F	0.61	0/1818	0.62	0/2443
2	3G	0.61	0/1818	0.62	0/2443
2	3H	0.61	0/1818	0.62	0/2443
2	3I	0.61	0/1818	0.62	0/2443
All	All	0.61	0/64782	0.63	0/87120

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	1758	0	1776	38	0
1	1B	1758	0	1776	66	0
1	1C	1758	0	1776	15	0
1	1D	1758	0	1776	11	0
1	1E	1758	0	1776	12	0
1	1F	1758	0	1776	16	0
1	1G	1758	0	1776	24	0
1	1H	1758	0	1776	43	0
1	1I	1758	0	1776	36	0
1	4A	1758	0	1776	38	0
1	4B	1758	0	1776	43	0
1	4C	1758	0	1776	23	0
1	4D	1758	0	1776	16	0
1	4E	1758	0	1776	12	0
1	4F	1758	0	1776	12	0
1	4G	1758	0	1776	12	0
1	4H	1758	0	1776	58	0
1	4I	1758	0	1776	30	0
2	2A	1790	0	1773	12	0
2	2B	1790	0	1773	11	0
2	2C	1790	0	1773	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	2D	1790	0	1773	6	0
2	2E	1790	0	1773	6	0
2	2F	1790	0	1773	5	0
2	2G	1790	0	1773	8	0
2	2H	1790	0	1773	10	0
2	2I	1790	0	1773	10	0
2	3A	1790	0	1773	9	0
2	3B	1790	0	1773	9	0
2	3C	1790	0	1773	8	0
2	3D	1790	0	1773	7	0
2	3E	1790	0	1773	7	0
2	3F	1790	0	1773	6	0
2	3G	1790	0	1773	8	0
2	3H	1790	0	1773	10	0
2	3I	1790	0	1773	12	0
3	1B	31	0	12	5	0
3	1C	31	0	12	1	0
3	1D	31	0	12	1	0
3	1E	31	0	12	0	0
3	1F	31	0	12	0	0
3	1G	31	0	12	1	0
3	1H	31	0	12	4	0
3	1I	31	0	12	7	0
3	4A	31	0	12	7	0
3	4B	31	0	12	4	0
3	4C	31	0	12	1	0
3	4D	31	0	12	0	0
3	4E	31	0	12	0	0
3	4F	31	0	12	1	0
3	4G	31	0	12	1	0
3	4H	31	0	12	3	0
All	All	64360	0	64074	495	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (495) 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)
1:4H:47:LYS:HE3	1:4I:234:SER:HB3	1.44	0.99
1:1A:234:SER:HB3	1:1B:47:LYS:HE3	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:23:GLN:NE2	1:1B:61:THR:HG21	1.81	0.94
1:4A:67:GLY:O	1:4B:20:ILE:HG13	1.69	0.92
1:1H:20:ILE:HG13	1:1I:67:GLY:O	1.69	0.91
1:1A:29:TYR:HE1	1:1B:62:THR:HG1	1.22	0.87
1:1A:234:SER:CB	1:1B:47:LYS:HE3	2.05	0.85
1:4H:47:LYS:HE3	1:4I:234:SER:CB	2.06	0.85
1:1I:14:GLN:NE2	2:2I:82:ASN:HD22	1.75	0.84
2:3B:82:ASN:HD22	1:4B:14:GLN:NE2	1.75	0.84
2:2A:85:PHE:CD2	1:1B:77:HIS:HD2	1.95	0.84
1:1H:14:GLN:NE2	2:2H:82:ASN:HD22	1.75	0.84
1:4H:77:HIS:HD2	2:3I:85:PHE:CD2	1.96	0.84
1:4H:57:ASN:OD1	1:4I:143:ARG:HD3	1.79	0.83
1:1A:143:ARG:HD3	1:1B:57:ASN:OD1	1.77	0.82
2:3A:82:ASN:HD22	1:4A:14:GLN:NE2	1.75	0.82
1:4A:42:THR:HG22	3:4A:301:AGS:O1B	1.80	0.82
1:1B:49:ASN:HB2	1:1B:66:ASP:HB3	1.62	0.81
1:1I:42:THR:HG22	3:1I:301:AGS:O1B	1.80	0.81
2:3B:82:ASN:HD22	1:4B:14:GLN:HE22	1.30	0.80
1:1G:17:VAL:HG22	1:1H:70:VAL:HB	1.64	0.80
1:4B:70:VAL:HB	1:4C:17:VAL:HG22	1.64	0.80
1:1H:14:GLN:HE22	2:2H:82:ASN:HD22	1.30	0.79
2:2A:85:PHE:CG	1:1B:77:HIS:CD2	2.71	0.78
2:3A:82:ASN:HD22	1:4A:14:GLN:HE22	1.30	0.77
1:4H:77:HIS:CD2	2:3I:85:PHE:CG	2.73	0.77
1:1I:14:GLN:HE22	2:2I:82:ASN:HD22	1.30	0.77
2:2A:85:PHE:CG	1:1B:77:HIS:HD2	2.03	0.76
1:4H:92:LEU:HD21	1:4I:17:VAL:HG11	1.67	0.76
2:2A:85:PHE:CD2	1:1B:77:HIS:CD2	2.74	0.75
1:1A:23:GLN:CD	1:1B:61:THR:HG21	2.06	0.74
1:4H:77:HIS:CD2	2:3I:85:PHE:CD2	2.76	0.74
1:4H:62:THR:OG1	1:4I:29:TYR:HE1	1.72	0.73
1:4H:77:HIS:HD2	2:3I:85:PHE:CG	2.05	0.73
1:1A:29:TYR:HE1	1:1B:62:THR:OG1	1.70	0.72
1:1H:12:LEU:HB2	1:1I:91:GLN:NE2	2.05	0.71
1:1A:29:TYR:CE1	1:1B:62:THR:OG1	2.43	0.71
1:4B:63:VAL:O	1:4C:233:SER:HA	1.90	0.71
1:1G:233:SER:HA	1:1H:63:VAL:O	1.89	0.71
1:4A:91:GLN:NE2	1:4B:12:LEU:HB2	2.05	0.71
1:1B:46:THR:HB	1:1B:64:THR:HG23	1.73	0.70
1:4H:62:THR:OG1	1:4I:29:TYR:CE1	2.43	0.70
1:1A:234:SER:OG	1:1B:47:LYS:CD	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1H:20:ILE:HD12	1:1I:67:GLY:CA	2.22	0.69
1:4H:63:VAL:HG22	1:4I:231:ARG:HB3	1.75	0.69
1:4A:67:GLY:CA	1:4B:20:ILE:HD12	2.23	0.69
1:4H:47:LYS:CD	1:4I:234:SER:OG	2.41	0.69
1:1A:234:SER:OG	1:1B:47:LYS:HD3	1.94	0.68
1:1A:231:ARG:HB3	1:1B:63:VAL:HG22	1.76	0.66
2:2A:87:GLY:HA3	1:1B:73:LYS:HZ2	1.60	0.66
1:4B:69:VAL:HG12	1:4C:20:ILE:HG12	1.78	0.66
1:4H:73:LYS:HZ2	2:3I:87:GLY:HA3	1.60	0.65
1:4H:47:LYS:HD3	1:4I:234:SER:OG	1.94	0.65
1:4H:62:THR:HG1	1:4I:29:TYR:HE1	1.38	0.65
1:1G:20:ILE:HG12	1:1H:69:VAL:HG12	1.78	0.64
1:1H:40:GLY:HA3	3:1H:301:AGS:C8	2.28	0.64
1:4B:40:GLY:HA3	3:4B:301:AGS:C8	2.28	0.64
1:4A:91:GLN:OE1	1:4B:11:ILE:HG23	1.97	0.63
2:3H:19:ARG:NH1	2:3H:22:LYS:HD3	2.14	0.62
2:2B:19:ARG:NH1	2:2B:22:LYS:HD3	2.15	0.62
1:1B:40:GLY:HA2	3:1B:301:AGS:O1A	2.00	0.62
1:1H:11:ILE:HG23	1:1I:91:GLN:OE1	2.01	0.61
1:4H:214:TYR:CE2	1:4I:222:PRO:HD2	2.36	0.61
1:1G:17:VAL:HG22	1:1H:70:VAL:CB	2.31	0.60
1:1H:20:ILE:CG1	1:1I:67:GLY:O	2.47	0.60
1:1A:27:LYS:NZ	1:1B:59:ASP:OD2	2.21	0.60
1:1G:147:LYS:HG3	2:2G:90:VAL:HG21	1.83	0.60
1:4H:92:LEU:HD22	1:4H:99:ILE:HG13	1.82	0.60
1:4B:70:VAL:CB	1:4C:17:VAL:HG22	2.31	0.60
1:1A:222:PRO:HD2	1:1B:214:TYR:CE2	2.36	0.60
2:3C:90:VAL:HG21	1:4C:147:LYS:HG3	1.83	0.59
1:4H:49:ASN:HB2	1:4H:66:ASP:HB3	1.84	0.59
1:4F:67:GLY:O	1:4G:20:ILE:HG13	2.03	0.59
1:4H:37:PHE:HA	3:4H:301:AGS:S1G	2.43	0.59
1:1B:37:PHE:HA	3:1B:301:AGS:S1G	2.43	0.58
1:4H:88:ILE:HD11	1:4I:15:LEU:HG	1.83	0.58
1:4H:40:GLY:HA2	3:4H:301:AGS:O1A	2.04	0.57
1:4A:62:THR:CG2	1:4B:231:ARG:HD3	2.35	0.57
2:2B:20:VAL:O	2:2B:24:VAL:HG22	2.05	0.57
2:2A:20:VAL:O	2:2A:24:VAL:HG22	2.05	0.57
2:3D:20:VAL:O	2:3D:24:VAL:HG22	2.05	0.57
2:2E:20:VAL:O	2:2E:24:VAL:HG22	2.05	0.57
2:3E:20:VAL:O	2:3E:24:VAL:HG22	2.05	0.57
2:3F:20:VAL:O	2:3F:24:VAL:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1B:88:ILE:O	1:1B:92:LEU:HD12	2.04	0.57
2:2C:20:VAL:O	2:2C:24:VAL:HG22	2.05	0.57
1:1B:92:LEU:HD22	1:1B:99:ILE:HG13	1.86	0.57
2:3A:20:VAL:O	2:3A:24:VAL:HG22	2.05	0.57
1:1C:20:ILE:HG13	1:1D:67:GLY:O	2.03	0.57
2:2H:20:VAL:O	2:2H:24:VAL:HG22	2.05	0.57
2:3I:20:VAL:O	2:3I:24:VAL:HG22	2.05	0.57
2:3C:20:VAL:O	2:3C:24:VAL:HG22	2.05	0.56
2:2F:20:VAL:O	2:2F:24:VAL:HG22	2.05	0.56
2:2G:20:VAL:O	2:2G:24:VAL:HG22	2.05	0.56
2:3H:17:ILE:HG23	2:3H:31:LEU:HD23	1.87	0.56
1:1A:12:LEU:HD13	1:1B:92:LEU:HG	1.88	0.56
1:1A:23:GLN:NE2	1:1B:61:THR:CG2	2.61	0.56
1:4A:67:GLY:O	1:4B:20:ILE:CG1	2.47	0.56
2:2B:17:ILE:HG23	2:2B:31:LEU:HD23	1.86	0.56
2:2B:19:ARG:HH11	2:2B:22:LYS:HD3	1.70	0.56
2:3B:20:VAL:O	2:3B:24:VAL:HG22	2.05	0.56
2:3G:20:VAL:O	2:3G:24:VAL:HG22	2.05	0.56
2:3H:20:VAL:O	2:3H:24:VAL:HG22	2.05	0.56
2:2I:20:VAL:O	2:2I:24:VAL:HG22	2.05	0.56
2:2D:20:VAL:O	2:2D:24:VAL:HG22	2.05	0.56
1:1H:231:ARG:HD3	1:1I:62:THR:CG2	2.35	0.56
2:3H:19:ARG:HH11	2:3H:22:LYS:HD3	1.70	0.56
1:1I:63:VAL:CG2	3:1I:301:AGS:H5'1	2.35	0.56
1:1A:24:ASN:ND2	1:1B:61:THR:O	2.36	0.56
1:4H:84:MET:O	1:4H:88:ILE:HG13	2.05	0.56
1:1D:17:VAL:HG22	1:1E:70:VAL:HB	1.89	0.55
1:4A:91:GLN:CD	1:4B:12:LEU:HB2	2.27	0.55
1:1H:12:LEU:HB2	1:1I:91:GLN:CD	2.26	0.55
1:4A:63:VAL:CG2	3:4A:301:AGS:H5'1	2.37	0.55
1:4B:40:GLY:HA3	3:4B:301:AGS:H8	1.89	0.55
1:1H:20:ILE:HG13	1:1I:67:GLY:C	2.26	0.54
1:1E:17:VAL:HG22	1:1F:70:VAL:HB	1.89	0.54
1:4H:88:ILE:O	1:4H:92:LEU:HD12	2.08	0.54
1:4A:67:GLY:C	1:4B:20:ILE:HG13	2.27	0.54
1:1H:20:ILE:CD1	1:1I:67:GLY:C	2.76	0.54
1:1D:42:THR:HG22	3:1D:301:AGS:O1B	2.07	0.54
1:4D:70:VAL:HB	1:4E:17:VAL:HG22	1.89	0.53
1:4E:70:VAL:HB	1:4F:17:VAL:HG22	1.89	0.53
1:4F:42:THR:HG22	3:4F:301:AGS:O1B	2.07	0.53
1:4A:67:GLY:C	1:4B:20:ILE:CD1	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1H:40:GLY:HA3	3:1H:301:AGS:H8	1.89	0.53
1:4B:216:TYR:CE2	3:4B:301:AGS:C4	2.92	0.53
1:1H:20:ILE:HD12	1:1I:67:GLY:C	2.29	0.53
1:1H:216:TYR:CE2	3:1H:301:AGS:C4	2.92	0.53
1:1I:63:VAL:HG21	3:1I:301:AGS:H5'1	1.90	0.53
1:1B:84:MET:O	1:1B:88:ILE:HG13	2.09	0.53
1:4H:203:ILE:HD13	1:4H:216:TYR:CE2	2.44	0.53
1:1B:203:ILE:HD13	1:1B:216:TYR:CE2	2.44	0.52
1:1H:233:SER:HA	1:1I:63:VAL:O	2.09	0.52
1:1A:11:ILE:HG22	1:1B:91:GLN:OE1	2.10	0.52
1:1A:27:LYS:HD3	1:1B:62:THR:HB	1.92	0.52
1:1I:14:GLN:NE2	2:2I:82:ASN:HB3	2.25	0.52
2:3A:82:ASN:HB3	1:4A:14:GLN:NE2	2.26	0.51
1:4H:52:LEU:HD11	1:4I:17:VAL:HG22	1.90	0.51
1:4H:91:GLN:OE1	1:4I:11:ILE:HG22	2.11	0.51
1:1H:14:GLN:NE2	2:2H:82:ASN:HB3	2.25	0.51
1:4H:41:LYS:HG2	3:4H:301:AGS:O1B	2.10	0.51
2:3B:82:ASN:HB3	1:4B:14:GLN:NE2	2.26	0.51
1:4A:67:GLY:C	1:4B:20:ILE:HD12	2.31	0.51
2:2B:205:LEU:O	2:2B:209:ILE:HG13	2.11	0.51
2:2C:205:LEU:O	2:2C:209:ILE:HG13	2.11	0.51
2:3A:205:LEU:O	2:3A:209:ILE:HG13	2.11	0.51
1:4A:63:VAL:HG21	3:4A:301:AGS:H5'1	1.93	0.51
2:3D:205:LEU:O	2:3D:209:ILE:HG13	2.11	0.51
2:2H:205:LEU:O	2:2H:209:ILE:HG13	2.11	0.51
1:1A:24:ASN:ND2	1:1B:64:THR:O	2.44	0.51
2:2E:205:LEU:O	2:2E:209:ILE:HG13	2.11	0.51
2:3C:205:LEU:O	2:3C:209:ILE:HG13	2.11	0.51
2:2F:205:LEU:O	2:2F:209:ILE:HG13	2.11	0.51
2:3F:205:LEU:O	2:3F:209:ILE:HG13	2.11	0.51
2:2I:205:LEU:O	2:2I:209:ILE:HG13	2.11	0.51
2:2D:205:LEU:O	2:2D:209:ILE:HG13	2.11	0.50
2:3I:205:LEU:O	2:3I:209:ILE:HG13	2.11	0.50
2:3B:205:LEU:O	2:3B:209:ILE:HG13	2.11	0.50
2:2G:205:LEU:O	2:2G:209:ILE:HG13	2.11	0.50
2:3G:205:LEU:O	2:3G:209:ILE:HG13	2.11	0.50
1:1G:20:ILE:HG12	1:1H:69:VAL:CG1	2.41	0.50
2:3H:205:LEU:O	2:3H:209:ILE:HG13	2.11	0.50
1:1H:12:LEU:CB	1:1I:91:GLN:NE2	2.75	0.50
1:1A:17:VAL:HA	1:1B:69:VAL:O	2.12	0.50
1:1B:35:GLY:CA	1:1B:41:LYS:HD3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2A:205:LEU:O	2:2A:209:ILE:HG13	2.11	0.49
1:4B:69:VAL:CG1	1:4C:20:ILE:HG12	2.41	0.49
1:1I:42:THR:CG2	3:1I:301:AGS:O1A	2.60	0.49
2:3E:205:LEU:O	2:3E:209:ILE:HG13	2.11	0.49
1:1H:20:ILE:HD12	1:1I:67:GLY:HA3	1.94	0.49
1:1C:42:THR:HG22	3:1C:301:AGS:O1B	2.13	0.49
1:1B:46:THR:HB	1:1B:64:THR:CG2	2.41	0.49
1:4C:97:LYS:HE2	1:4D:19:ASP:OD2	2.13	0.49
1:4C:70:VAL:HB	1:4D:17:VAL:HG22	1.94	0.49
1:1F:19:ASP:OD2	1:1G:97:LYS:HE2	2.13	0.49
1:4H:62:THR:HB	1:4I:27:LYS:HD3	1.95	0.48
1:1A:23:GLN:OE1	1:1B:69:VAL:HG11	2.13	0.48
1:1F:17:VAL:HG22	1:1G:70:VAL:HB	1.94	0.48
1:4A:91:GLN:NE2	1:4B:12:LEU:CB	2.75	0.48
1:4A:145:ILE:HG21	1:4A:156:LEU:HD13	1.96	0.48
1:1B:145:ILE:HG21	1:1B:156:LEU:HD13	1.96	0.48
1:4B:145:ILE:HG21	1:4B:156:LEU:HD13	1.96	0.48
1:1B:41:LYS:HG2	3:1B:301:AGS:O1B	2.13	0.48
1:1D:145:ILE:HG21	1:1D:156:LEU:HD13	1.96	0.48
1:4G:42:THR:HG22	3:4G:301:AGS:O1B	2.13	0.48
1:4H:92:LEU:HG	1:4I:12:LEU:HD13	1.95	0.48
1:4A:63:VAL:O	1:4B:233:SER:HA	2.12	0.48
1:1A:143:ARG:CD	1:1B:57:ASN:OD1	2.58	0.48
1:4H:37:PHE:HE1	1:4H:161:HIS:HD1	1.62	0.48
1:4H:145:ILE:HG21	1:4H:156:LEU:HD13	1.96	0.48
1:4A:91:GLN:OE1	1:4B:11:ILE:CG2	2.62	0.48
1:4C:69:VAL:HG12	1:4D:20:ILE:HG12	1.96	0.48
1:4F:145:ILE:HG21	1:4F:156:LEU:HD13	1.96	0.48
1:1B:37:PHE:HE1	1:1B:161:HIS:HD1	1.62	0.47
1:1A:12:LEU:HD22	1:1B:95:ASN:ND2	2.29	0.47
1:1G:42:THR:HG22	3:1G:301:AGS:O1B	2.14	0.47
1:4D:145:ILE:HG21	1:4D:156:LEU:HD13	1.96	0.47
1:1I:145:ILE:HG21	1:1I:156:LEU:HD13	1.96	0.47
1:1A:28:PHE:CZ	1:1A:153:GLN:HB3	2.50	0.47
1:4G:28:PHE:CZ	1:4G:153:GLN:HB3	2.50	0.47
1:1H:145:ILE:HG21	1:1H:156:LEU:HD13	1.96	0.47
1:1D:28:PHE:CZ	1:1D:153:GLN:HB3	2.50	0.47
1:4D:28:PHE:CZ	1:4D:153:GLN:HB3	2.50	0.47
1:1C:28:PHE:CZ	1:1C:153:GLN:HB3	2.50	0.47
1:1B:28:PHE:CZ	1:1B:153:GLN:HB3	2.49	0.47
1:1E:233:SER:HA	1:1F:63:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4E:28:PHE:CZ	1:4E:153:GLN:HB3	2.50	0.47
1:4E:145:ILE:HG21	1:4E:156:LEU:HD13	1.96	0.47
1:1F:28:PHE:CZ	1:1F:153:GLN:HB3	2.50	0.47
1:1F:145:ILE:HG21	1:1F:156:LEU:HD13	1.96	0.47
1:4F:28:PHE:CZ	1:4F:153:GLN:HB3	2.50	0.47
1:1G:28:PHE:CZ	1:1G:153:GLN:HB3	2.50	0.47
1:1H:28:PHE:CZ	1:1H:153:GLN:HB3	2.50	0.47
1:4H:214:TYR:CD2	1:4I:222:PRO:HD2	2.50	0.47
1:1A:145:ILE:HG21	1:1A:156:LEU:HD13	1.96	0.47
1:4D:63:VAL:O	1:4E:233:SER:HA	2.14	0.47
2:2E:84:VAL:HB	2:2E:96:HIS:O	2.15	0.47
1:4C:42:THR:HG22	3:4C:301:AGS:O1B	2.14	0.47
2:2D:84:VAL:HB	2:2D:96:HIS:O	2.15	0.47
1:1E:145:ILE:HG21	1:1E:156:LEU:HD13	1.96	0.47
1:4H:28:PHE:CZ	1:4H:153:GLN:HB3	2.50	0.47
2:3I:84:VAL:HB	2:3I:96:HIS:O	2.15	0.47
1:4I:28:PHE:CZ	1:4I:153:GLN:HB3	2.50	0.47
2:2A:84:VAL:HB	2:2A:96:HIS:O	2.15	0.47
1:1I:42:THR:HG22	3:1I:301:AGS:O1A	2.15	0.47
2:3A:84:VAL:HB	2:3A:96:HIS:O	2.15	0.46
1:4A:42:THR:CG2	3:4A:301:AGS:O1A	2.63	0.46
2:3C:84:VAL:HB	2:3C:96:HIS:O	2.15	0.46
1:1E:28:PHE:CZ	1:1E:153:GLN:HB3	2.50	0.46
1:1F:20:ILE:HG12	1:1G:69:VAL:HG12	1.96	0.46
1:1I:28:PHE:CZ	1:1I:153:GLN:HB3	2.50	0.46
1:1C:145:ILE:HG21	1:1C:156:LEU:HD13	1.96	0.46
1:1G:145:ILE:HG21	1:1G:156:LEU:HD13	1.96	0.46
2:2G:84:VAL:HB	2:2G:96:HIS:O	2.15	0.46
2:2C:84:VAL:HB	2:2C:96:HIS:O	2.15	0.46
2:2F:84:VAL:HB	2:2F:96:HIS:O	2.15	0.46
2:3G:82:ASN:HD22	1:4G:14:GLN:NE2	2.14	0.46
1:4H:95:ASN:ND2	1:4I:12:LEU:HD22	2.30	0.46
1:1A:222:PRO:HD2	1:1B:214:TYR:CD2	2.51	0.46
2:3B:84:VAL:HB	2:3B:96:HIS:O	2.15	0.46
2:3F:84:VAL:HB	2:3F:96:HIS:O	2.15	0.46
1:4G:145:ILE:HG21	1:4G:156:LEU:HD13	1.96	0.46
1:1C:14:GLN:NE2	2:2C:82:ASN:HD22	2.14	0.46
2:3H:84:VAL:HB	2:3H:96:HIS:O	2.15	0.46
1:4H:35:GLY:CA	1:4H:41:LYS:HD3	2.45	0.46
1:4C:145:ILE:HG21	1:4C:156:LEU:HD13	1.96	0.46
1:4C:28:PHE:CZ	1:4C:153:GLN:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3E:84:VAL:HB	2:3E:96:HIS:O	2.15	0.46
1:4A:28:PHE:CZ	1:4A:153:GLN:HB3	2.50	0.46
1:4B:28:PHE:CZ	1:4B:153:GLN:HB3	2.50	0.46
1:4D:149:GLN:HG3	1:4D:154:PHE:O	2.16	0.46
1:4H:149:GLN:HG3	1:4H:154:PHE:O	2.16	0.46
1:1B:35:GLY:H	1:1B:41:LYS:HD3	1.80	0.46
2:2B:84:VAL:HB	2:2B:96:HIS:O	2.15	0.46
2:2H:84:VAL:HB	2:2H:96:HIS:O	2.15	0.46
1:4I:145:ILE:HG21	1:4I:156:LEU:HD13	1.96	0.46
1:1A:20:ILE:HG21	1:1B:64:THR:HB	1.98	0.46
1:1A:149:GLN:HG3	1:1A:154:PHE:O	2.16	0.46
1:4C:149:GLN:HG3	1:4C:154:PHE:O	2.16	0.46
1:4E:149:GLN:HG3	1:4E:154:PHE:O	2.16	0.46
1:1F:149:GLN:HG3	1:1F:154:PHE:O	2.16	0.46
2:3G:84:VAL:HB	2:3G:96:HIS:O	2.15	0.46
2:2I:84:VAL:HB	2:2I:96:HIS:O	2.15	0.46
1:4A:149:GLN:HG3	1:4A:154:PHE:O	2.16	0.45
1:1D:149:GLN:HG3	1:1D:154:PHE:O	2.16	0.45
1:4H:63:VAL:CG2	1:4I:231:ARG:HB3	2.45	0.45
1:1B:88:ILE:HG22	1:1B:92:LEU:HD11	1.97	0.45
2:3D:84:VAL:HB	2:3D:96:HIS:O	2.15	0.45
1:4H:35:GLY:H	1:4H:41:LYS:HD3	1.79	0.45
1:4H:46:THR:HB	1:4H:64:THR:HG23	1.98	0.45
1:4A:67:GLY:HA3	1:4B:20:ILE:HD12	1.94	0.45
1:1B:149:GLN:HG3	1:1B:154:PHE:O	2.16	0.45
1:4I:149:GLN:HG3	1:4I:154:PHE:O	2.16	0.45
2:3G:61:PHE:HD2	2:3G:62:PHE:CE1	2.35	0.45
1:4B:149:GLN:HG3	1:4B:154:PHE:O	2.16	0.45
2:3C:195:PHE:CE2	1:4C:144:TYR:CD2	3.05	0.45
1:4C:63:VAL:O	1:4D:233:SER:HA	2.16	0.45
1:1E:149:GLN:HG3	1:1E:154:PHE:O	2.16	0.45
2:3F:61:PHE:HD2	2:3F:62:PHE:CE1	2.35	0.45
2:2A:61:PHE:HD2	2:2A:62:PHE:CE1	2.35	0.45
1:4B:97:LYS:HE2	1:4C:19:ASP:OD2	2.17	0.45
1:1G:149:GLN:HG3	1:1G:154:PHE:O	2.16	0.45
1:1A:27:LYS:CD	1:1B:62:THR:HB	2.47	0.45
1:4B:61:THR:OG1	1:4C:20:ILE:HG23	2.17	0.45
2:2G:61:PHE:HD2	2:2G:62:PHE:CE1	2.35	0.45
2:2I:61:PHE:HD2	2:2I:62:PHE:CE1	2.35	0.45
1:1A:27:LYS:HE2	1:1B:62:THR:HB	1.99	0.45
2:2B:122:ASP:HB3	2:2C:16:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:61:PHE:HD2	2:3B:62:PHE:CE1	2.35	0.45
1:1F:233:SER:HA	1:1G:63:VAL:O	2.16	0.45
1:4F:149:GLN:HG3	1:4F:154:PHE:O	2.16	0.45
2:3H:61:PHE:HD2	2:3H:62:PHE:CE1	2.35	0.45
2:3A:61:PHE:HD2	2:3A:62:PHE:CE1	2.35	0.44
1:1H:149:GLN:HG3	1:1H:154:PHE:O	2.16	0.44
1:1I:149:GLN:HG3	1:1I:154:PHE:O	2.16	0.44
2:2D:61:PHE:HD2	2:2D:62:PHE:CE1	2.35	0.44
2:3D:61:PHE:HD2	2:3D:62:PHE:CE1	2.35	0.44
1:1H:11:ILE:CG2	1:1I:91:GLN:OE1	2.66	0.44
1:1H:40:GLY:CA	3:1H:301:AGS:H8	2.47	0.44
1:1B:35:GLY:HA3	1:1B:41:LYS:HD3	1.99	0.44
1:1C:149:GLN:HG3	1:1C:154:PHE:O	2.16	0.44
2:2F:61:PHE:HD2	2:2F:62:PHE:CE1	2.35	0.44
2:3G:16:LYS:NZ	2:3H:122:ASP:HB3	2.32	0.44
2:2H:61:PHE:HD2	2:2H:62:PHE:CE1	2.35	0.44
1:1B:217:VAL:HG21	1:1B:242:ARG:HB3	1.98	0.44
2:3E:61:PHE:HD2	2:3E:62:PHE:CE1	2.35	0.44
1:1G:19:ASP:OD2	1:1H:97:LYS:HE2	2.17	0.44
2:3C:61:PHE:HD2	2:3C:62:PHE:CE1	2.35	0.44
1:1G:20:ILE:HG23	1:1H:61:THR:OG1	2.17	0.44
1:1G:144:TYR:CD2	2:2G:195:PHE:CE2	3.05	0.44
1:4G:149:GLN:HG3	1:4G:154:PHE:O	2.16	0.44
1:1H:12:LEU:CB	1:1I:91:GLN:HE22	2.31	0.44
1:4H:41:LYS:O	1:4H:45:LEU:HG	2.17	0.44
2:2C:61:PHE:HD2	2:2C:62:PHE:CE1	2.35	0.44
2:3I:61:PHE:HD2	2:3I:62:PHE:CE1	2.35	0.44
1:1H:234:SER:HB3	1:1I:47:LYS:HE3	2.00	0.44
1:4H:216:TYR:CD1	1:4H:216:TYR:N	2.86	0.44
2:2A:86:GLU:O	2:2A:86:GLU:HG2	2.18	0.43
2:2B:61:PHE:HD2	2:2B:62:PHE:CE1	2.35	0.43
1:4B:40:GLY:CA	3:4B:301:AGS:H8	2.47	0.43
2:2D:86:GLU:O	2:2D:86:GLU:HG2	2.18	0.43
1:1H:14:GLN:HE21	2:2H:82:ASN:HB3	1.83	0.43
1:4A:42:THR:HG22	3:4A:301:AGS:O1A	2.18	0.43
2:2F:86:GLU:O	2:2F:86:GLU:HG2	2.18	0.43
1:1B:216:TYR:CD1	1:1B:216:TYR:N	2.86	0.43
1:1D:85:LEU:O	1:1D:89:ILE:HG13	2.19	0.43
2:2E:86:GLU:O	2:2E:86:GLU:HG2	2.19	0.43
1:1B:41:LYS:O	1:1B:44:PHE:HB3	2.18	0.43
2:3B:82:ASN:HB3	1:4B:14:GLN:HE21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4B:85:LEU:O	1:4B:89:ILE:HG13	2.19	0.43
1:4D:97:LYS:HE2	1:4E:19:ASP:OD2	2.18	0.43
1:1E:85:LEU:O	1:1E:89:ILE:HG13	2.19	0.43
2:2E:61:PHE:HD2	2:2E:62:PHE:CE1	2.35	0.43
2:3E:86:GLU:O	2:3E:86:GLU:HG2	2.18	0.43
1:4G:85:LEU:O	1:4G:89:ILE:HG13	2.19	0.43
1:4H:54:LEU:HG	1:4H:70:VAL:CG1	2.48	0.43
2:3F:86:GLU:HG2	2:3F:86:GLU:O	2.18	0.43
2:3G:86:GLU:O	2:3G:86:GLU:HG2	2.18	0.43
1:1I:85:LEU:O	1:1I:89:ILE:HG13	2.19	0.43
2:2B:10:LEU:O	2:2B:14:GLY:N	2.51	0.43
2:3D:86:GLU:O	2:3D:86:GLU:HG2	2.18	0.43
1:4D:85:LEU:O	1:4D:89:ILE:HG13	2.19	0.43
2:2G:86:GLU:O	2:2G:86:GLU:HG2	2.18	0.43
2:3A:82:ASN:HB3	1:4A:14:GLN:HE21	1.83	0.43
2:2B:86:GLU:O	2:2B:86:GLU:HG2	2.18	0.43
2:2C:86:GLU:O	2:2C:86:GLU:HG2	2.18	0.43
1:4C:85:LEU:O	1:4C:89:ILE:HG13	2.19	0.43
2:3A:86:GLU:O	2:3A:86:GLU:HG2	2.18	0.43
1:4A:47:LYS:HE3	1:4B:234:SER:HB3	2.00	0.43
1:1F:85:LEU:O	1:1F:89:ILE:HG13	2.19	0.43
1:1H:85:LEU:O	1:1H:89:ILE:HG13	2.19	0.43
2:3B:86:GLU:HG2	2:3B:86:GLU:O	2.18	0.43
1:4E:84:MET:O	1:4E:88:ILE:HG13	2.19	0.43
2:2H:86:GLU:HG2	2:2H:86:GLU:O	2.18	0.43
1:1I:43:THR:HG21	3:1I:301:AGS:N7	2.33	0.43
1:1A:85:LEU:O	1:1A:89:ILE:HG13	2.19	0.42
1:1B:35:GLY:N	1:1B:41:LYS:HD3	2.33	0.42
1:1C:85:LEU:O	1:1C:89:ILE:HG13	2.19	0.42
1:1E:19:ASP:OD2	1:1F:97:LYS:HE2	2.19	0.42
1:1H:84:MET:O	1:1H:88:ILE:HG13	2.19	0.42
1:4I:85:LEU:O	1:4I:89:ILE:HG13	2.19	0.42
1:1B:42:THR:O	1:1B:43:THR:C	2.58	0.42
1:1C:84:MET:O	1:1C:88:ILE:HG13	2.19	0.42
1:4F:85:LEU:O	1:4F:89:ILE:HG13	2.19	0.42
1:4G:84:MET:O	1:4G:88:ILE:HG13	2.19	0.42
2:3H:10:LEU:O	2:3H:14:GLY:N	2.51	0.42
1:4A:84:MET:O	1:4A:88:ILE:HG13	2.19	0.42
1:4B:84:MET:O	1:4B:88:ILE:HG13	2.19	0.42
1:4H:57:ASN:OD1	1:4I:143:ARG:CD	2.60	0.42
2:3I:86:GLU:O	2:3I:86:GLU:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4A:43:THR:HG21	3:4A:301:AGS:N7	2.34	0.42
1:4C:84:MET:O	1:4C:88:ILE:HG13	2.20	0.42
1:4F:84:MET:O	1:4F:88:ILE:HG13	2.20	0.42
1:4H:217:VAL:HG21	1:4H:242:ARG:HB3	1.99	0.42
1:4A:85:LEU:O	1:4A:89:ILE:HG13	2.19	0.42
1:1B:17:VAL:HG22	1:1C:70:VAL:HB	2.02	0.42
2:3C:86:GLU:O	2:3C:86:GLU:HG2	2.18	0.42
2:3H:86:GLU:O	2:3H:86:GLU:HG2	2.18	0.42
1:4I:84:MET:O	1:4I:88:ILE:HG13	2.19	0.42
1:1E:84:MET:O	1:1E:88:ILE:HG13	2.19	0.42
1:1G:84:MET:O	1:1G:88:ILE:HG13	2.19	0.42
2:2I:86:GLU:O	2:2I:86:GLU:HG2	2.18	0.42
1:1D:84:MET:O	1:1D:88:ILE:HG13	2.20	0.42
1:4D:84:MET:O	1:4D:88:ILE:HG13	2.19	0.42
1:1G:17:VAL:HG22	1:1H:70:VAL:CG2	2.50	0.42
1:1G:85:LEU:O	1:1G:89:ILE:HG13	2.19	0.42
1:1I:14:GLN:HE21	2:2I:82:ASN:HB3	1.83	0.42
1:1I:84:MET:O	1:1I:88:ILE:HG13	2.19	0.42
1:4H:35:GLY:N	1:4H:41:LYS:HD3	2.35	0.42
1:4H:47:LYS:CE	1:4I:234:SER:CB	2.89	0.42
1:4B:70:VAL:CG2	1:4C:17:VAL:HG22	2.50	0.42
1:4E:85:LEU:O	1:4E:89:ILE:HG13	2.19	0.42
1:4A:91:GLN:HE22	1:4B:12:LEU:CB	2.32	0.41
1:1B:217:VAL:CG2	1:1B:242:ARG:HB3	2.50	0.41
1:4G:69:VAL:HG12	1:4H:20:ILE:HG12	2.01	0.41
1:1H:137:ARG:O	1:1H:141:ILE:HG13	2.20	0.41
1:1I:41:LYS:HG2	3:1I:301:AGS:O2B	2.19	0.41
1:4B:82:ILE:HG23	1:4B:145:ILE:HD11	2.03	0.41
1:1E:137:ARG:O	1:1E:141:ILE:HG13	2.20	0.41
1:1F:84:MET:O	1:1F:88:ILE:HG13	2.19	0.41
1:1H:12:LEU:HB2	1:1I:91:GLN:HE22	1.85	0.41
1:1A:84:MET:O	1:1A:88:ILE:HG13	2.19	0.41
1:1A:137:ARG:O	1:1A:141:ILE:HG13	2.20	0.41
1:1A:231:ARG:HB3	1:1B:63:VAL:CG2	2.48	0.41
1:1A:234:SER:CB	1:1B:47:LYS:CE	2.88	0.41
2:2A:87:GLY:CA	1:1B:73:LYS:HZ2	2.28	0.41
1:1B:20:ILE:HG12	1:1C:69:VAL:HG12	2.01	0.41
1:1B:41:LYS:O	1:1B:45:LEU:HG	2.21	0.41
1:1C:137:ARG:O	1:1C:141:ILE:HG13	2.20	0.41
1:4F:82:ILE:HG23	1:4F:145:ILE:HD11	2.03	0.41
1:4F:137:ARG:O	1:4F:141:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1H:82:ILE:HG23	1:1H:145:ILE:HD11	2.03	0.41
1:4C:137:ARG:O	1:4C:141:ILE:HG13	2.20	0.41
1:1F:82:ILE:HG23	1:1F:145:ILE:HD11	2.03	0.41
1:1A:107:ILE:HG21	1:1A:181:ILE:HD11	2.03	0.41
1:4B:107:ILE:HG21	1:4B:181:ILE:HD11	2.03	0.41
1:1D:233:SER:HA	1:1E:63:VAL:O	2.20	0.41
1:4D:137:ARG:O	1:4D:141:ILE:HG13	2.20	0.41
1:4G:70:VAL:HB	1:4H:17:VAL:HG22	2.02	0.41
1:4H:82:ILE:HG23	1:4H:145:ILE:HD11	2.03	0.41
1:1A:82:ILE:HG23	1:1A:145:ILE:HD11	2.03	0.41
1:4A:137:ARG:O	1:4A:141:ILE:HG13	2.20	0.41
1:1B:40:GLY:HA3	3:1B:301:AGS:H8	2.02	0.41
1:1G:137:ARG:O	1:1G:141:ILE:HG13	2.20	0.41
1:1C:107:ILE:HG21	1:1C:181:ILE:HD11	2.03	0.41
1:4E:63:VAL:O	1:4F:233:SER:HA	2.20	0.41
1:4E:82:ILE:HG23	1:4E:145:ILE:HD11	2.03	0.41
1:1F:137:ARG:O	1:1F:141:ILE:HG13	2.21	0.41
1:1H:107:ILE:HG21	1:1H:181:ILE:HD11	2.03	0.41
1:4H:217:VAL:CG2	1:4H:242:ARG:HB3	2.51	0.41
1:4I:82:ILE:HG23	1:4I:145:ILE:HD11	2.02	0.41
1:4I:107:ILE:HG21	1:4I:181:ILE:HD11	2.03	0.41
1:1A:184:GLN:HB3	1:1A:186:GLN:OE1	2.21	0.41
1:4A:41:LYS:HG2	3:4A:301:AGS:O2B	2.21	0.41
1:4A:67:GLY:C	1:4B:20:ILE:CG1	2.88	0.41
1:4A:82:ILE:HG23	1:4A:145:ILE:HD11	2.03	0.41
1:1C:82:ILE:HG23	1:1C:145:ILE:HD11	2.03	0.41
1:4C:82:ILE:HG23	1:4C:145:ILE:HD11	2.03	0.41
1:1E:82:ILE:HG23	1:1E:145:ILE:HD11	2.03	0.41
1:1F:184:GLN:HB3	1:1F:186:GLN:OE1	2.21	0.41
1:1G:184:GLN:HB3	1:1G:186:GLN:OE1	2.21	0.41
1:4H:42:THR:O	1:4H:43:THR:C	2.59	0.41
1:4H:88:ILE:HG22	1:4H:92:LEU:HD11	2.02	0.41
1:4H:107:ILE:HG21	1:4H:181:ILE:HD11	2.03	0.41
1:4H:137:ARG:O	1:4H:141:ILE:HG13	2.20	0.41
1:4H:184:GLN:HB3	1:4H:186:GLN:OE1	2.21	0.41
1:1I:82:ILE:HG23	1:1I:145:ILE:HD11	2.03	0.41
2:2A:78:ASN:HB2	2:2A:104:ASP:OD1	2.21	0.41
1:4A:184:GLN:HB3	1:4A:186:GLN:OE1	2.21	0.41
1:1D:137:ARG:O	1:1D:141:ILE:HG13	2.21	0.41
1:4D:107:ILE:HG21	1:4D:181:ILE:HD11	2.03	0.41
2:3E:78:ASN:HB2	2:3E:104:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1H:20:ILE:CG1	1:1I:67:GLY:C	2.87	0.41
1:4I:137:ARG:O	1:4I:141:ILE:HG13	2.20	0.41
2:2B:78:ASN:HB2	2:2B:104:ASP:OD1	2.22	0.40
1:4B:137:ARG:O	1:4B:141:ILE:HG13	2.20	0.40
1:4C:107:ILE:HG21	1:4C:181:ILE:HD11	2.03	0.40
2:2H:78:ASN:HB2	2:2H:104:ASP:OD1	2.22	0.40
1:4H:55:ASP:OD1	1:4H:71:GLN:HA	2.22	0.40
1:1I:184:GLN:HB3	1:1I:186:GLN:OE1	2.21	0.40
1:4A:107:ILE:HG21	1:4A:181:ILE:HD11	2.03	0.40
1:1C:184:GLN:HB3	1:1C:186:GLN:OE1	2.21	0.40
2:2D:192:GLU:OE2	2:2D:192:GLU:N	2.54	0.40
2:3D:192:GLU:OE2	2:3D:192:GLU:N	2.54	0.40
1:1H:184:GLN:HB3	1:1H:186:GLN:OE1	2.21	0.40
1:1B:137:ARG:O	1:1B:141:ILE:HG13	2.20	0.40
1:1B:245:ASN:HA	3:1B:301:AGS:HN62	1.86	0.40
1:4D:184:GLN:HB3	1:4D:186:GLN:OE1	2.21	0.40
1:4E:77:HIS:HD2	2:3F:85:PHE:CE2	2.39	0.40
1:1G:82:ILE:HG23	1:1G:145:ILE:HD11	2.03	0.40
2:2G:78:ASN:HB2	2:2G:104:ASP:OD1	2.22	0.40
1:4G:137:ARG:O	1:4G:141:ILE:HG13	2.20	0.40
1:4H:73:LYS:HZ2	2:3I:87:GLY:CA	2.31	0.40
1:4H:203:ILE:HG12	1:4H:216:TYR:CD2	2.56	0.40
2:2I:78:ASN:HB2	2:2I:104:ASP:OD1	2.21	0.40
1:1B:184:GLN:HB3	1:1B:186:GLN:OE1	2.21	0.40
1:4B:184:GLN:HB3	1:4B:186:GLN:OE1	2.21	0.40
2:2C:192:GLU:OE2	2:2C:192:GLU:N	2.54	0.40
2:3C:78:ASN:HB2	2:3C:104:ASP:OD1	2.22	0.40
1:1D:184:GLN:HB3	1:1D:186:GLN:OE1	2.21	0.40
1:4D:101:VAL:HA	1:4D:155:HIS:O	2.22	0.40
2:2E:78:ASN:HB2	2:2E:104:ASP:OD1	2.22	0.40
2:3E:192:GLU:OE2	2:3E:192:GLU:N	2.54	0.40
1:1F:101:VAL:HA	1:1F:155:HIS:O	2.22	0.40
1:4F:184:GLN:HB3	1:4F:186:GLN:OE1	2.21	0.40
2:3G:78:ASN:HB2	2:3G:104:ASP:OD1	2.22	0.40
1:4G:101:VAL:HA	1:4G:155:HIS:O	2.22	0.40
1:4A:34:TYR:CZ	1:4A:200:ARG:HB2	2.57	0.40
1:4B:34:TYR:CZ	1:4B:200:ARG:HB2	2.57	0.40
1:1C:34:TYR:CZ	1:1C:200:ARG:HB2	2.57	0.40
2:3D:78:ASN:HB2	2:3D:104:ASP:OD1	2.22	0.40
1:1G:101:VAL:HA	1:1G:155:HIS:O	2.22	0.40
2:3I:24:VAL:HG11	2:3I:50:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4I:184:GLN:HB3	1:4I:186:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	1B	211/279 (76%)	206 (98%)	5 (2%)	0	100	100
1	1C	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	1D	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	1E	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	1F	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	1G	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	1H	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	1I	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	4A	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	4B	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	4C	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	4D	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	4E	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	4F	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	4G	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
1	4H	211/279 (76%)	207 (98%)	4 (2%)	0	100	100
1	4I	211/279 (76%)	209 (99%)	2 (1%)	0	100	100
2	2A	214/232 (92%)	209 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2B	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	2C	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	2D	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	2E	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	2F	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	2G	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	2H	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	2I	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	3A	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	3B	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	3C	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	3D	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	3E	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	3F	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	3G	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	3H	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
2	3I	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
All	All	7650/9198 (83%)	7519 (98%)	131 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	196/250 (78%)	196 (100%)	0	100	100
1	1B	196/250 (78%)	196 (100%)	0	100	100
1	1C	196/250 (78%)	196 (100%)	0	100	100
1	1D	196/250 (78%)	196 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1E	196/250 (78%)	196 (100%)	0	100	100
1	1F	196/250 (78%)	196 (100%)	0	100	100
1	1G	196/250 (78%)	196 (100%)	0	100	100
1	1H	196/250 (78%)	196 (100%)	0	100	100
1	1I	196/250 (78%)	196 (100%)	0	100	100
1	4A	196/250 (78%)	196 (100%)	0	100	100
1	4B	196/250 (78%)	196 (100%)	0	100	100
1	4C	196/250 (78%)	196 (100%)	0	100	100
1	4D	196/250 (78%)	196 (100%)	0	100	100
1	4E	196/250 (78%)	196 (100%)	0	100	100
1	4F	196/250 (78%)	196 (100%)	0	100	100
1	4G	196/250 (78%)	196 (100%)	0	100	100
1	4H	196/250 (78%)	196 (100%)	0	100	100
1	4I	196/250 (78%)	196 (100%)	0	100	100
2	2A	206/219 (94%)	206 (100%)	0	100	100
2	2B	206/219 (94%)	206 (100%)	0	100	100
2	2C	206/219 (94%)	206 (100%)	0	100	100
2	2D	206/219 (94%)	206 (100%)	0	100	100
2	2E	206/219 (94%)	206 (100%)	0	100	100
2	2F	206/219 (94%)	206 (100%)	0	100	100
2	2G	206/219 (94%)	206 (100%)	0	100	100
2	2H	206/219 (94%)	206 (100%)	0	100	100
2	2I	206/219 (94%)	206 (100%)	0	100	100
2	3A	206/219 (94%)	206 (100%)	0	100	100
2	3B	206/219 (94%)	206 (100%)	0	100	100
2	3C	206/219 (94%)	206 (100%)	0	100	100
2	3D	206/219 (94%)	206 (100%)	0	100	100
2	3E	206/219 (94%)	206 (100%)	0	100	100
2	3F	206/219 (94%)	206 (100%)	0	100	100
2	3G	206/219 (94%)	206 (100%)	0	100	100
2	3H	206/219 (94%)	206 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	3I	206/219 (94%)	206 (100%)	0	100	100
All	All	7236/8442 (86%)	7236 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	4A	14	GLN
1	1B	77	HIS
1	4B	14	GLN
1	1C	14	GLN
1	1D	14	GLN
1	4D	77	HIS
1	1E	77	HIS
1	4E	77	HIS
1	1F	77	HIS
1	4F	14	GLN
1	4G	14	GLN
1	1H	14	GLN
1	4H	77	HIS
1	1I	14	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AGS	1C	301	-	26,33,33	0.83	1 (3%)	26,52,52	0.79	1 (3%)
3	AGS	4B	301	-	26,33,33	0.85	1 (3%)	26,52,52	0.79	1 (3%)
3	AGS	1B	301	-	26,33,33	0.84	1 (3%)	26,52,52	0.78	1 (3%)
3	AGS	4D	301	-	26,33,33	0.83	1 (3%)	26,52,52	0.79	1 (3%)
3	AGS	1G	301	-	26,33,33	0.83	1 (3%)	26,52,52	0.80	1 (3%)
3	AGS	1I	301	-	26,33,33	0.83	1 (3%)	26,52,52	0.79	1 (3%)
3	AGS	1F	301	-	26,33,33	0.82	1 (3%)	26,52,52	0.78	1 (3%)
3	AGS	4G	301	-	26,33,33	0.83	1 (3%)	26,52,52	0.78	1 (3%)
3	AGS	1H	301	-	26,33,33	0.84	1 (3%)	26,52,52	0.79	1 (3%)
3	AGS	4E	301	-	26,33,33	0.83	1 (3%)	26,52,52	0.78	1 (3%)
3	AGS	4C	301	-	26,33,33	0.84	1 (3%)	26,52,52	0.79	1 (3%)
3	AGS	1D	301	-	26,33,33	0.83	1 (3%)	26,52,52	0.79	1 (3%)
3	AGS	4A	301	-	26,33,33	0.83	1 (3%)	26,52,52	0.79	1 (3%)
3	AGS	4H	301	-	26,33,33	0.83	1 (3%)	26,52,52	0.78	1 (3%)
3	AGS	1E	301	-	26,33,33	0.84	1 (3%)	26,52,52	0.79	1 (3%)
3	AGS	4F	301	-	26,33,33	0.84	1 (3%)	26,52,52	0.78	1 (3%)

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	AGS	1C	301	-	-	2/17/38/38	0/3/3/3
3	AGS	4B	301	-	-	2/17/38/38	0/3/3/3
3	AGS	1B	301	-	-	2/17/38/38	0/3/3/3
3	AGS	4D	301	-	-	2/17/38/38	0/3/3/3
3	AGS	1G	301	-	-	2/17/38/38	0/3/3/3
3	AGS	1I	301	-	-	2/17/38/38	0/3/3/3
3	AGS	1F	301	-	-	2/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	4G	301	-	-	2/17/38/38	0/3/3/3
3	AGS	1H	301	-	-	2/17/38/38	0/3/3/3
3	AGS	4E	301	-	-	2/17/38/38	0/3/3/3
3	AGS	4C	301	-	-	2/17/38/38	0/3/3/3
3	AGS	1D	301	-	-	2/17/38/38	0/3/3/3
3	AGS	4A	301	-	-	2/17/38/38	0/3/3/3
3	AGS	4H	301	-	-	2/17/38/38	0/3/3/3
3	AGS	1E	301	-	-	2/17/38/38	0/3/3/3
3	AGS	4F	301	-	-	2/17/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1E	301	AGS	PG-S1G	2.17	1.95	1.90
3	4B	301	AGS	PG-S1G	2.17	1.95	1.90
3	1B	301	AGS	PG-S1G	2.16	1.95	1.90
3	1C	301	AGS	PG-S1G	2.16	1.95	1.90
3	4C	301	AGS	PG-S1G	2.16	1.95	1.90
3	1G	301	AGS	PG-S1G	2.16	1.95	1.90
3	4G	301	AGS	PG-S1G	2.16	1.95	1.90
3	1H	301	AGS	PG-S1G	2.15	1.95	1.90
3	4F	301	AGS	PG-S1G	2.15	1.95	1.90
3	4E	301	AGS	PG-S1G	2.14	1.95	1.90
3	4H	301	AGS	PG-S1G	2.14	1.95	1.90
3	1D	301	AGS	PG-S1G	2.14	1.95	1.90
3	4A	301	AGS	PG-S1G	2.13	1.95	1.90
3	1I	301	AGS	PG-S1G	2.13	1.95	1.90
3	4D	301	AGS	PG-S1G	2.12	1.95	1.90
3	1F	301	AGS	PG-S1G	2.09	1.95	1.90

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1D	301	AGS	C5-C6-N6	2.30	123.85	120.35
3	1G	301	AGS	C5-C6-N6	2.30	123.85	120.35
3	1E	301	AGS	C5-C6-N6	2.29	123.83	120.35
3	1C	301	AGS	C5-C6-N6	2.28	123.82	120.35
3	1B	301	AGS	C5-C6-N6	2.27	123.81	120.35
3	4D	301	AGS	C5-C6-N6	2.26	123.79	120.35
3	4F	301	AGS	C5-C6-N6	2.26	123.78	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4C	301	AGS	C5-C6-N6	2.24	123.76	120.35
3	1F	301	AGS	C5-C6-N6	2.23	123.74	120.35
3	4B	301	AGS	C5-C6-N6	2.22	123.73	120.35
3	1H	301	AGS	C5-C6-N6	2.22	123.73	120.35
3	4G	301	AGS	C5-C6-N6	2.21	123.71	120.35
3	4H	301	AGS	C5-C6-N6	2.21	123.71	120.35
3	1I	301	AGS	C5-C6-N6	2.21	123.71	120.35
3	4A	301	AGS	C5-C6-N6	2.21	123.70	120.35
3	4E	301	AGS	C5-C6-N6	2.20	123.69	120.35

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	4A	301	AGS	C5'-O5'-PA-O2A
3	1B	301	AGS	C5'-O5'-PA-O2A
3	4B	301	AGS	C5'-O5'-PA-O2A
3	1C	301	AGS	C5'-O5'-PA-O2A
3	4C	301	AGS	C5'-O5'-PA-O2A
3	1D	301	AGS	C5'-O5'-PA-O2A
3	4D	301	AGS	C5'-O5'-PA-O2A
3	1E	301	AGS	C5'-O5'-PA-O2A
3	4E	301	AGS	C5'-O5'-PA-O2A
3	1F	301	AGS	C5'-O5'-PA-O2A
3	4F	301	AGS	C5'-O5'-PA-O2A
3	1G	301	AGS	C5'-O5'-PA-O2A
3	4G	301	AGS	C5'-O5'-PA-O2A
3	1H	301	AGS	C5'-O5'-PA-O2A
3	4H	301	AGS	C5'-O5'-PA-O2A
3	1I	301	AGS	C5'-O5'-PA-O2A
3	4A	301	AGS	C5'-O5'-PA-O3A
3	1B	301	AGS	C5'-O5'-PA-O3A
3	4B	301	AGS	C5'-O5'-PA-O3A
3	1C	301	AGS	C5'-O5'-PA-O3A
3	4C	301	AGS	C5'-O5'-PA-O3A
3	1D	301	AGS	C5'-O5'-PA-O3A
3	4D	301	AGS	C5'-O5'-PA-O3A
3	1E	301	AGS	C5'-O5'-PA-O3A
3	4E	301	AGS	C5'-O5'-PA-O3A
3	1F	301	AGS	C5'-O5'-PA-O3A
3	4F	301	AGS	C5'-O5'-PA-O3A
3	1G	301	AGS	C5'-O5'-PA-O3A

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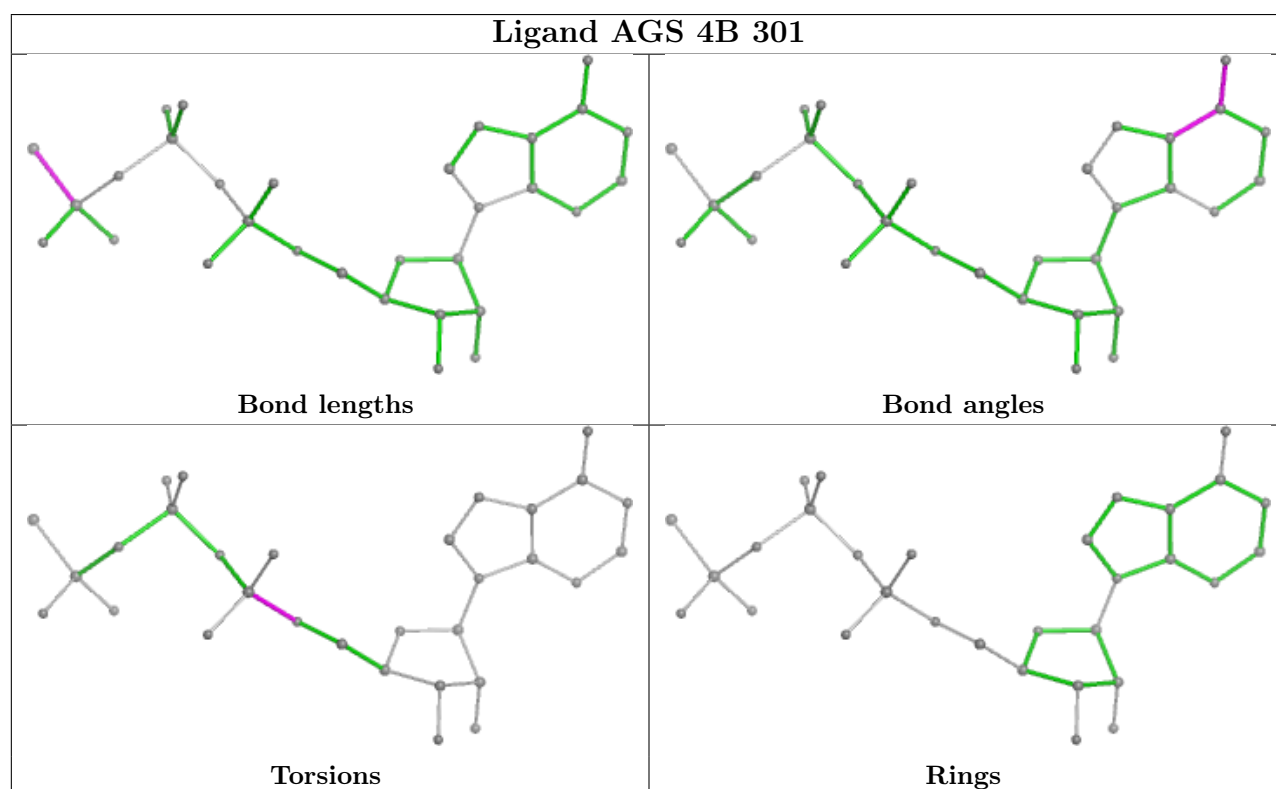
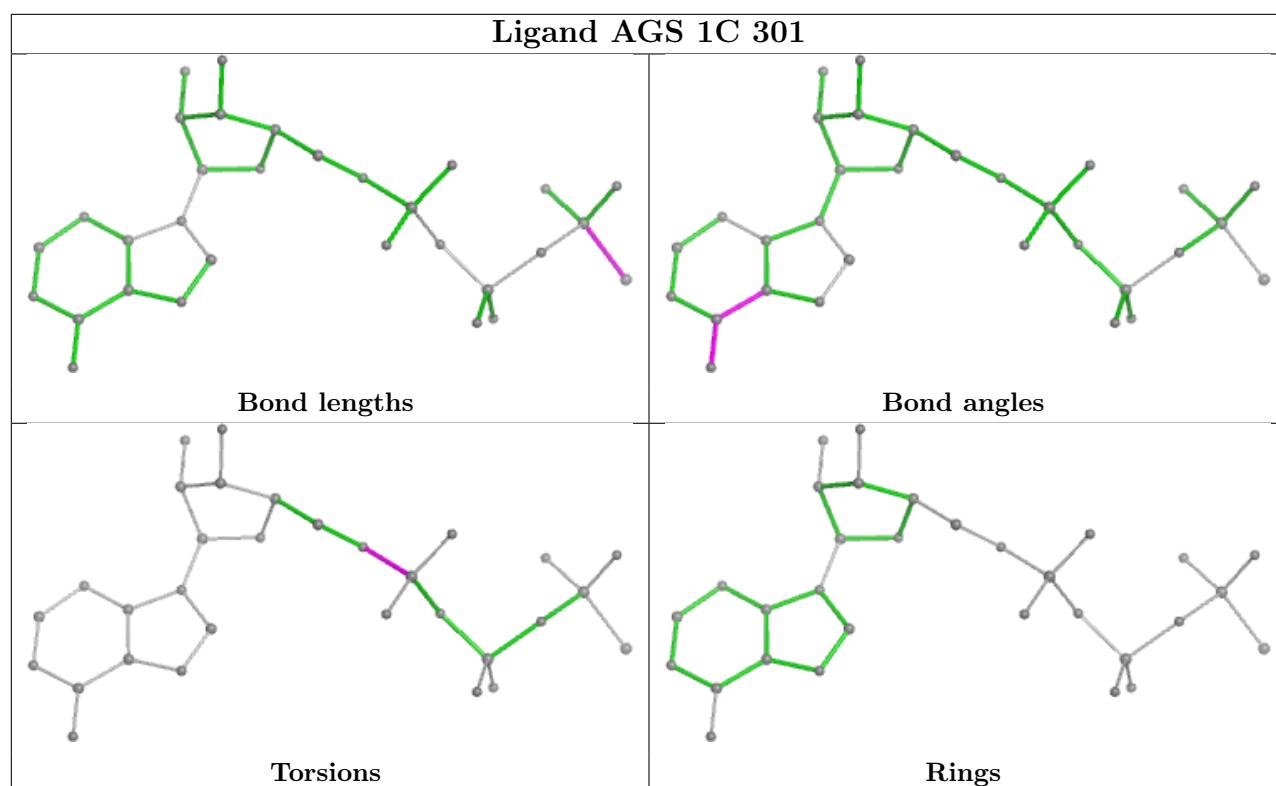
Mol	Chain	Res	Type	Atoms
3	4G	301	AGS	C5'-O5'-PA-O3A
3	1H	301	AGS	C5'-O5'-PA-O3A
3	4H	301	AGS	C5'-O5'-PA-O3A
3	1I	301	AGS	C5'-O5'-PA-O3A

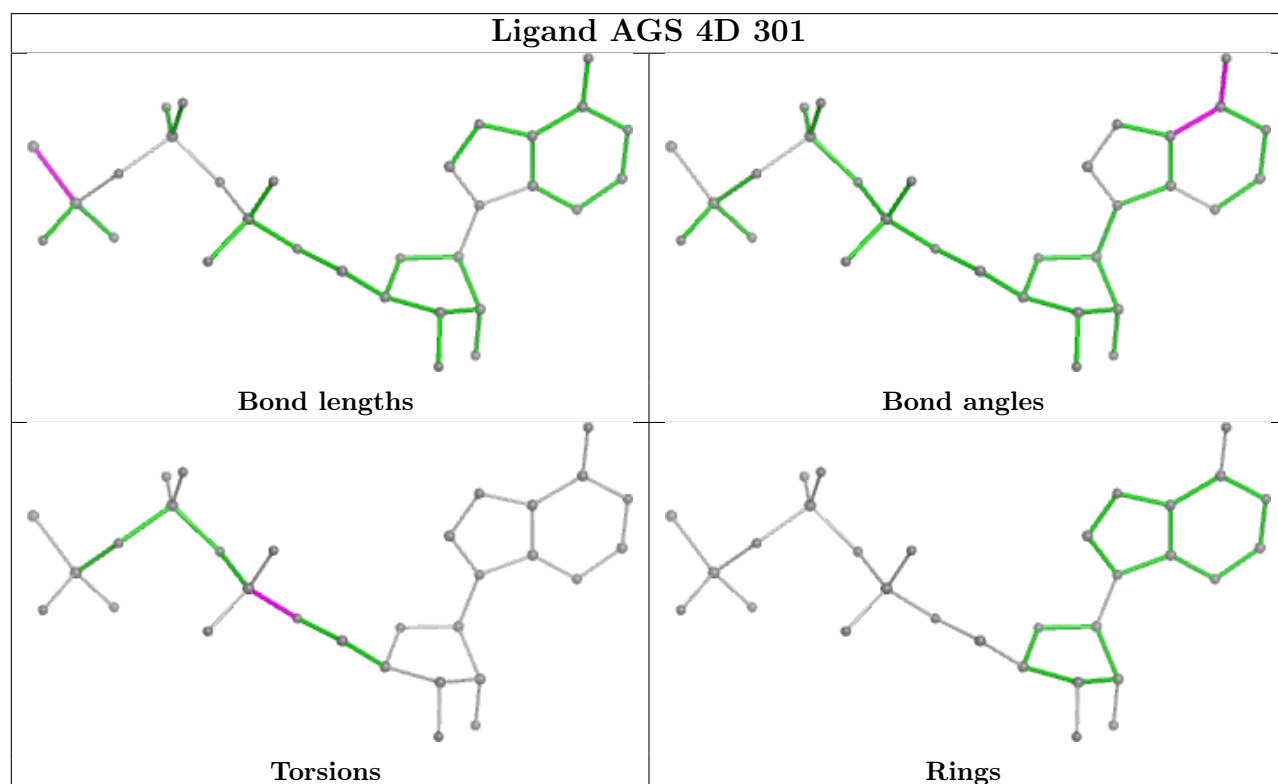
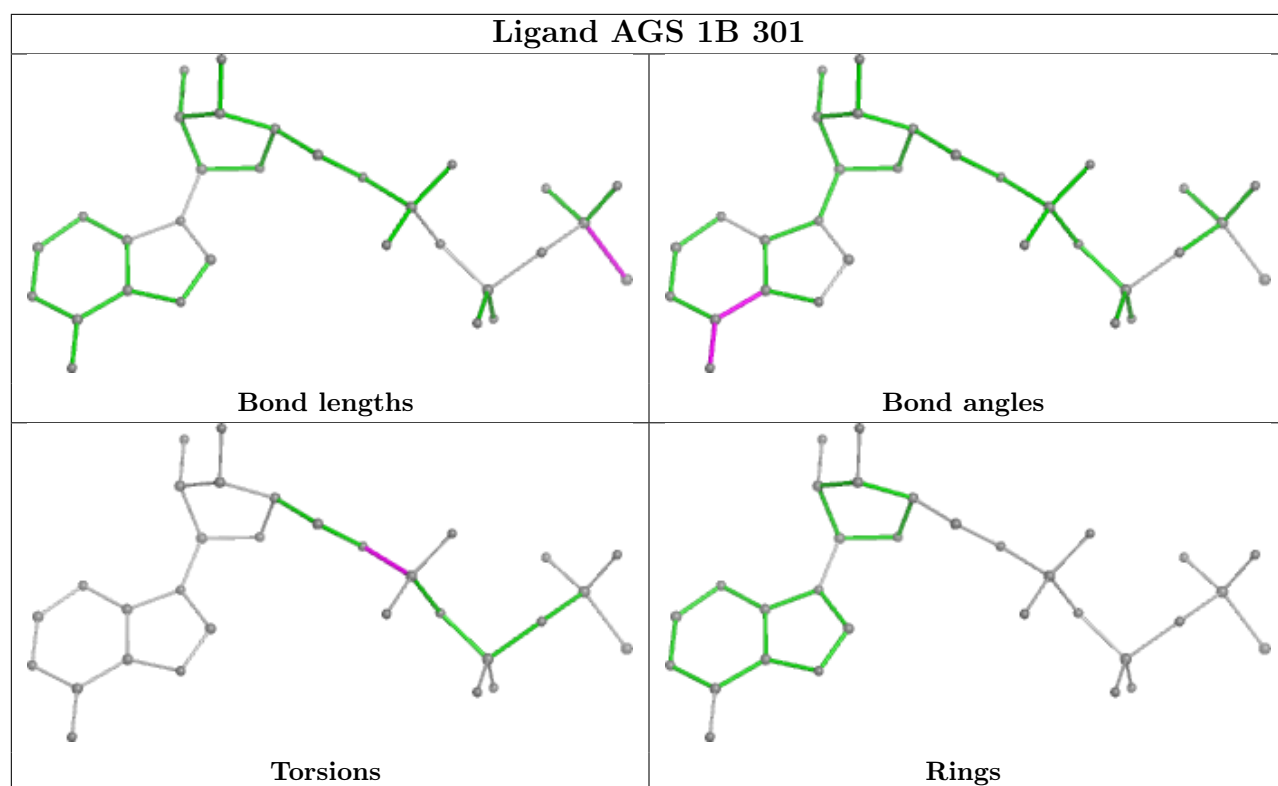
There are no ring outliers.

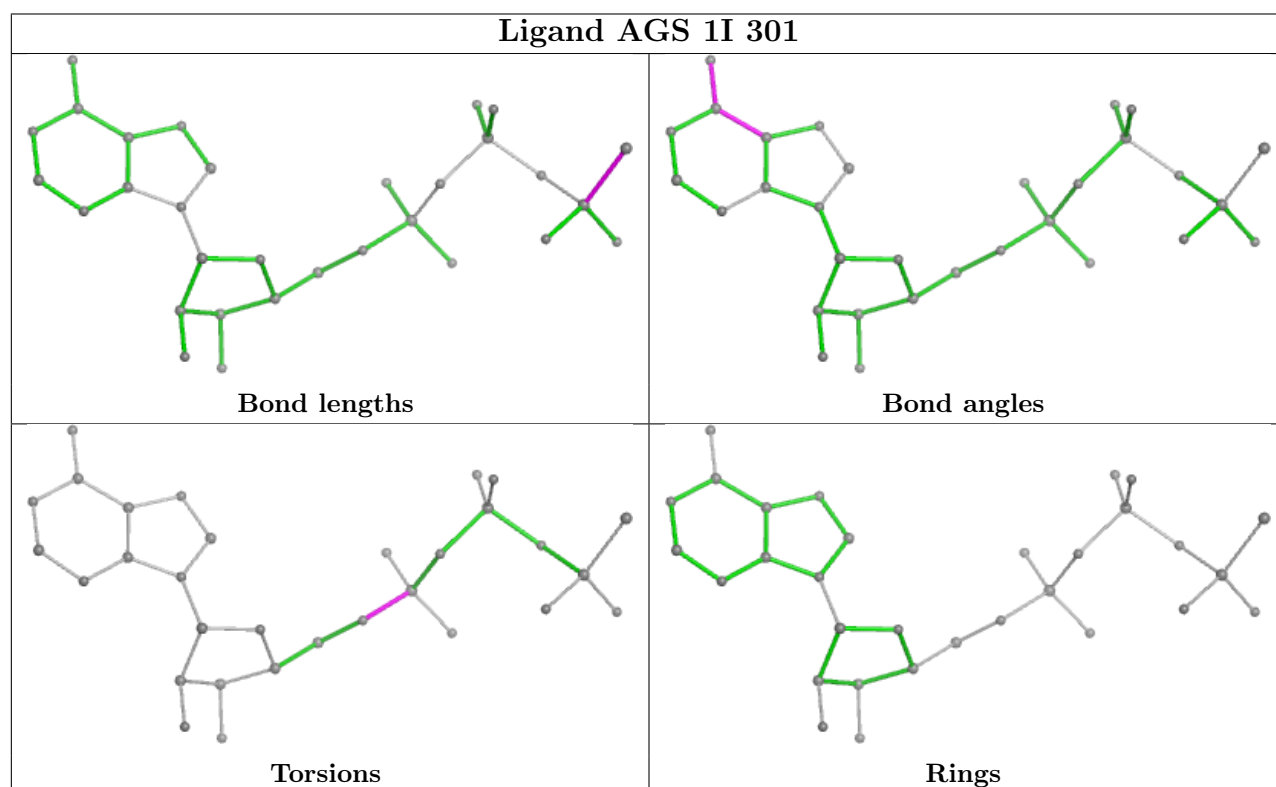
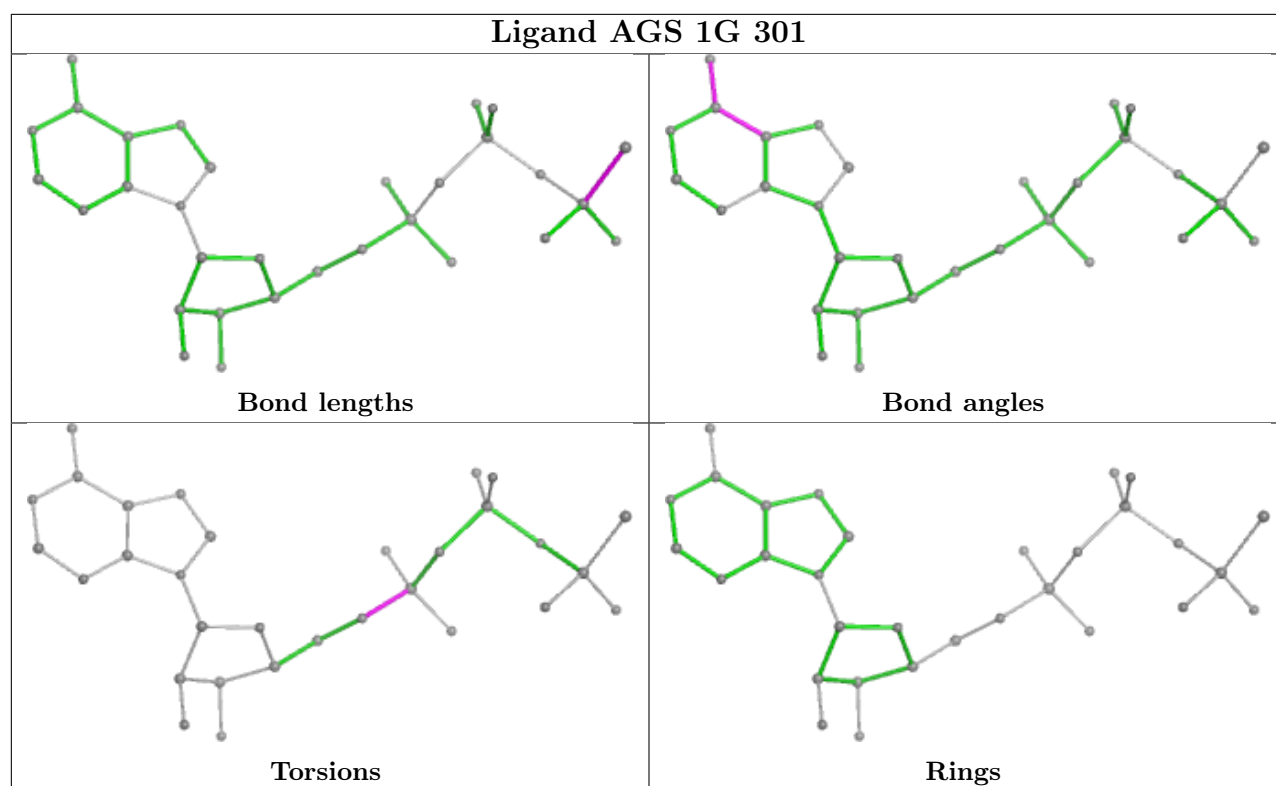
12 monomers are involved in 36 short contacts:

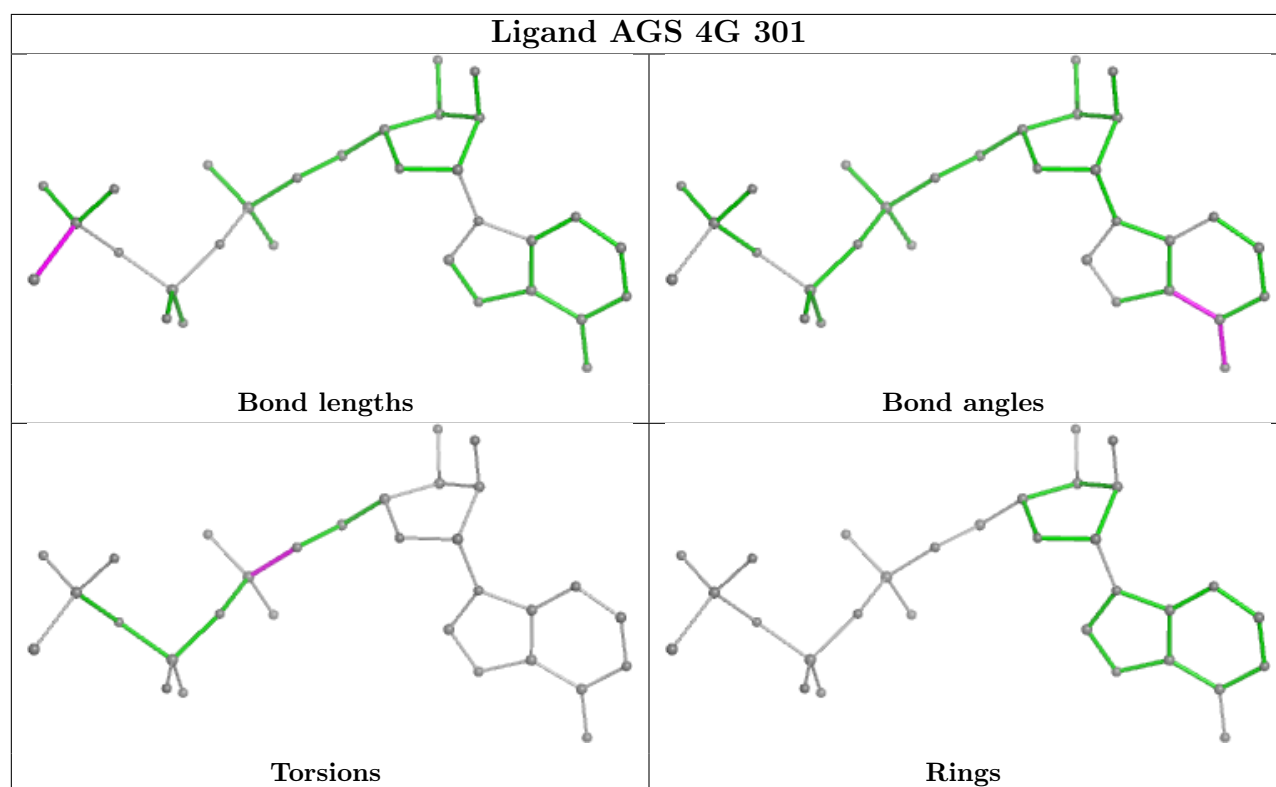
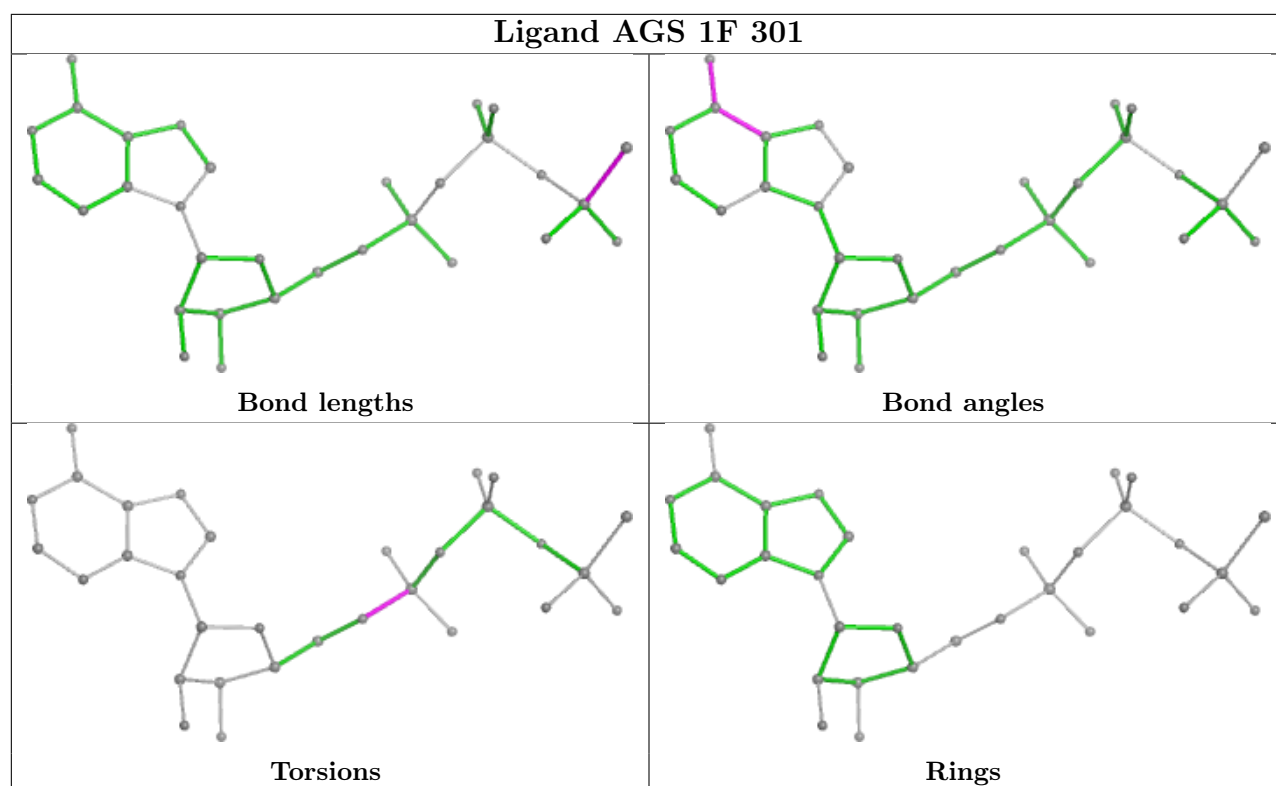
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1C	301	AGS	1	0
3	4B	301	AGS	4	0
3	1B	301	AGS	5	0
3	1G	301	AGS	1	0
3	1I	301	AGS	7	0
3	4G	301	AGS	1	0
3	1H	301	AGS	4	0
3	4C	301	AGS	1	0
3	1D	301	AGS	1	0
3	4A	301	AGS	7	0
3	4H	301	AGS	3	0
3	4F	301	AGS	1	0

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

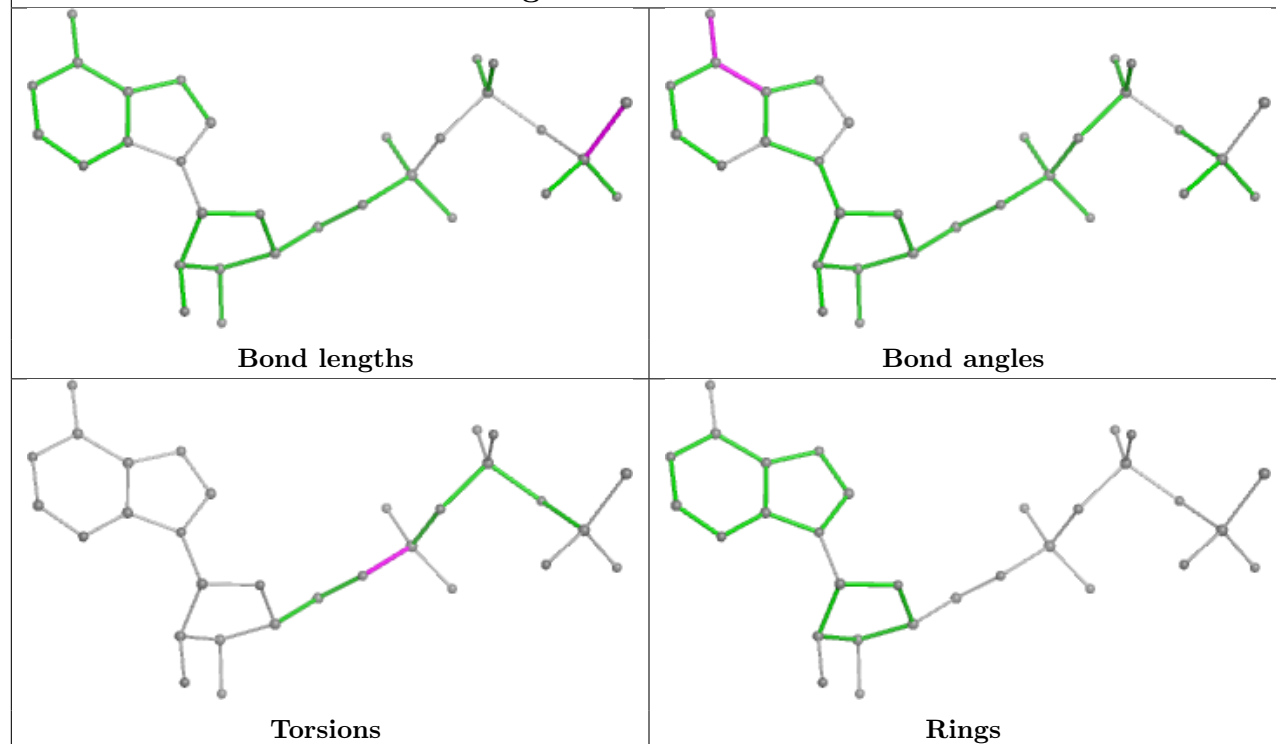




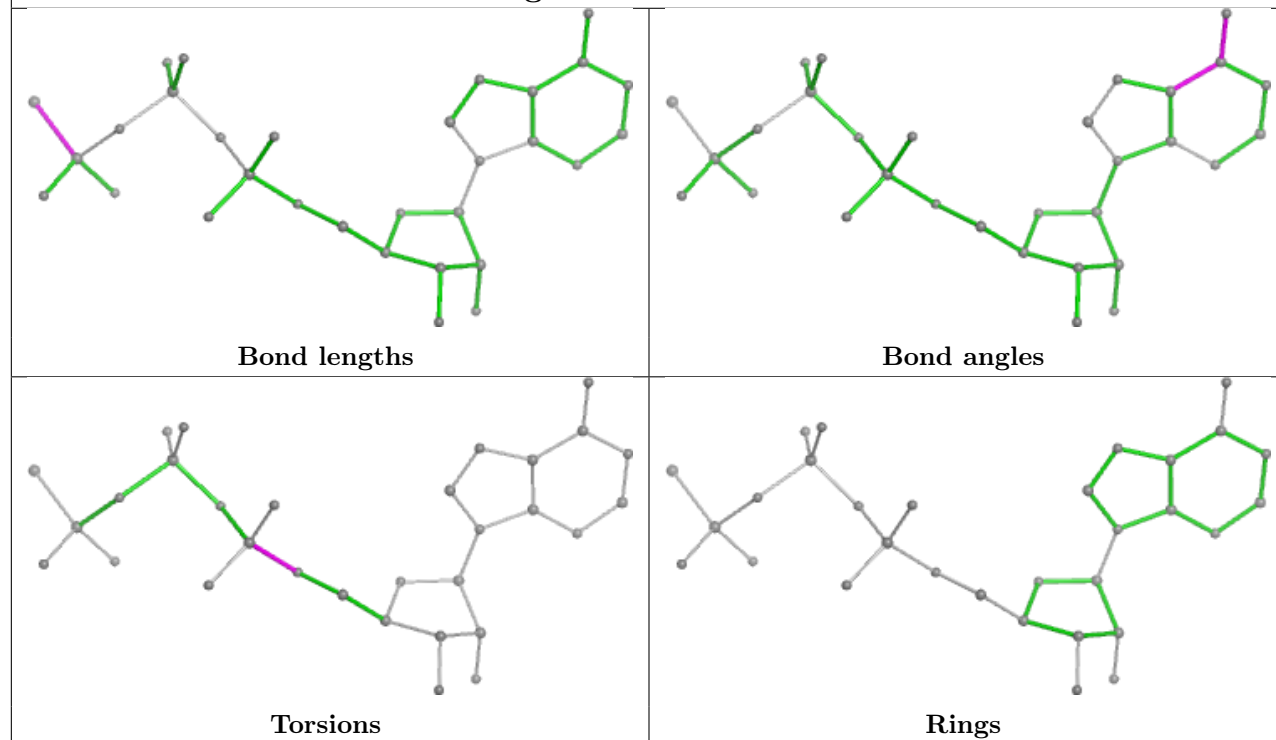


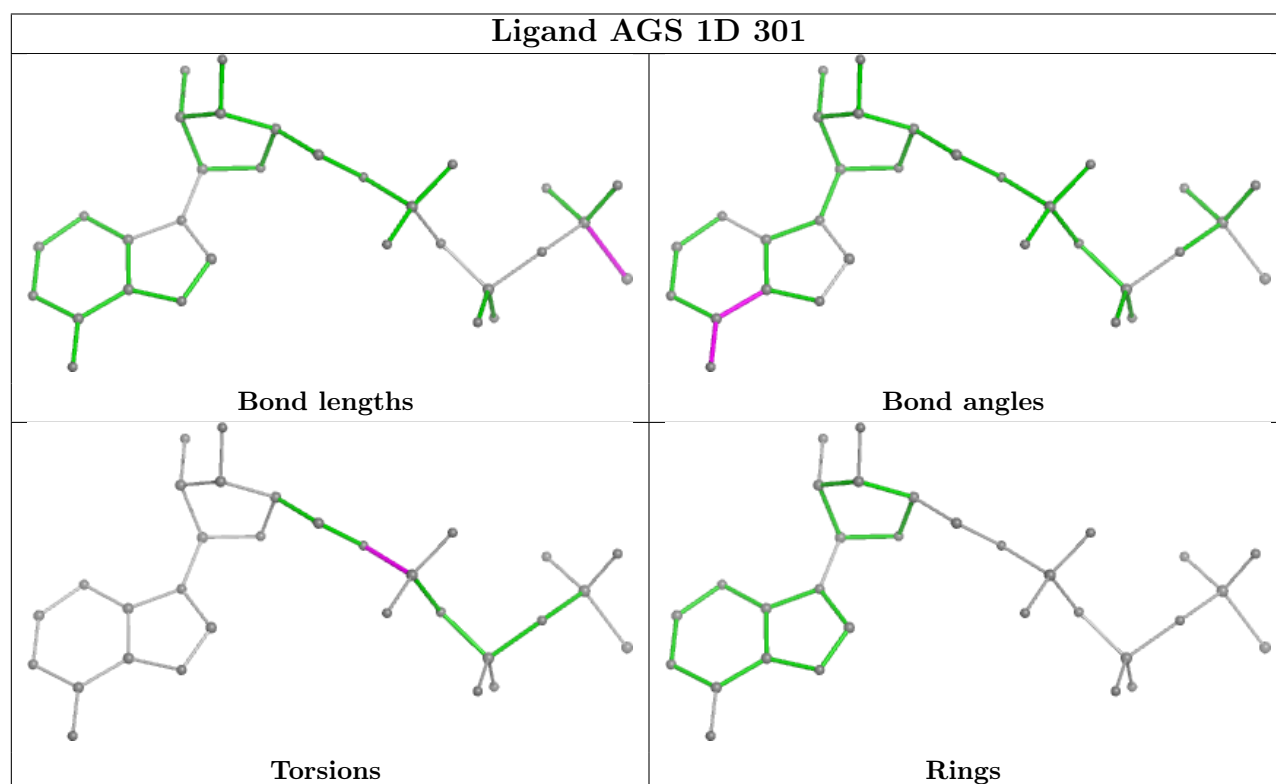
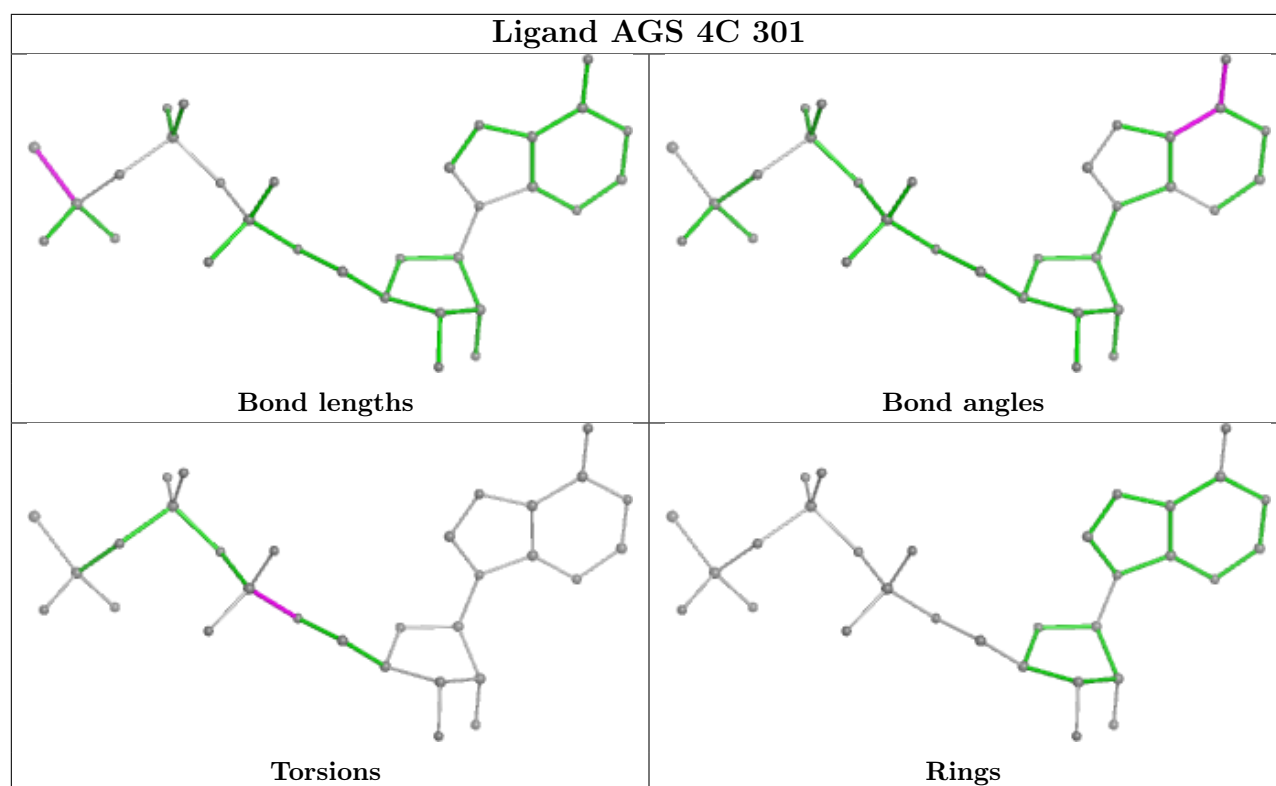


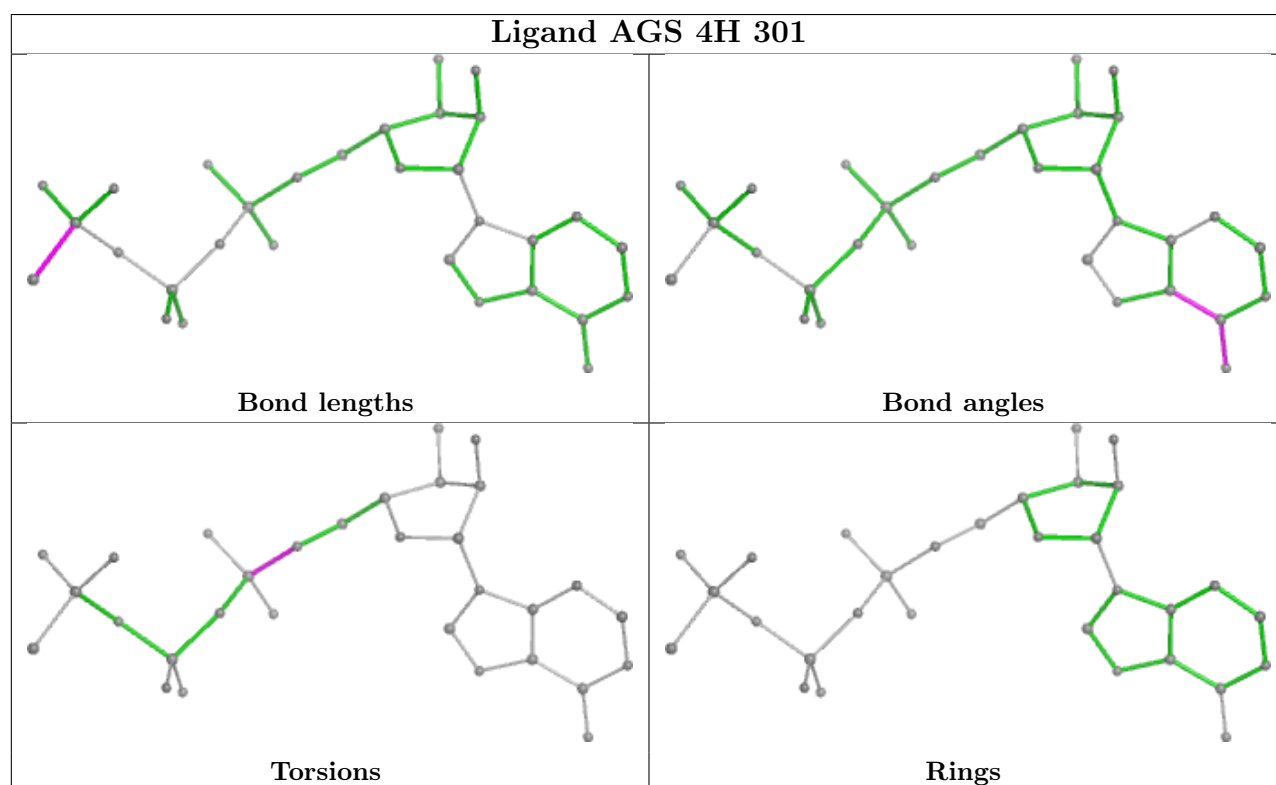
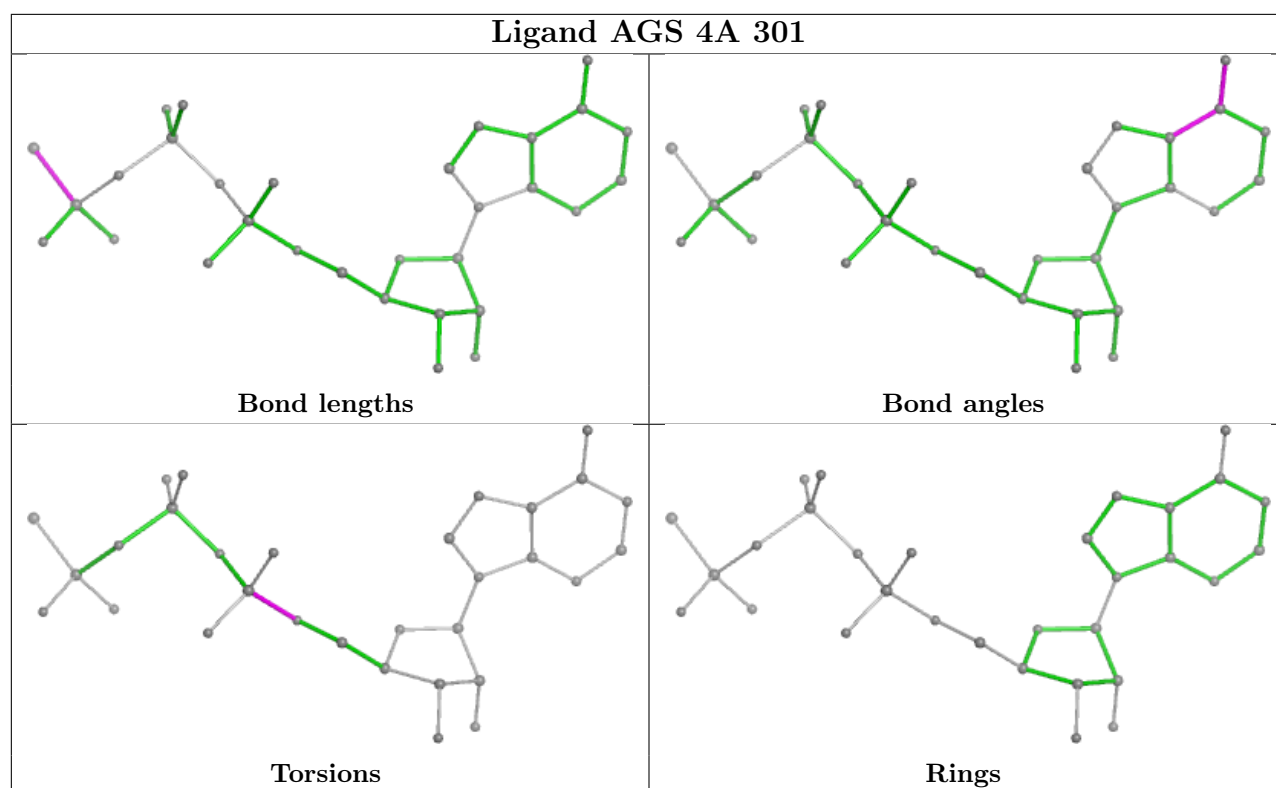
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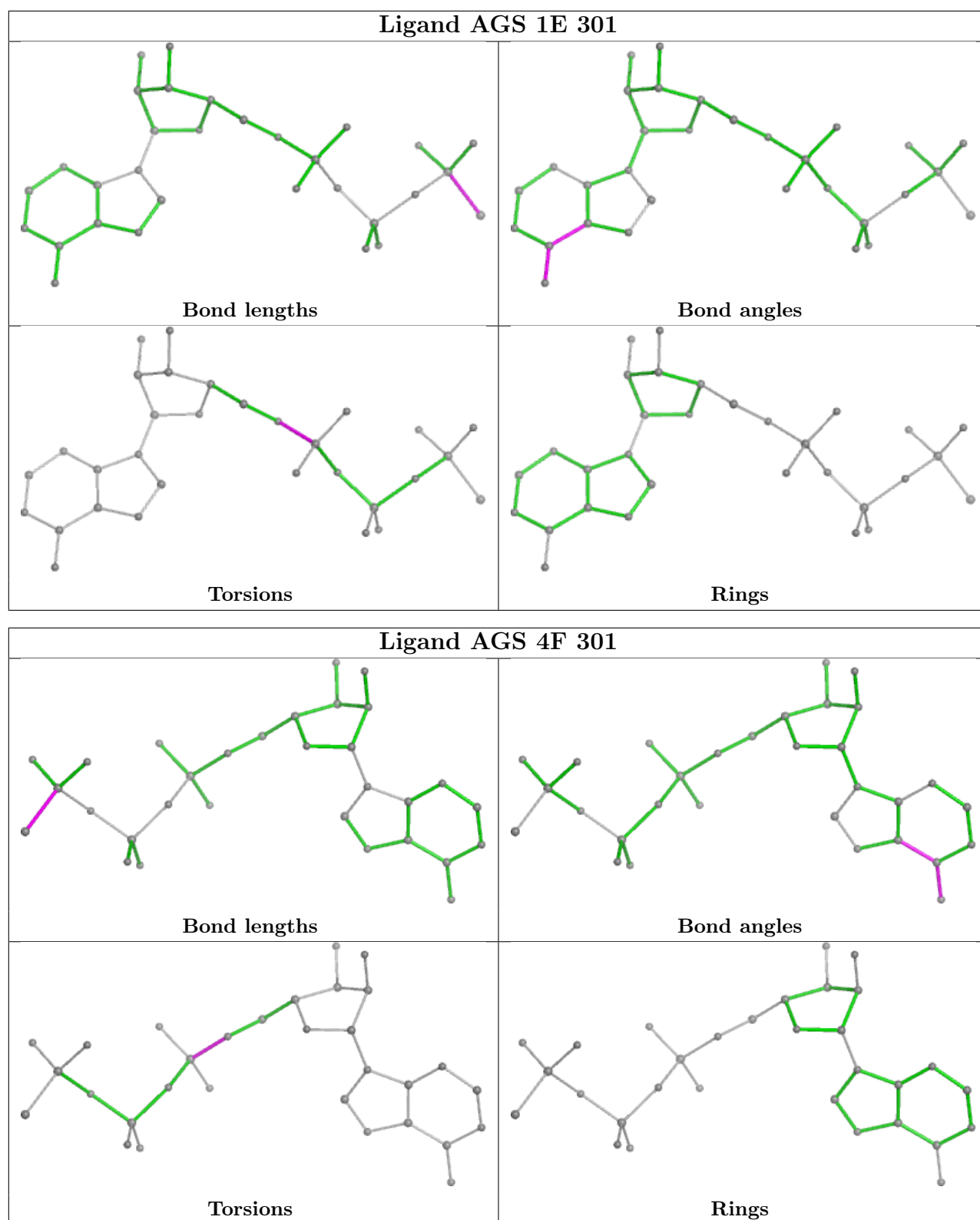


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5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.