



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2023 – 04:00 AM EDT

PDB ID : 2Q4B  
Title : Ensemble refinement of the protein crystal structure of selenomethionyl gene product from Arabidopsis thaliana At5g02240 in space group P21212  
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)  
Deposited on : 2007-05-31  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

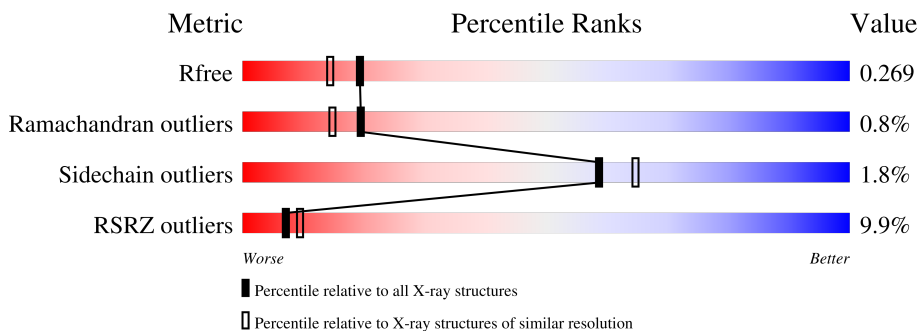
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



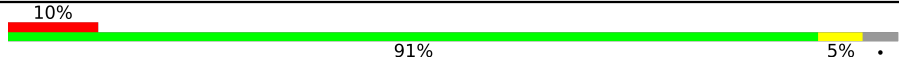

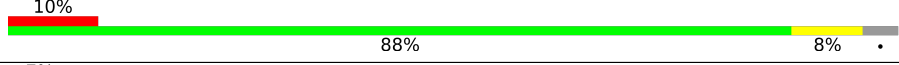

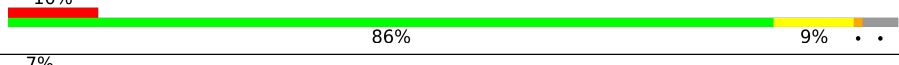
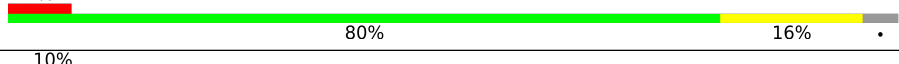
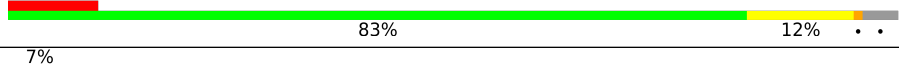

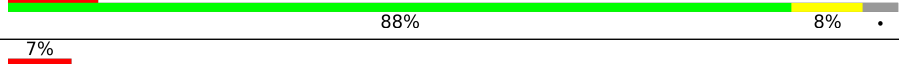

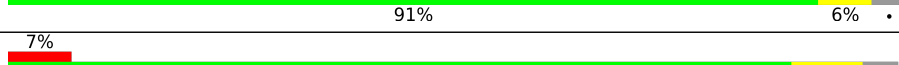
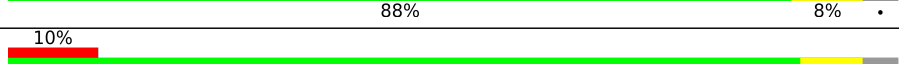

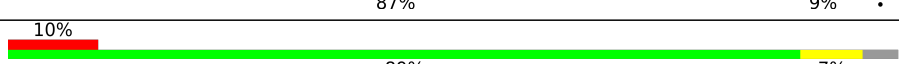
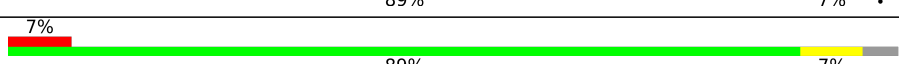
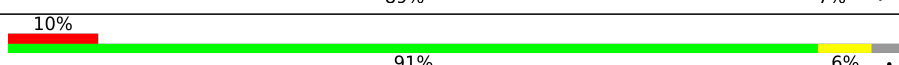
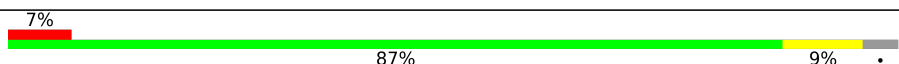
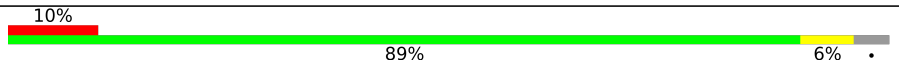
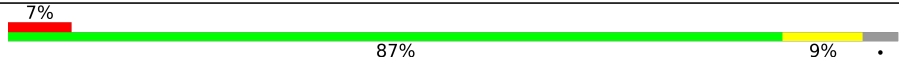
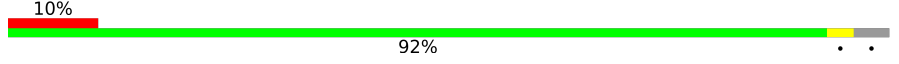

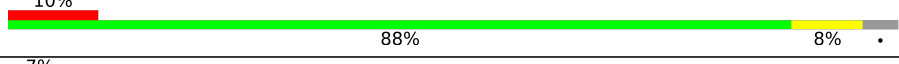
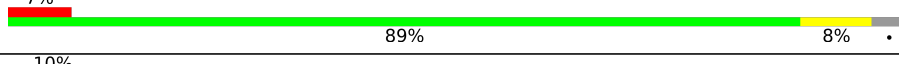
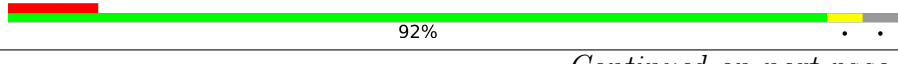

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	1-A	253	
1	1-B	253	
1	10-A	253	
1	10-B	253	
1	11-A	253	
1	11-B	253	

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Mol	Chain	Length	Quality of chain
1	12-A	253	 10% 91% 5%
1	12-B	253	 7% 87% 9%
1	13-A	253	 10% 88% 8%
1	13-B	253	 7% 81% 15%
1	14-A	253	 10% 86% 9%
1	14-B	253	 7% 80% 16%
1	15-A	253	 10% 83% 12%
1	15-B	253	 7% 78% 17%
1	16-A	253	 10% 88% 8%
1	16-B	253	 7% 80% 15%
1	2-A	253	 10% 91% 6%
1	2-B	253	 7% 88% 8%
1	3-A	253	 10% 89% 7%
1	3-B	253	 7% 87% 9%
1	4-A	253	 10% 89% 7%
1	4-B	253	 7% 89% 7%
1	5-A	253	 10% 91% 6%
1	5-B	253	 7% 87% 9%
1	6-A	253	 10% 89% 6%
1	6-B	253	 7% 87% 9%
1	7-A	253	 10% 92%
1	7-B	253	 7% 86% 10%
1	8-A	253	 10% 88% 8%
1	8-B	253	 7% 89% 8%
1	9-A	253	 10% 92%

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Mol	Chain	Length	Quality of chain
1	9-B	253	<p>7% 88% 8%</p>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAP	1-A	400	X	-	-	-
2	NAP	1-B	401	X	-	-	-
2	NAP	10-A	400	X	-	-	-
2	NAP	10-B	401	X	-	-	-
2	NAP	11-A	400	X	-	-	-
2	NAP	11-B	401	X	-	-	-
2	NAP	12-A	400	X	-	-	-
2	NAP	12-B	401	X	-	-	-
2	NAP	13-A	400	X	-	-	-
2	NAP	13-B	401	X	-	-	-
2	NAP	14-A	400	X	-	-	-
2	NAP	14-B	401	X	-	-	-
2	NAP	15-A	400	X	-	-	-
2	NAP	16-A	400	X	-	-	-
2	NAP	2-A	400	X	-	-	-
2	NAP	2-B	401	X	-	-	-
2	NAP	3-A	400	X	-	-	-
2	NAP	3-B	401	X	-	-	-
2	NAP	4-A	400	X	-	-	-
2	NAP	4-B	401	X	-	-	-
2	NAP	5-A	400	X	-	-	-
2	NAP	5-B	401	X	-	-	-
2	NAP	6-A	400	X	-	-	-
2	NAP	6-B	401	X	-	-	-
2	NAP	7-A	400	X	-	-	-
2	NAP	7-B	401	X	-	-	-
2	NAP	8-A	400	X	-	-	-
2	NAP	8-B	401	X	-	-	-
2	NAP	9-A	400	X	-	-	-
2	NAP	9-B	401	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 66192 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 At5g02240.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	2-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	3-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	4-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	5-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	6-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	7-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	8-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	9-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	10-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	11-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	12-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	13-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	14-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	15-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0
1	16-A	243	Total 1836	C 1163	N 312	O 358	S 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	2-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	3-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	4-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	5-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	6-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	7-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	8-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	9-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	10-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	11-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	12-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	13-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	14-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	15-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			
1	16-B	243	Total	C	N	O	S	0	0	0
			1836	1163	312	358	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q94EG6
B	1	SER	-	expression tag	UNP Q94EG6

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	15-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	16-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	1-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	2-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	3-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	4-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	5-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	6-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	7-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	8-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	9-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	10-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	11-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	12-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	13-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	14-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	15-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	16-B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	146	Total	O	0	0
			146	146		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	2-A	147	Total 147	O 147	0	0
3	3-A	147	Total 147	O 147	0	0
3	4-A	146	Total 146	O 146	0	0
3	5-A	147	Total 147	O 147	0	0
3	6-A	145	Total 145	O 145	0	0
3	7-A	145	Total 145	O 145	0	0
3	8-A	146	Total 146	O 146	0	0
3	9-A	146	Total 146	O 146	0	0
3	10-A	147	Total 147	O 147	0	0
3	11-A	146	Total 146	O 146	0	0
3	12-A	147	Total 147	O 147	0	0
3	13-A	146	Total 146	O 146	0	0
3	14-A	146	Total 146	O 146	0	0
3	15-A	147	Total 147	O 147	0	0
3	16-A	147	Total 147	O 147	0	0
3	1-B	223	Total 223	O 223	0	0
3	2-B	222	Total 222	O 222	0	0
3	3-B	222	Total 222	O 222	0	0
3	4-B	223	Total 223	O 223	0	0
3	5-B	222	Total 222	O 222	0	0
3	6-B	224	Total 224	O 224	0	0

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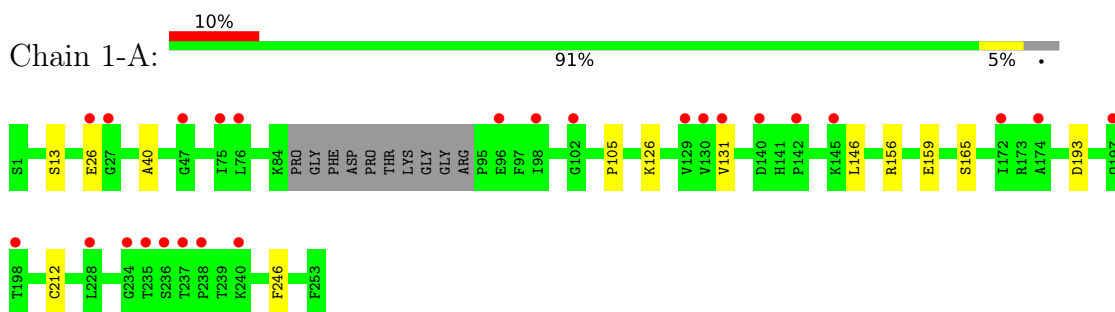
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	7-B	224	Total 224	O 224	0	0
3	8-B	223	Total 223	O 223	0	0
3	9-B	223	Total 223	O 223	0	0
3	10-B	222	Total 222	O 222	0	0
3	11-B	223	Total 223	O 223	0	0
3	12-B	222	Total 222	O 222	0	0
3	13-B	223	Total 223	O 223	0	0
3	14-B	223	Total 223	O 223	0	0
3	15-B	222	Total 222	O 222	0	0
3	16-B	222	Total 222	O 222	0	0

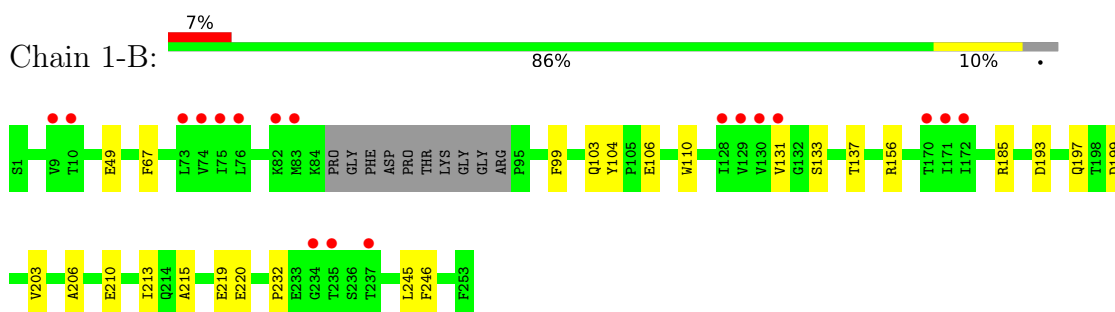
### 3 Residue-property plots [i](#)

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

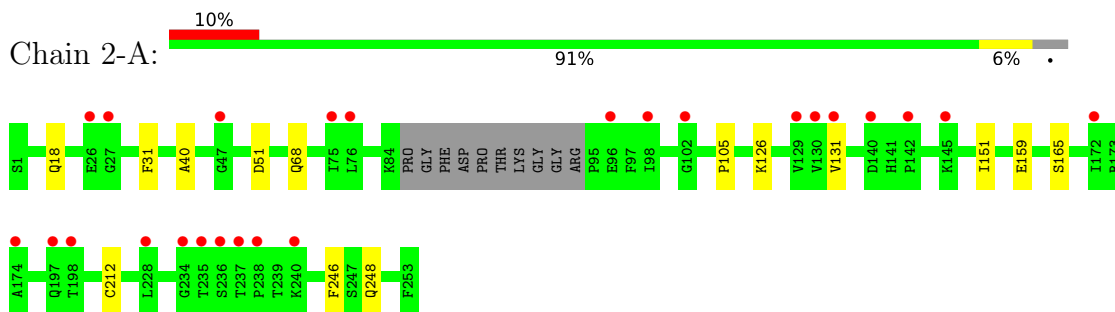
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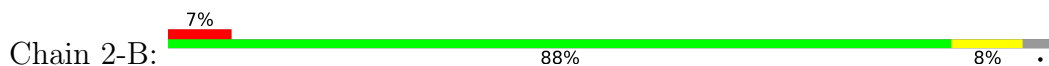
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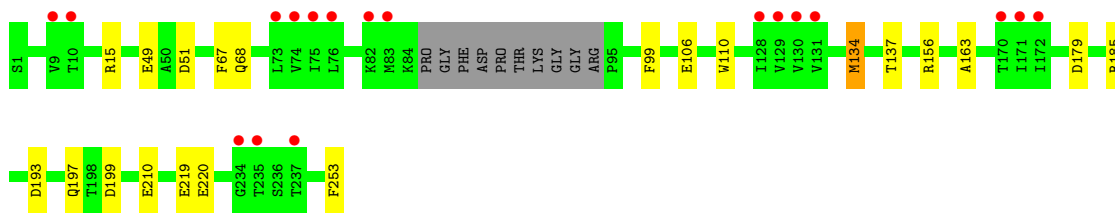


- Molecule 1: Protein At5g02240

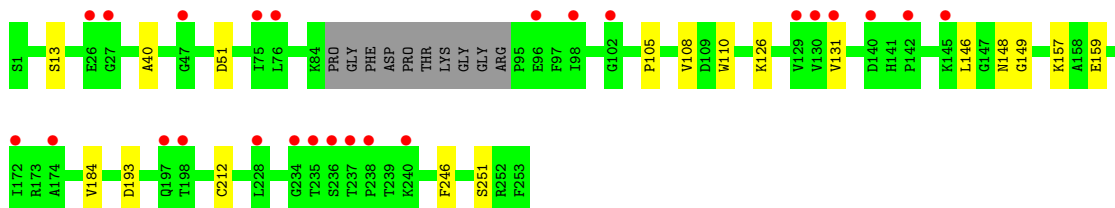
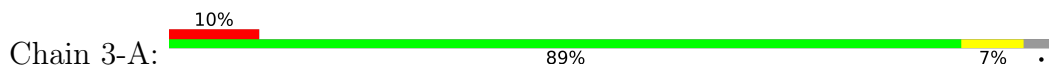


- Molecule 1: Protein At5g02240

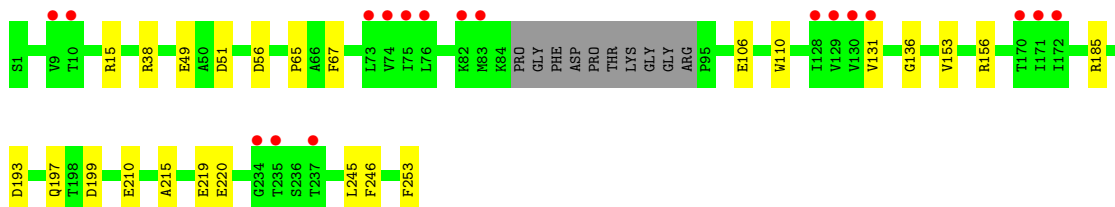
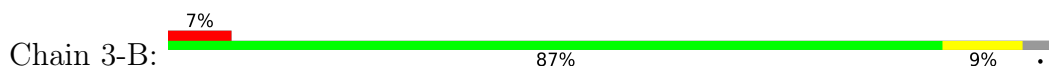




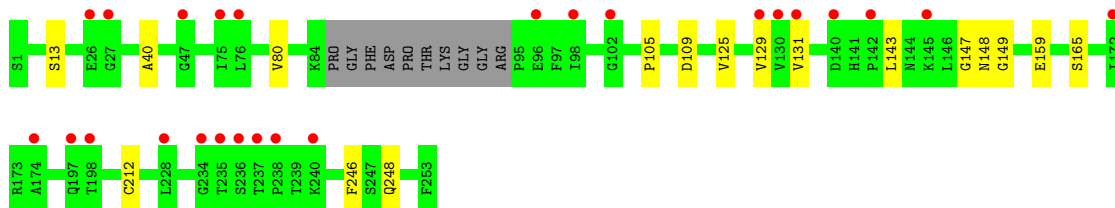
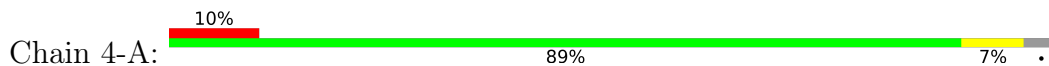
- Molecule 1: Protein At5g02240



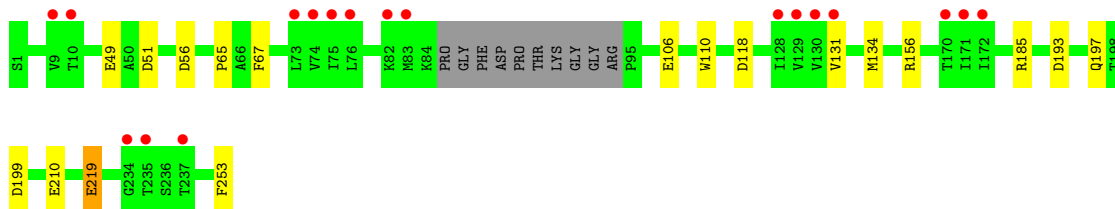
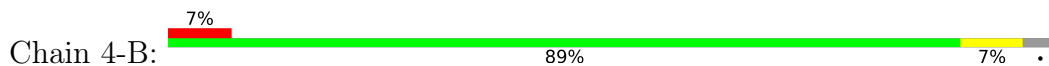
- Molecule 1: Protein At5g02240



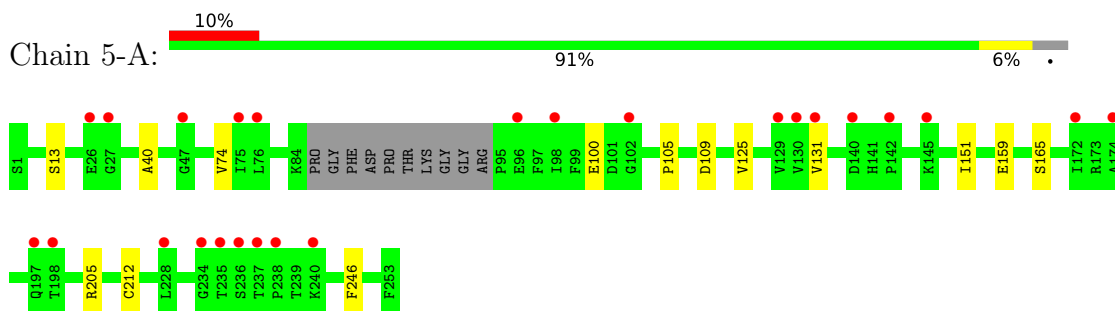
- Molecule 1: Protein At5g02240



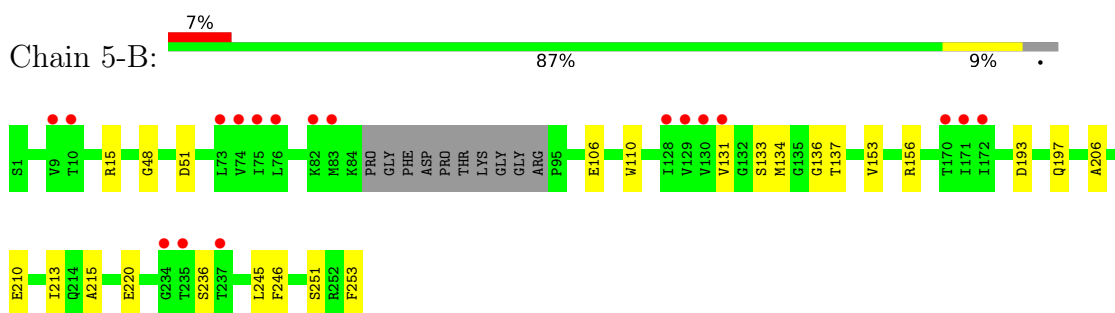
- Molecule 1: Protein At5g02240



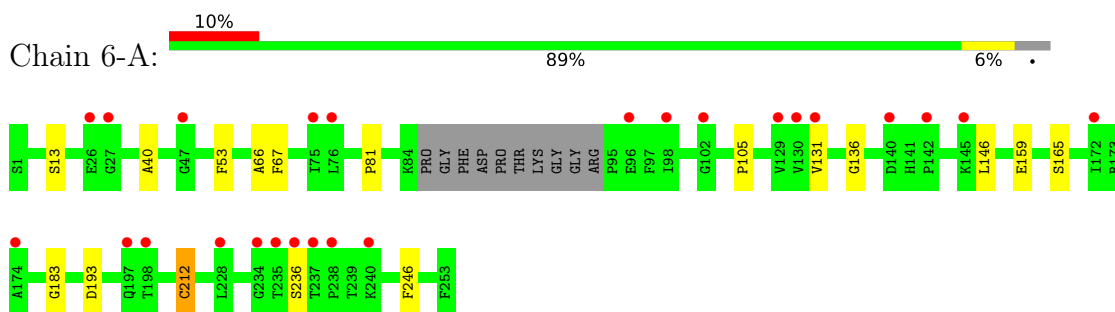
- Molecule 1: Protein At5g02240



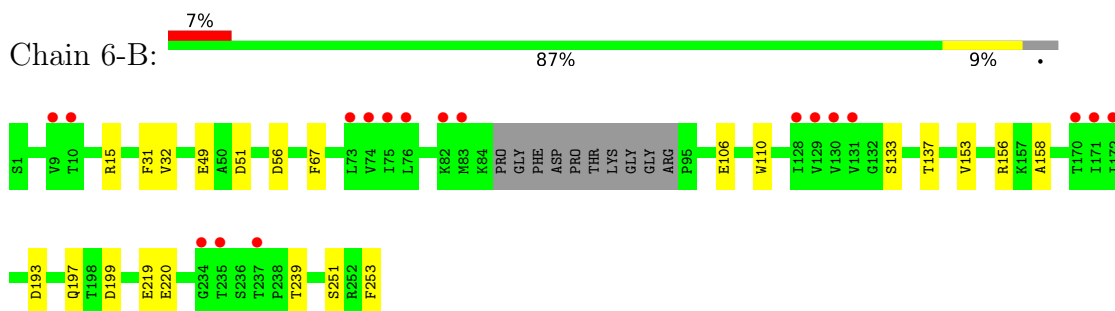
- Molecule 1: Protein At5g02240



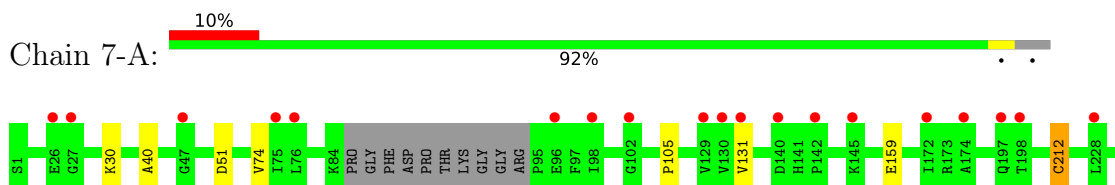
- Molecule 1: Protein At5g02240

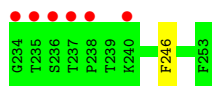


- Molecule 1: Protein At5g02240

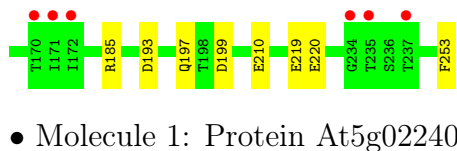
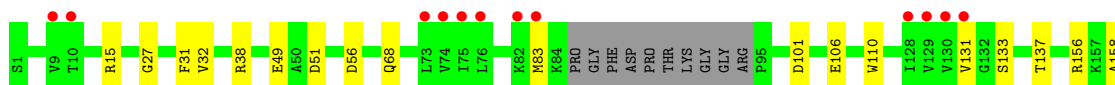
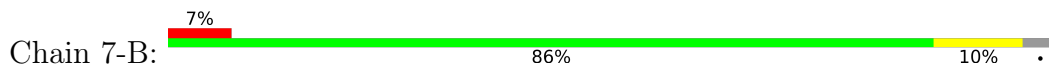


- Molecule 1: Protein At5g02240

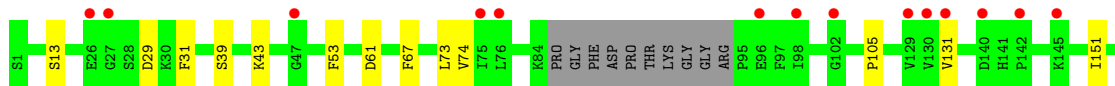
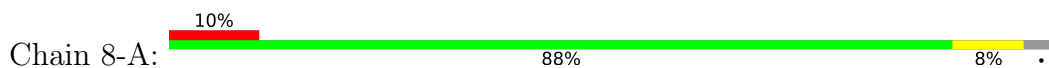




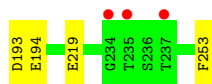
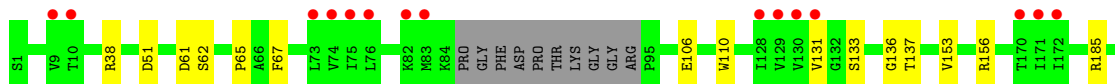
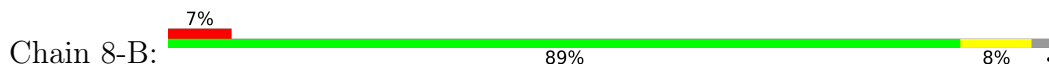
- Molecule 1: Protein At5g02240



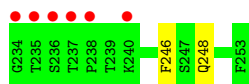
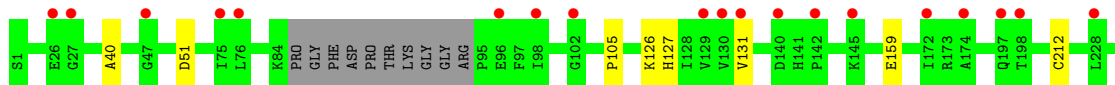
- Molecule 1: Protein At5g02240



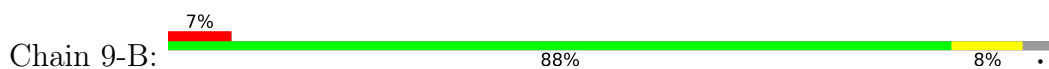
- Molecule 1: Protein At5g02240

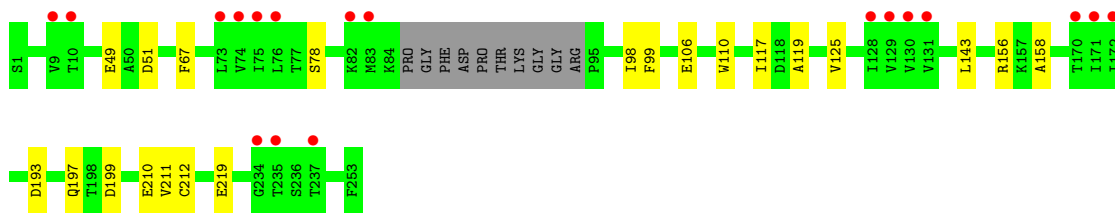


- Molecule 1: Protein At5g02240

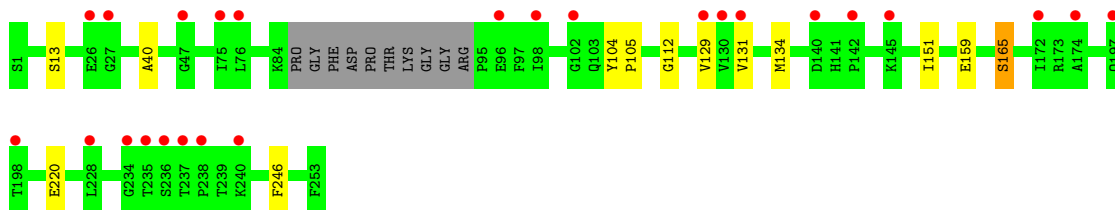


- Molecule 1: Protein At5g02240

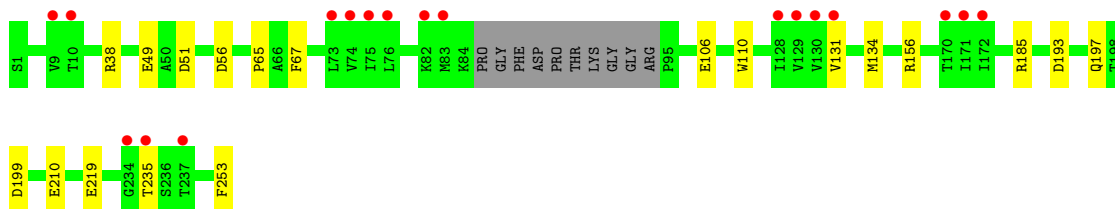
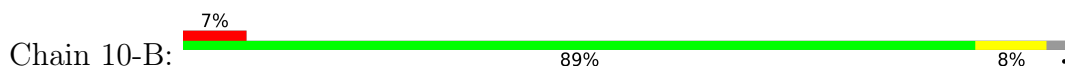




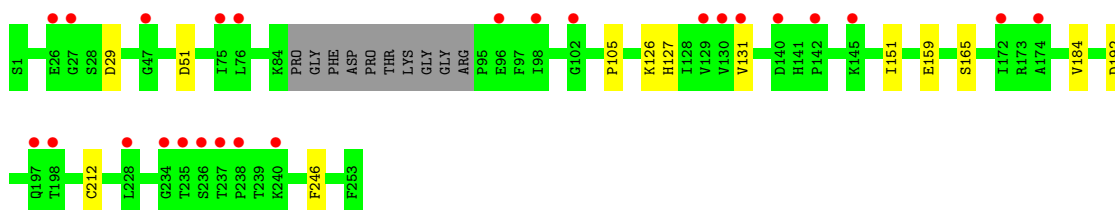
- Molecule 1: Protein At5g02240



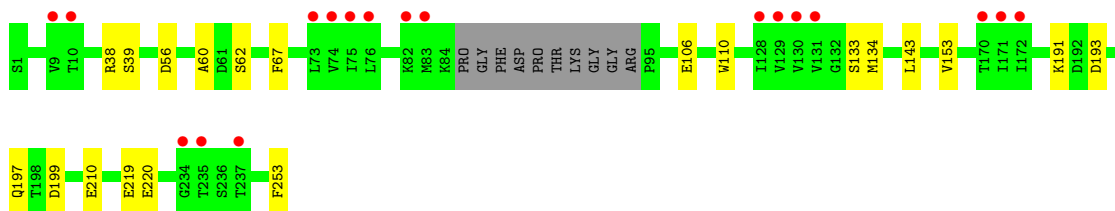
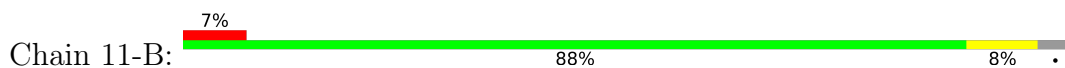
- Molecule 1: Protein At5g02240



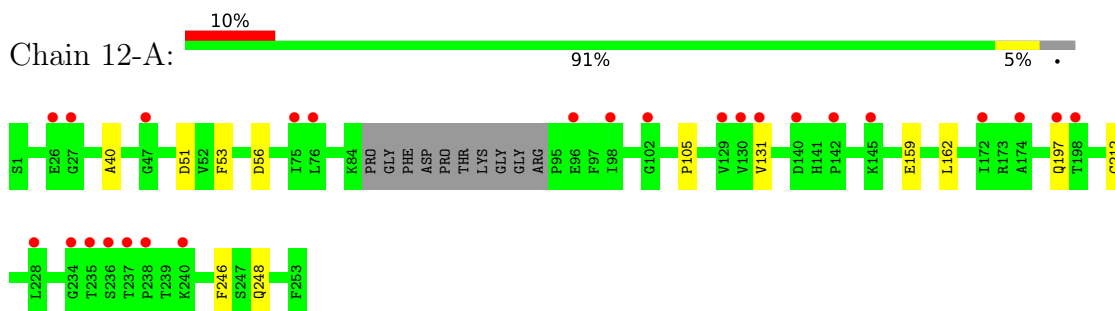
- Molecule 1: Protein At5g02240



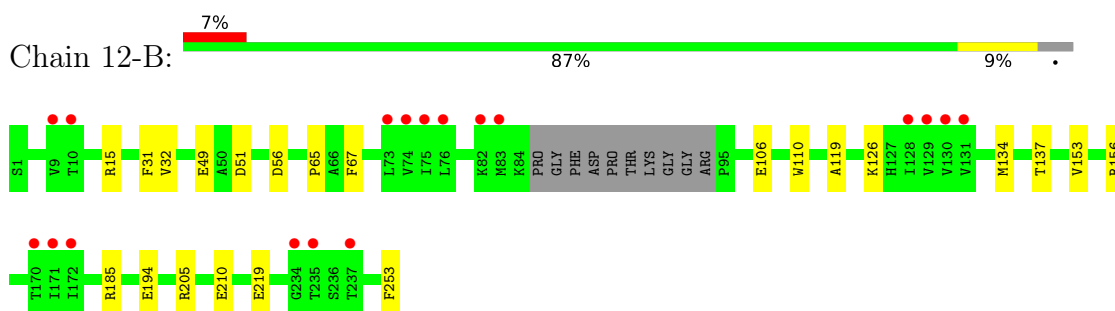
- Molecule 1: Protein At5g02240



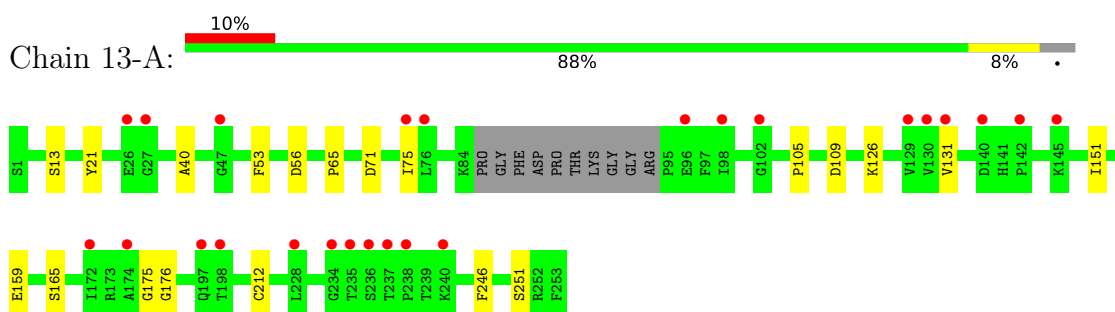
- Molecule 1: Protein At5g02240



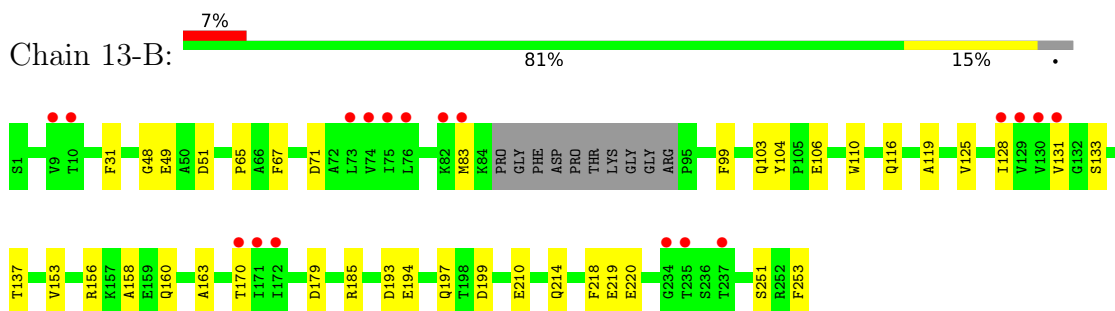
- Molecule 1: Protein At5g02240



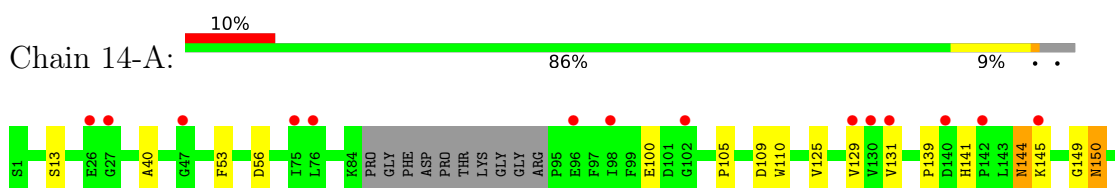
- Molecule 1: Protein At5g02240



- Molecule 1: Protein At5g02240



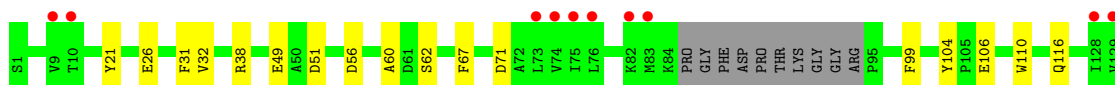
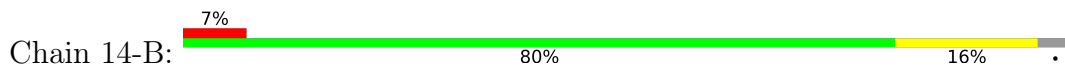
- Molecule 1: Protein At5g02240



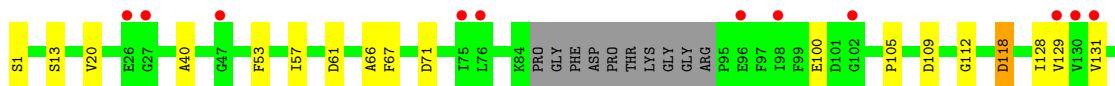
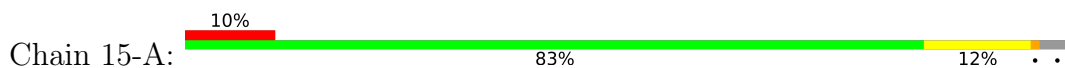




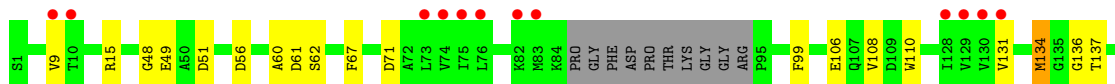
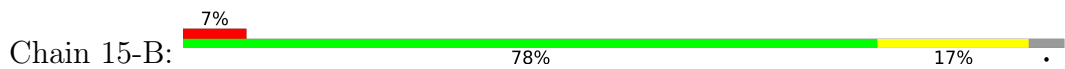
- Molecule 1: Protein At5g02240



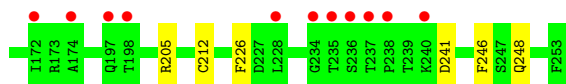
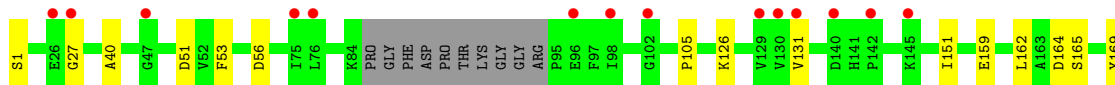
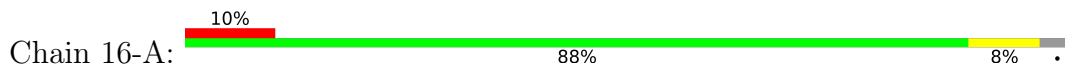
- Molecule 1: Protein At5g02240



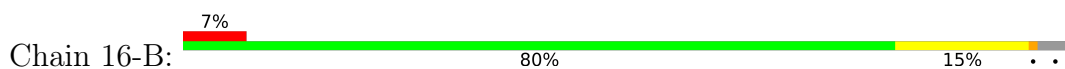
- Molecule 1: Protein At5g02240

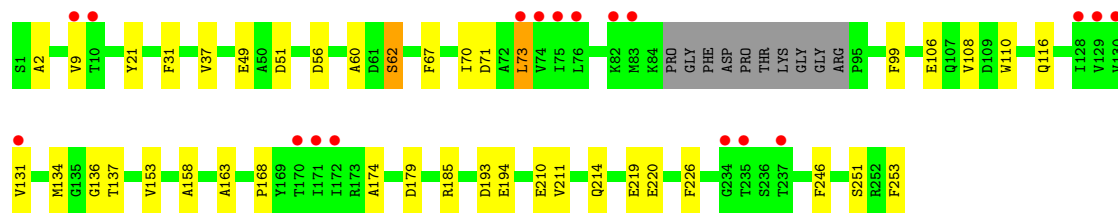


- Molecule 1: Protein At5g02240



- Molecule 1: Protein At5g02240





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.63Å 77.29Å 92.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.09 – 2.10 29.09 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.9 (29.09-2.10) 92.7 (29.09-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.16 (at 2.10Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.180 , 0.257 0.190 , 0.269	Depositor DCC
$R_{free}$ test set	1525 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 70.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.027 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	66192	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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

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	1-A	1.35	9/1865 (0.5%)	1.01	1/2516 (0.0%)
1	1-B	1.60	18/1865 (1.0%)	1.12	3/2516 (0.1%)
1	2-A	1.36	11/1865 (0.6%)	1.00	1/2516 (0.0%)
1	2-B	1.59	14/1865 (0.8%)	1.10	5/2516 (0.2%)
1	3-A	1.41	8/1865 (0.4%)	1.01	3/2516 (0.1%)
1	3-B	1.60	15/1865 (0.8%)	1.13	7/2516 (0.3%)
1	4-A	1.37	10/1865 (0.5%)	1.01	2/2516 (0.1%)
1	4-B	1.60	11/1865 (0.6%)	1.11	6/2516 (0.2%)
1	5-A	1.39	12/1865 (0.6%)	1.02	2/2516 (0.1%)
1	5-B	1.59	16/1865 (0.9%)	1.11	4/2516 (0.2%)
1	6-A	1.32	9/1865 (0.5%)	1.01	1/2516 (0.0%)
1	6-B	1.59	13/1865 (0.7%)	1.10	5/2516 (0.2%)
1	7-A	1.39	8/1865 (0.4%)	1.00	2/2516 (0.1%)
1	7-B	1.59	13/1865 (0.7%)	1.12	7/2516 (0.3%)
1	8-A	1.40	15/1865 (0.8%)	1.02	1/2516 (0.0%)
1	8-B	1.57	12/1865 (0.6%)	1.11	4/2516 (0.2%)
1	9-A	1.36	7/1865 (0.4%)	1.01	1/2516 (0.0%)
1	9-B	1.58	10/1865 (0.5%)	1.11	4/2516 (0.2%)
1	10-A	1.37	12/1865 (0.6%)	0.99	0/2516
1	10-B	1.61	11/1865 (0.6%)	1.11	6/2516 (0.2%)
1	11-A	1.44	8/1865 (0.4%)	1.01	2/2516 (0.1%)
1	11-B	1.60	13/1865 (0.7%)	1.09	3/2516 (0.1%)
1	12-A	1.50	8/1865 (0.4%)	1.01	1/2516 (0.0%)
1	12-B	1.60	14/1865 (0.8%)	1.13	7/2516 (0.3%)
1	13-A	1.58	19/1865 (1.0%)	1.11	3/2516 (0.1%)
1	13-B	1.84	28/1865 (1.5%)	1.22	8/2516 (0.3%)
1	14-A	1.64	19/1865 (1.0%)	1.09	3/2516 (0.1%)
1	14-B	1.87	35/1865 (1.9%)	1.26	9/2516 (0.4%)
1	15-A	1.61	18/1865 (1.0%)	1.11	3/2516 (0.1%)
1	15-B	1.83	38/1865 (2.0%)	1.25	10/2516 (0.4%)
1	16-A	1.59	18/1865 (1.0%)	1.09	1/2516 (0.0%)
1	16-B	1.85	37/1865 (2.0%)	1.22	5/2516 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	1.56	489/59680 (0.8%)	1.09	120/80512 (0.1%)

The worst 5 of 489 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	12-A	212	CYS	CB-SG	-27.96	1.34	1.82
1	11-A	212	CYS	CB-SG	-21.73	1.45	1.82
1	14-A	212	CYS	CB-SG	19.59	2.15	1.82
1	3-A	212	CYS	CB-SG	-19.56	1.49	1.82
1	15-A	212	CYS	CB-SG	-18.22	1.51	1.82

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	14-B	156	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	7-B	156	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	15-B	173	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	13-A	212	CYS	CA-CB-SG	-8.40	98.89	114.00
1	14-B	156	ARG	NE-CZ-NH1	8.33	124.46	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1-A	1836	0	1866	0	0
1	1-B	1836	0	1866	0	0
1	2-A	1836	0	1866	0	0
1	2-B	1836	0	1866	0	0
1	3-A	1836	0	1866	0	0
1	3-B	1836	0	1866	0	0
1	4-A	1836	0	1866	0	0
1	4-B	1836	0	1866	0	0
1	5-A	1836	0	1866	0	0
1	5-B	1836	0	1866	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	6-A	1836	0	1866	0	0
1	6-B	1836	0	1866	0	0
1	7-A	1836	0	1866	0	0
1	7-B	1836	0	1866	0	0
1	8-A	1836	0	1866	0	0
1	8-B	1836	0	1866	0	0
1	9-A	1836	0	1866	0	0
1	9-B	1836	0	1866	0	0
1	10-A	1836	0	1866	0	0
1	10-B	1836	0	1866	0	0
1	11-A	1836	0	1866	0	0
1	11-B	1836	0	1866	0	0
1	12-A	1836	0	1866	0	0
1	12-B	1836	0	1866	0	0
1	13-A	1836	0	1866	0	0
1	13-B	1836	0	1866	0	0
1	14-A	1836	0	1866	0	0
1	14-B	1836	0	1866	0	0
1	15-A	1836	0	1866	0	0
1	15-B	1836	0	1866	0	0
1	16-A	1836	0	1866	0	0
1	16-B	1836	0	1866	0	0
2	1-A	48	0	24	0	0
2	1-B	48	0	23	0	0
2	2-A	48	0	24	0	0
2	2-B	48	0	24	0	0
2	3-A	48	0	24	0	0
2	3-B	48	0	24	0	0
2	4-A	48	0	24	0	0
2	4-B	48	0	24	0	0
2	5-A	48	0	24	0	0
2	5-B	48	0	24	0	0
2	6-A	48	0	24	0	0
2	6-B	48	0	24	0	0
2	7-A	48	0	24	0	0
2	7-B	48	0	24	0	0
2	8-A	48	0	24	0	0
2	8-B	48	0	23	0	0
2	9-A	48	0	24	0	0
2	9-B	48	0	23	0	0
2	10-A	48	0	24	0	0
2	10-B	48	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	11-A	48	0	24	0	0
2	11-B	48	0	24	0	0
2	12-A	48	0	23	0	0
2	12-B	48	0	24	0	0
2	13-A	48	0	24	0	0
2	13-B	48	0	23	0	0
2	14-A	48	0	23	0	0
2	14-B	48	0	22	0	0
2	15-A	48	0	23	0	0
2	15-B	48	0	21	0	0
2	16-A	48	0	24	0	0
2	16-B	48	0	23	0	0
3	1-A	146	0	0	0	0
3	1-B	223	0	0	0	0
3	2-A	147	0	0	0	0
3	2-B	222	0	0	0	0
3	3-A	147	0	0	0	0
3	3-B	222	0	0	0	0
3	4-A	146	0	0	0	0
3	4-B	223	0	0	0	0
3	5-A	147	0	0	0	0
3	5-B	222	0	0	0	0
3	6-A	145	0	0	0	0
3	6-B	224	0	0	0	0
3	7-A	145	0	0	0	0
3	7-B	224	0	0	0	0
3	8-A	146	0	0	0	0
3	8-B	223	0	0	0	0
3	9-A	146	0	0	0	0
3	9-B	223	0	0	0	0
3	10-A	147	0	0	0	0
3	10-B	222	0	0	0	0
3	11-A	146	0	0	0	0
3	11-B	223	0	0	0	0
3	12-A	147	0	0	0	0
3	12-B	222	0	0	0	0
3	13-A	146	0	0	0	0
3	13-B	223	0	0	0	0
3	14-A	146	0	0	0	0
3	14-B	223	0	0	0	0
3	15-A	147	0	0	0	0
3	15-B	222	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	16-A	147	0	0	0	0
3	16-B	222	0	0	0	0
All	All	66192	0	60467	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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 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	1-A	239/253 (94%)	224 (94%)	12 (5%)	3 (1%)	12	7
1	1-B	239/253 (94%)	226 (95%)	12 (5%)	1 (0%)	34	32
1	2-A	239/253 (94%)	220 (92%)	19 (8%)	0	100	100
1	2-B	239/253 (94%)	228 (95%)	10 (4%)	1 (0%)	34	32
1	3-A	239/253 (94%)	214 (90%)	21 (9%)	4 (2%)	9	4
1	3-B	239/253 (94%)	226 (95%)	12 (5%)	1 (0%)	34	32
1	4-A	239/253 (94%)	220 (92%)	16 (7%)	3 (1%)	12	7
1	4-B	239/253 (94%)	228 (95%)	11 (5%)	0	100	100
1	5-A	239/253 (94%)	218 (91%)	20 (8%)	1 (0%)	34	32
1	5-B	239/253 (94%)	225 (94%)	11 (5%)	3 (1%)	12	7
1	6-A	239/253 (94%)	215 (90%)	17 (7%)	7 (3%)	4	1
1	6-B	239/253 (94%)	227 (95%)	11 (5%)	1 (0%)	34	32
1	7-A	239/253 (94%)	220 (92%)	18 (8%)	1 (0%)	34	32
1	7-B	239/253 (94%)	229 (96%)	8 (3%)	2 (1%)	19	15
1	8-A	239/253 (94%)	214 (90%)	22 (9%)	3 (1%)	12	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	8-B	239/253 (94%)	226 (95%)	12 (5%)	1 (0%)	34	32
1	9-A	239/253 (94%)	223 (93%)	15 (6%)	1 (0%)	34	32
1	9-B	239/253 (94%)	226 (95%)	12 (5%)	1 (0%)	34	32
1	10-A	239/253 (94%)	222 (93%)	16 (7%)	1 (0%)	34	32
1	10-B	239/253 (94%)	229 (96%)	9 (4%)	1 (0%)	34	32
1	11-A	239/253 (94%)	218 (91%)	17 (7%)	4 (2%)	9	4
1	11-B	239/253 (94%)	223 (93%)	15 (6%)	1 (0%)	34	32
1	12-A	239/253 (94%)	222 (93%)	17 (7%)	0	100	100
1	12-B	239/253 (94%)	230 (96%)	9 (4%)	0	100	100
1	13-A	239/253 (94%)	221 (92%)	18 (8%)	0	100	100
1	13-B	239/253 (94%)	225 (94%)	13 (5%)	1 (0%)	34	32
1	14-A	239/253 (94%)	209 (87%)	21 (9%)	9 (4%)	3	1
1	14-B	239/253 (94%)	228 (95%)	10 (4%)	1 (0%)	34	32
1	15-A	239/253 (94%)	206 (86%)	29 (12%)	4 (2%)	9	4
1	15-B	239/253 (94%)	225 (94%)	12 (5%)	2 (1%)	19	15
1	16-A	239/253 (94%)	222 (93%)	16 (7%)	1 (0%)	34	32
1	16-B	239/253 (94%)	220 (92%)	19 (8%)	0	100	100
All	All	7648/8096 (94%)	7109 (93%)	480 (6%)	59 (1%)	19	15

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	26	GLU
1	1-A	146	LEU
1	3-A	184	VAL
1	6-A	146	LEU
1	7-A	30	LYS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	196/203 (97%)	194 (99%)	2 (1%)	76	82
1	1-B	196/203 (97%)	192 (98%)	4 (2%)	55	60
1	2-A	196/203 (97%)	191 (97%)	5 (3%)	46	50
1	2-B	196/203 (97%)	193 (98%)	3 (2%)	65	71
1	3-A	196/203 (97%)	191 (97%)	5 (3%)	46	50
1	3-B	196/203 (97%)	194 (99%)	2 (1%)	76	82
1	4-A	196/203 (97%)	192 (98%)	4 (2%)	55	60
1	4-B	196/203 (97%)	194 (99%)	2 (1%)	76	82
1	5-A	196/203 (97%)	194 (99%)	2 (1%)	76	82
1	5-B	196/203 (97%)	195 (100%)	1 (0%)	88	92
1	6-A	196/203 (97%)	194 (99%)	2 (1%)	76	82
1	6-B	196/203 (97%)	193 (98%)	3 (2%)	65	71
1	7-A	196/203 (97%)	194 (99%)	2 (1%)	76	82
1	7-B	196/203 (97%)	192 (98%)	4 (2%)	55	60
1	8-A	196/203 (97%)	191 (97%)	5 (3%)	46	50
1	8-B	196/203 (97%)	194 (99%)	2 (1%)	76	82
1	9-A	196/203 (97%)	193 (98%)	3 (2%)	65	71
1	9-B	196/203 (97%)	190 (97%)	6 (3%)	40	43
1	10-A	196/203 (97%)	193 (98%)	3 (2%)	65	71
1	10-B	196/203 (97%)	195 (100%)	1 (0%)	88	92
1	11-A	196/203 (97%)	194 (99%)	2 (1%)	76	82
1	11-B	196/203 (97%)	193 (98%)	3 (2%)	65	71
1	12-A	196/203 (97%)	192 (98%)	4 (2%)	55	60
1	12-B	196/203 (97%)	194 (99%)	2 (1%)	76	82
1	13-A	196/203 (97%)	192 (98%)	4 (2%)	55	60
1	13-B	196/203 (97%)	193 (98%)	3 (2%)	65	71
1	14-A	196/203 (97%)	191 (97%)	5 (3%)	46	50
1	14-B	196/203 (97%)	194 (99%)	2 (1%)	76	82
1	15-A	196/203 (97%)	185 (94%)	11 (6%)	21	18
1	15-B	196/203 (97%)	193 (98%)	3 (2%)	65	71
1	16-A	196/203 (97%)	191 (97%)	5 (3%)	46	50
1	16-B	196/203 (97%)	191 (97%)	5 (3%)	46	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6272/6496 (97%)	6162 (98%)	110 (2%)	59 65

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	10-A	104	TYR
1	12-B	126	LYS
1	16-B	251	SER
1	15-B	219	GLU
1	10-A	220	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
1	9-B	18	GLN
1	16-A	160	GLN
1	12-A	64	ASN
1	15-B	103	GLN
1	15-A	103	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAP	8-A	400	-	45,52,52	3.09	12 (26%)	56,80,80	3.41	18 (32%)
2	NAP	9-B	401	-	45,52,52	3.32	16 (35%)	56,80,80	3.27	19 (33%)
2	NAP	8-B	401	-	45,52,52	3.48	19 (42%)	56,80,80	3.22	18 (32%)
2	NAP	2-A	400	-	45,52,52	2.79	17 (37%)	56,80,80	3.39	17 (30%)
2	NAP	16-A	400	-	45,52,52	2.83	16 (35%)	56,80,80	3.12	15 (26%)
2	NAP	13-A	400	-	45,52,52	2.98	17 (37%)	56,80,80	3.26	16 (28%)
2	NAP	9-A	400	-	45,52,52	2.52	13 (28%)	56,80,80	3.31	18 (32%)
2	NAP	5-B	401	-	45,52,52	4.21	16 (35%)	56,80,80	3.87	24 (42%)
2	NAP	13-B	401	-	45,52,52	5.20	22 (48%)	56,80,80	3.75	17 (30%)
2	NAP	7-B	401	-	45,52,52	4.18	16 (35%)	56,80,80	3.80	24 (42%)
2	NAP	3-A	400	-	45,52,52	2.97	15 (33%)	56,80,80	3.44	18 (32%)
2	NAP	15-A	400	-	45,52,52	2.81	17 (37%)	56,80,80	3.25	18 (32%)
2	NAP	12-B	401	-	45,52,52	4.17	18 (40%)	56,80,80	3.81	23 (41%)
2	NAP	12-A	400	-	45,52,52	2.76	18 (40%)	56,80,80	3.36	17 (30%)
2	NAP	4-A	400	-	45,52,52	2.80	15 (33%)	56,80,80	3.44	19 (33%)
2	NAP	11-A	400	-	45,52,52	3.00	16 (35%)	56,80,80	3.32	19 (33%)
2	NAP	1-A	400	-	45,52,52	2.69	16 (35%)	56,80,80	3.42	17 (30%)
2	NAP	11-B	401	-	45,52,52	3.19	15 (33%)	56,80,80	3.48	22 (39%)
2	NAP	14-B	401	-	45,52,52	5.27	20 (44%)	56,80,80	4.82	23 (41%)
2	NAP	2-B	401	-	45,52,52	3.18	14 (31%)	56,80,80	3.52	21 (37%)
2	NAP	4-B	401	-	45,52,52	3.26	12 (26%)	56,80,80	3.32	22 (39%)
2	NAP	5-A	400	-	45,52,52	2.94	17 (37%)	56,80,80	3.45	17 (30%)
2	NAP	16-B	401	-	45,52,52	4.07	13 (28%)	56,80,80	3.73	22 (39%)
2	NAP	15-B	401	-	45,52,52	4.72	19 (42%)	56,80,80	4.52	23 (41%)
2	NAP	7-A	400	-	45,52,52	2.68	15 (33%)	56,80,80	3.32	17 (30%)
2	NAP	10-A	400	-	45,52,52	2.77	16 (35%)	56,80,80	3.38	17 (30%)
2	NAP	14-A	400	-	45,52,52	2.88	18 (40%)	56,80,80	3.19	19 (33%)
2	NAP	6-A	400	-	45,52,52	3.12	15 (33%)	56,80,80	3.37	18 (32%)
2	NAP	3-B	401	-	45,52,52	4.19	15 (33%)	56,80,80	3.84	23 (41%)
2	NAP	10-B	401	-	45,52,52	3.21	17 (37%)	56,80,80	3.51	18 (32%)
2	NAP	6-B	401	-	45,52,52	3.17	14 (31%)	56,80,80	3.51	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAP	1-B	401	-	45,52,52	3.51	18 (40%)	56,80,80	3.25	19 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	8-A	400	-	1/1/12/12	15/31/67/67	0/5/5/5
2	NAP	9-B	401	-	1/1/12/12	18/31/67/67	0/5/5/5
2	NAP	8-B	401	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	2-A	400	-	1/1/12/12	11/31/67/67	0/5/5/5
2	NAP	16-A	400	-	1/1/12/12	20/31/67/67	0/5/5/5
2	NAP	13-A	400	-	1/1/12/12	11/31/67/67	0/5/5/5
2	NAP	9-A	400	-	1/1/12/12	15/31/67/67	0/5/5/5
2	NAP	5-B	401	-	1/1/12/12	9/31/67/67	0/5/5/5
2	NAP	13-B	401	-	1/1/12/12	12/31/67/67	0/5/5/5
2	NAP	7-B	401	-	1/1/12/12	9/31/67/67	0/5/5/5
2	NAP	3-A	400	-	1/1/12/12	13/31/67/67	0/5/5/5
2	NAP	15-A	400	-	1/1/12/12	17/31/67/67	0/5/5/5
2	NAP	12-B	401	-	1/1/12/12	12/31/67/67	0/5/5/5
2	NAP	12-A	400	-	1/1/12/12	16/31/67/67	0/5/5/5
2	NAP	4-A	400	-	1/1/12/12	17/31/67/67	0/5/5/5
2	NAP	11-A	400	-	1/1/12/12	7/31/67/67	0/5/5/5
2	NAP	1-A	400	-	1/1/12/12	15/31/67/67	0/5/5/5
2	NAP	11-B	401	-	1/1/12/12	9/31/67/67	0/5/5/5
2	NAP	14-B	401	-	1/1/12/12	12/31/67/67	0/5/5/5
2	NAP	2-B	401	-	1/1/12/12	9/31/67/67	0/5/5/5
2	NAP	4-B	401	-	1/1/12/12	16/31/67/67	0/5/5/5
2	NAP	5-A	400	-	1/1/12/12	12/31/67/67	0/5/5/5
2	NAP	16-B	401	-	-	19/31/67/67	0/5/5/5
2	NAP	15-B	401	-	-	13/31/67/67	0/5/5/5
2	NAP	7-A	400	-	1/1/12/12	11/31/67/67	0/5/5/5
2	NAP	10-A	400	-	1/1/12/12	11/31/67/67	0/5/5/5
2	NAP	14-A	400	-	1/1/12/12	11/31/67/67	0/5/5/5
2	NAP	6-A	400	-	1/1/12/12	9/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	3-B	401	-	1/1/12/12	9/31/67/67	0/5/5/5
2	NAP	10-B	401	-	1/1/12/12	11/31/67/67	0/5/5/5
2	NAP	6-B	401	-	1/1/12/12	9/31/67/67	0/5/5/5
2	NAP	1-B	401	-	1/1/12/12	15/31/67/67	0/5/5/5

The worst 5 of 517 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	14-B	401	NAP	O4B-C4B	27.32	2.06	1.45
2	15-B	401	NAP	O4B-C4B	23.55	1.97	1.45
2	16-B	401	NAP	O4B-C4B	18.92	1.87	1.45
2	5-B	401	NAP	O4B-C1B	16.82	1.64	1.41
2	13-B	401	NAP	O4B-C4B	16.79	1.82	1.45

The worst 5 of 620 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	14-B	401	NAP	O4B-C4B-C3B	-18.91	67.69	105.11
2	15-B	401	NAP	O4B-C4B-C3B	-16.84	71.78	105.11
2	14-B	401	NAP	O4B-C4B-C5B	-16.31	55.71	109.37
2	7-B	401	NAP	C5B-C4B-C3B	16.18	175.82	115.18
2	12-B	401	NAP	C5B-C4B-C3B	16.16	175.75	115.18

5 of 30 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	1-A	400	NAP	C4B
2	2-A	400	NAP	C4B
2	3-A	400	NAP	C4B
2	4-A	400	NAP	C4B
2	5-A	400	NAP	C4B

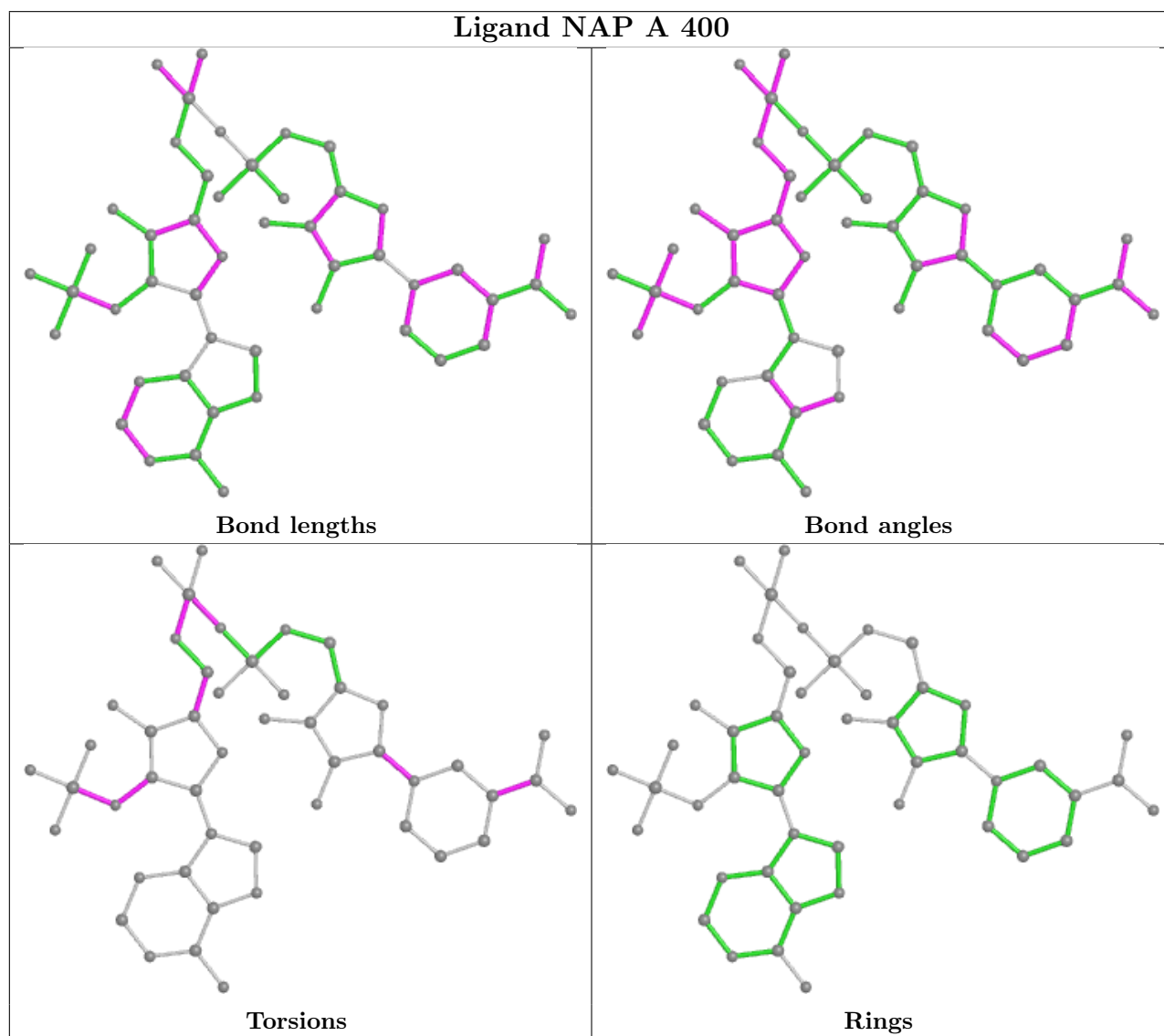
5 of 403 torsion outliers are listed below:

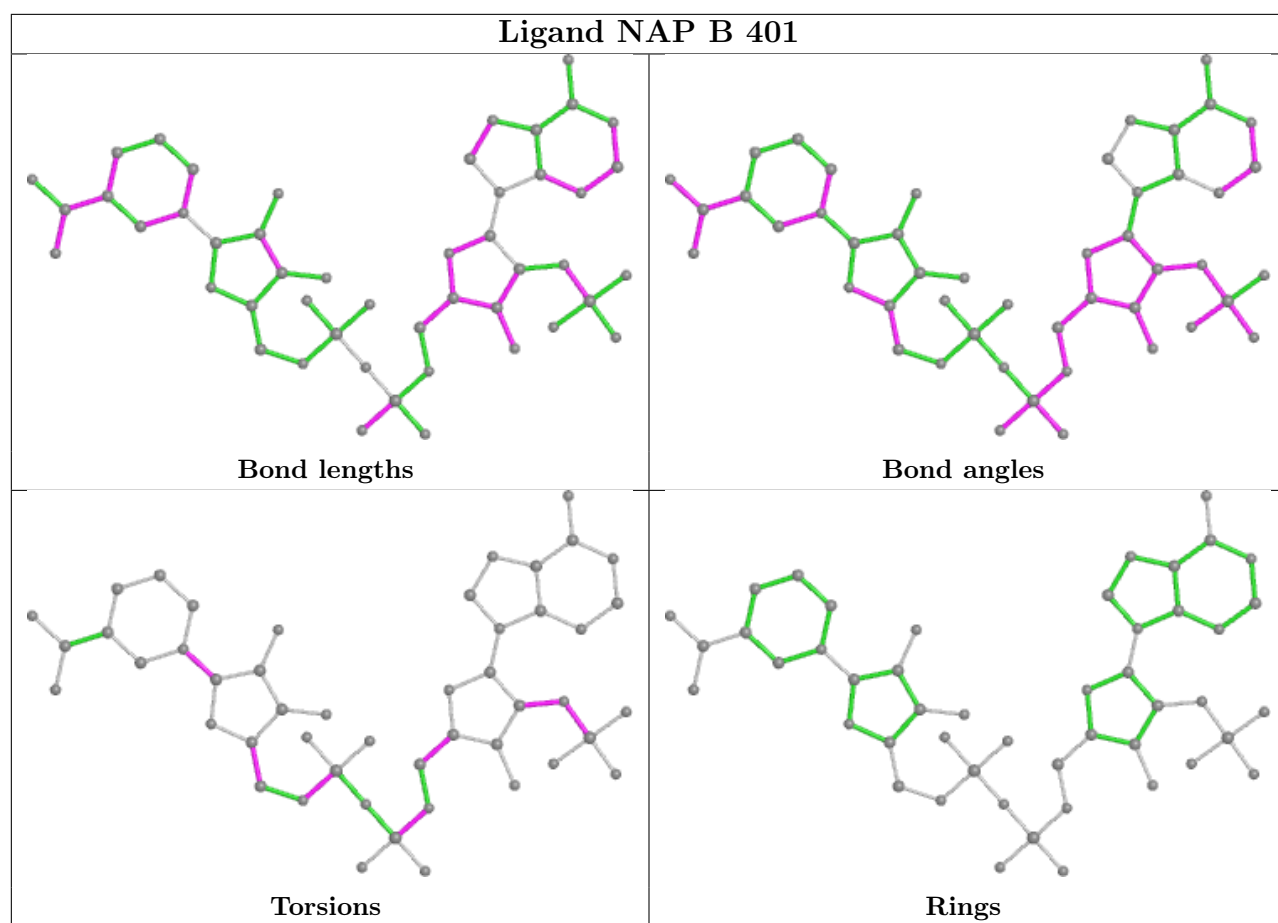
Mol	Chain	Res	Type	Atoms
2	1-A	400	NAP	C5B-O5B-PA-O2A
2	1-A	400	NAP	C5B-O5B-PA-O3
2	1-A	400	NAP	C3B-C4B-C5B-O5B
2	1-A	400	NAP	C3B-C2B-O2B-P2B
2	1-A	400	NAP	O4D-C1D-N1N-C6N

There are no ring outliers.

No monomer is involved in short contacts.

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





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

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.



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

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	1-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	2-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	2-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	3-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	3-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	4-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	4-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	5-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	5-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	6-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	6-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	7-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	7-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	8-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	8-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	9-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	9-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	10-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	10-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	11-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	11-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	12-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	12-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	13-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	13-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	14-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	14-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	15-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	15-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
1	16-A	243/253 (96%)	0.46	25 (10%) 6 8	16, 38, 66, 74	243 (100%)
1	16-B	243/253 (96%)	0.11	18 (7%) 14 18	20, 30, 50, 74	243 (100%)
All	All	7776/8096 (96%)	0.29	688 (8%) 7 12	16, 34, 62, 74	7776 (100%)

The worst 5 of 688 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	27	GLY	6.5
1	2-A	27	GLY	6.5
1	3-A	27	GLY	6.5
1	4-A	27	GLY	6.5
1	5-A	27	GLY	6.5

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAP	1-A	400	48/48	0.94	0.14	29,37,46,49	48
2	NAP	2-A	400	48/48	0.94	0.14	31,37,45,48	48

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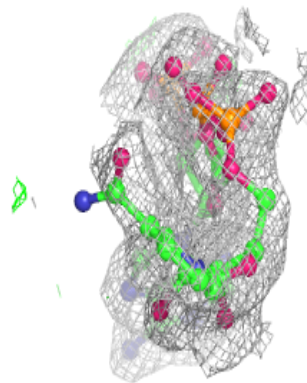
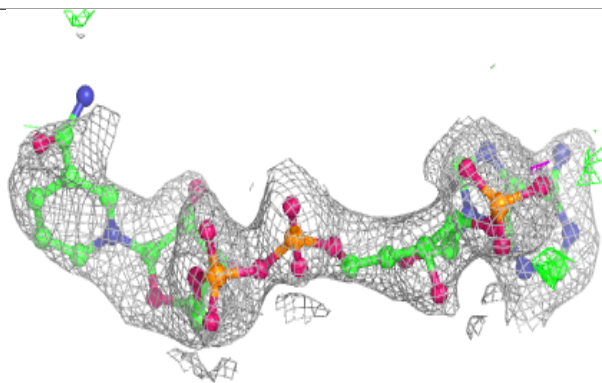
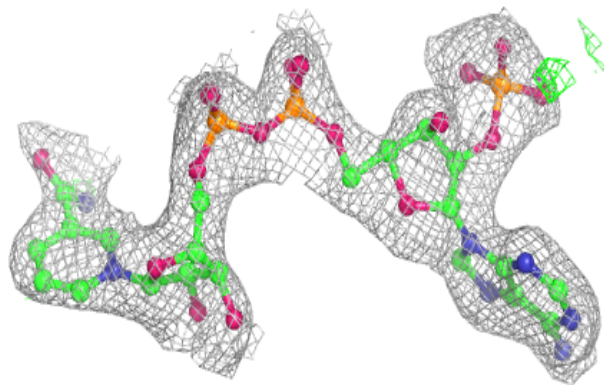
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	3-A	400	48/48	0.94	0.14	28,37,45,49	48
2	NAP	4-A	400	48/48	0.94	0.14	29,37,46,49	48
2	NAP	5-A	400	48/48	0.94	0.14	29,37,46,49	48
2	NAP	6-A	400	48/48	0.94	0.14	28,37,45,49	48
2	NAP	7-A	400	48/48	0.94	0.14	28,37,45,48	48
2	NAP	8-A	400	48/48	0.94	0.14	26,37,45,49	48
2	NAP	9-A	400	48/48	0.94	0.14	28,37,45,48	48
2	NAP	10-A	400	48/48	0.94	0.14	31,37,45,48	48
2	NAP	11-A	400	48/48	0.94	0.14	24,37,44,47	48
2	NAP	12-A	400	48/48	0.94	0.14	28,37,45,46	48
2	NAP	13-A	400	48/48	0.94	0.14	27,37,44,48	48
2	NAP	14-A	400	48/48	0.94	0.14	29,37,46,49	48
2	NAP	15-A	400	48/48	0.94	0.14	27,37,45,49	48
2	NAP	16-A	400	48/48	0.94	0.14	28,37,45,48	48
2	NAP	1-B	401	48/48	0.94	0.14	27,33,37,42	48
2	NAP	2-B	401	48/48	0.94	0.14	28,33,37,43	48
2	NAP	3-B	401	48/48	0.94	0.14	28,33,37,43	48
2	NAP	4-B	401	48/48	0.94	0.14	27,33,38,43	48
2	NAP	5-B	401	48/48	0.94	0.14	27,33,37,43	48
2	NAP	6-B	401	48/48	0.94	0.14	28,33,37,43	48
2	NAP	7-B	401	48/48	0.94	0.14	28,33,37,43	48
2	NAP	8-B	401	48/48	0.94	0.14	27,33,37,41	48
2	NAP	9-B	401	48/48	0.94	0.14	27,33,38,42	48
2	NAP	10-B	401	48/48	0.94	0.14	27,33,37,41	48
2	NAP	11-B	401	48/48	0.94	0.14	28,33,37,43	48
2	NAP	12-B	401	48/48	0.94	0.14	28,33,37,43	48
2	NAP	13-B	401	48/48	0.94	0.14	21,33,37,42	48
2	NAP	14-B	401	48/48	0.94	0.14	27,33,38,43	48
2	NAP	15-B	401	48/48	0.94	0.14	27,33,37,43	48
2	NAP	16-B	401	48/48	0.94	0.14	23,33,38,43	48

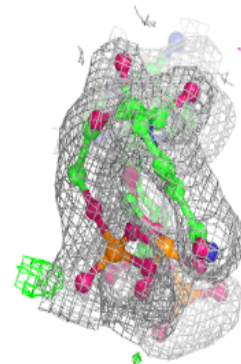
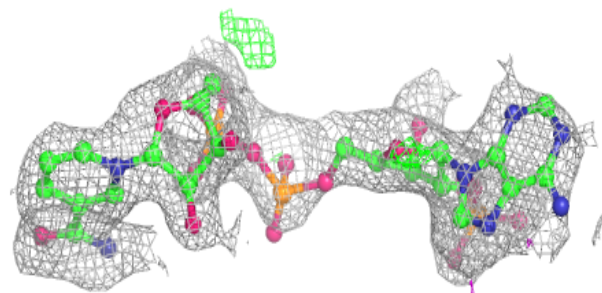
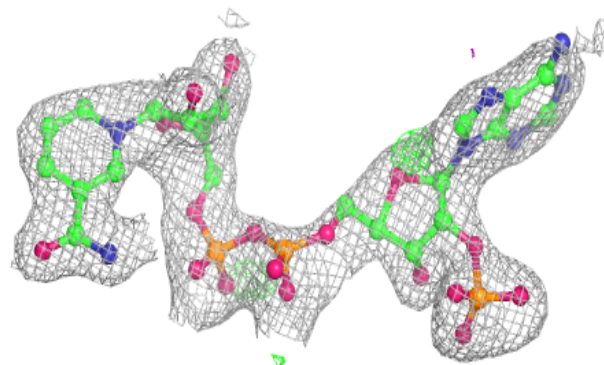
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP 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 NAP B 401:**

$2mF_o-DF_c$  (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.