



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 04:24 am BST

PDB ID : 2Q46
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At5g02240
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 : 1.80 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

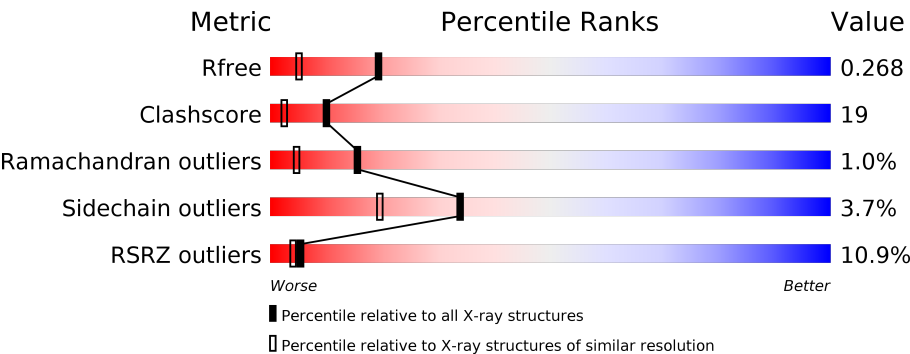
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	1-A	253	<div><div>11%</div><div><div></div><div>67%</div><div>29%</div><div>.</div></div></div>
1	1-B	253	<div><div>11%</div><div><div></div><div>67%</div><div>32%</div><div>.</div></div></div>
1	2-A	253	<div><div>11%</div><div><div></div><div>63%</div><div>33%</div><div>.</div></div></div>
1	2-B	253	<div><div>11%</div><div><div></div><div>64%</div><div>31%</div><div>.</div></div></div>
1	3-A	253	<div><div>11%</div><div><div></div><div>62%</div><div>34%</div><div>.</div></div></div>
1	3-B	253	<div><div>11%</div><div><div></div><div>67%</div><div>32%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	4-A	253	
1	4-B	253	
1	5-A	253	
1	5-B	253	
1	6-A	253	
1	6-B	253	
1	7-A	253	
1	7-B	253	
1	8-A	253	
1	8-B	253	

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	800	X	-	-	-
2	NAP	1-B	801	X	-	-	-
2	NAP	2-A	800	X	-	-	-
2	NAP	2-B	801	X	-	-	-
2	NAP	3-A	800	X	-	-	-
2	NAP	3-B	801	X	-	-	-
2	NAP	4-B	801	X	-	-	-
2	NAP	5-A	800	X	-	-	-
2	NAP	5-B	801	X	-	-	-
2	NAP	6-A	800	X	-	-	-
2	NAP	6-B	801	X	-	-	-
2	NAP	7-A	800	X	-	-	-
2	NAP	7-B	801	X	-	-	-
2	NAP	8-A	800	X	-	-	-
2	NAP	8-B	801	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34496 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.

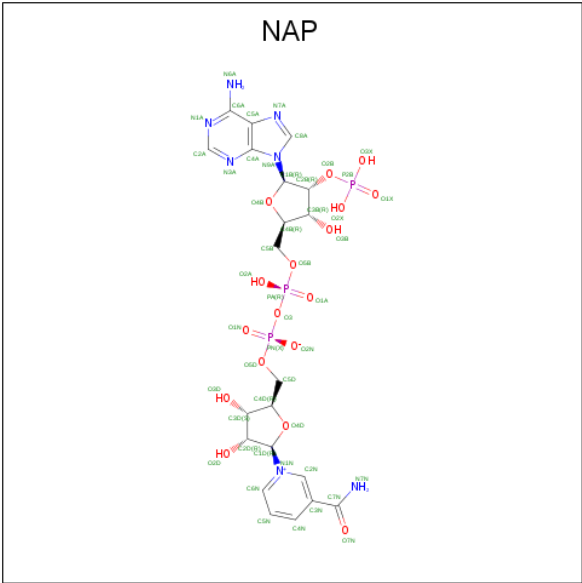
- Molecule 1 is a protein called Protein At5g02240.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	2-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	3-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	4-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	5-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	6-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	7-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	8-A	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	1-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	2-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	3-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	4-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	5-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	6-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	7-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0
1	8-B	253	Total 1908	C 1208	N 326	O 371	S 3	0	0	0

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: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	2-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	3-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	4-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	5-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	6-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	7-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	8-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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	204	Total	O	0	0
			204	204		
3	2-A	205	Total	O	0	0
			205	205		
3	3-A	205	Total	O	0	0
			205	205		
3	4-A	205	Total	O	0	0
			205	205		
3	5-A	205	Total	O	0	0
			205	205		
3	6-A	205	Total	O	0	0
			205	205		
3	7-A	205	Total	O	0	0
			205	205		
3	8-A	204	Total	O	0	0
			204	204		
3	1-B	196	Total	O	0	0
			196	196		
3	2-B	195	Total	O	0	0
			195	195		
3	3-B	195	Total	O	0	0
			195	195		
3	4-B	195	Total	O	0	0
			195	195		

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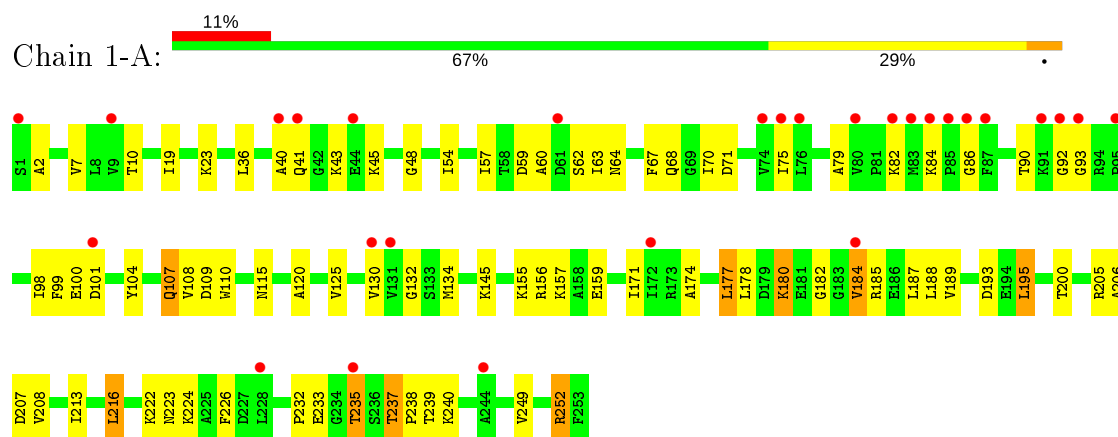
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	5-B	195	Total 195	O 195	0	0
3	6-B	195	Total 195	O 195	0	0
3	7-B	195	Total 195	O 195	0	0
3	8-B	196	Total 196	O 196	0	0

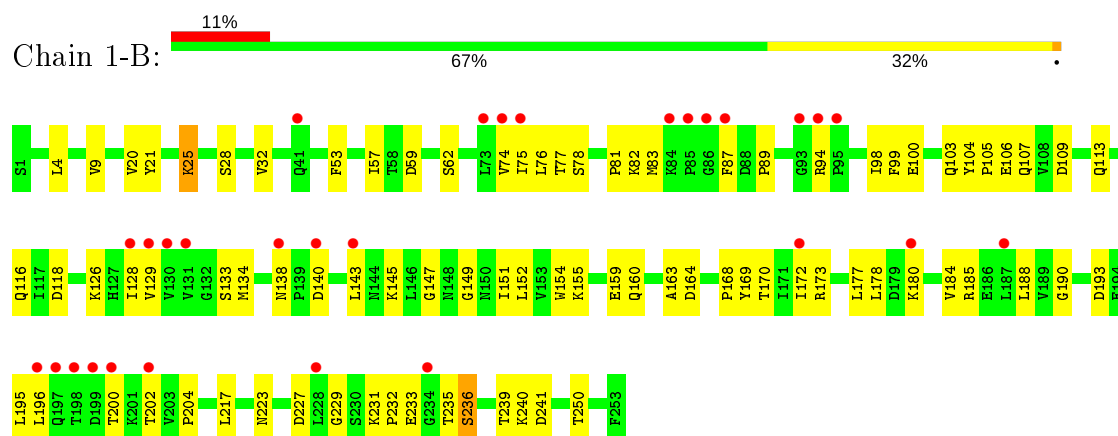
3 Residue-property plots [i](#)

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

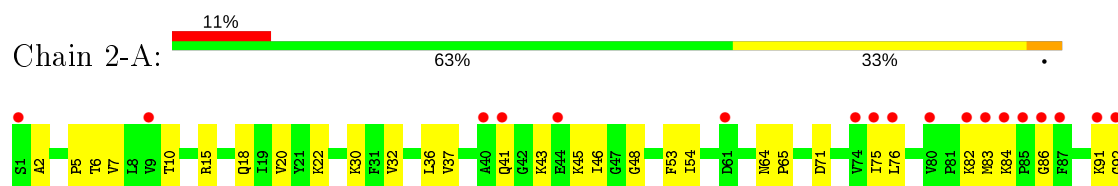
• Molecule 1: Protein At5g02240

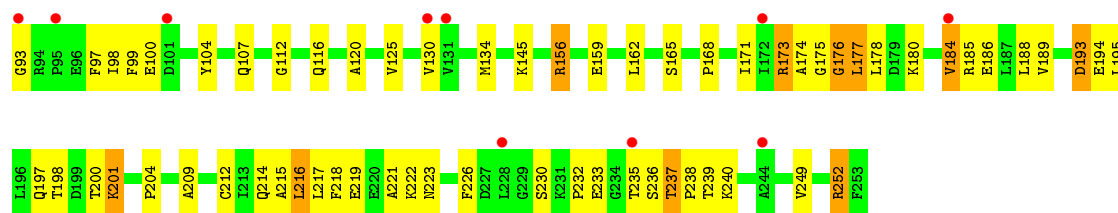


• Molecule 1: Protein At5g02240

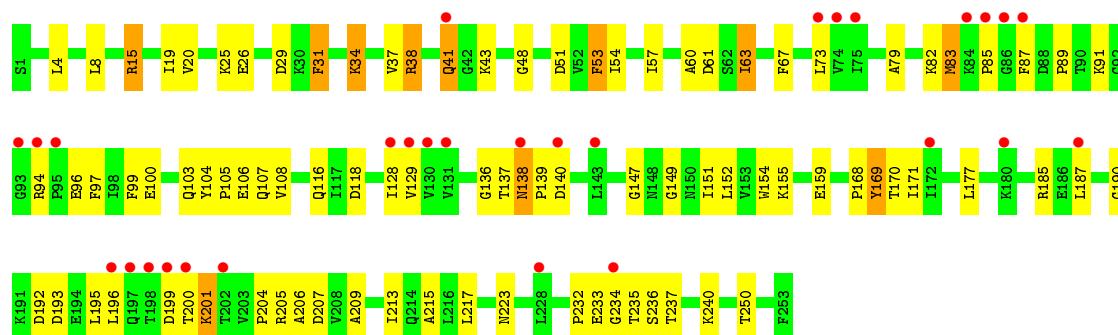


• Molecule 1: Protein At5g02240

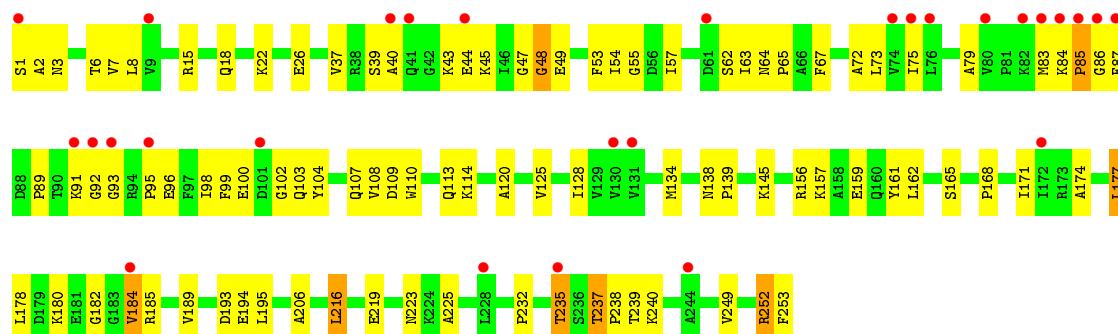




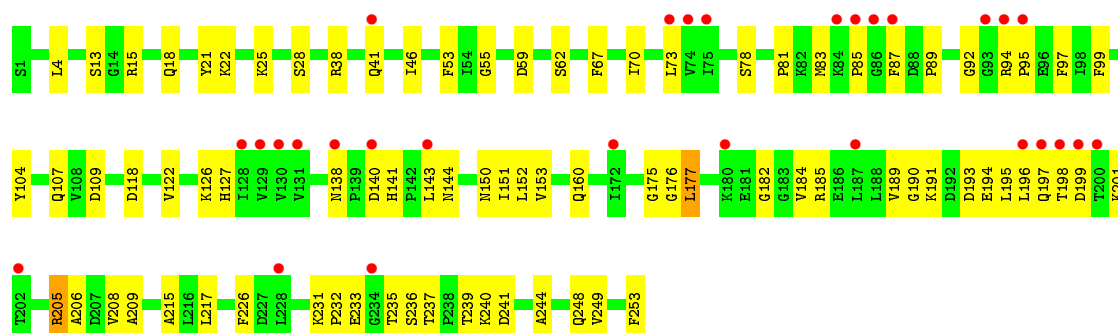
● Molecule 1: Protein At5g02240



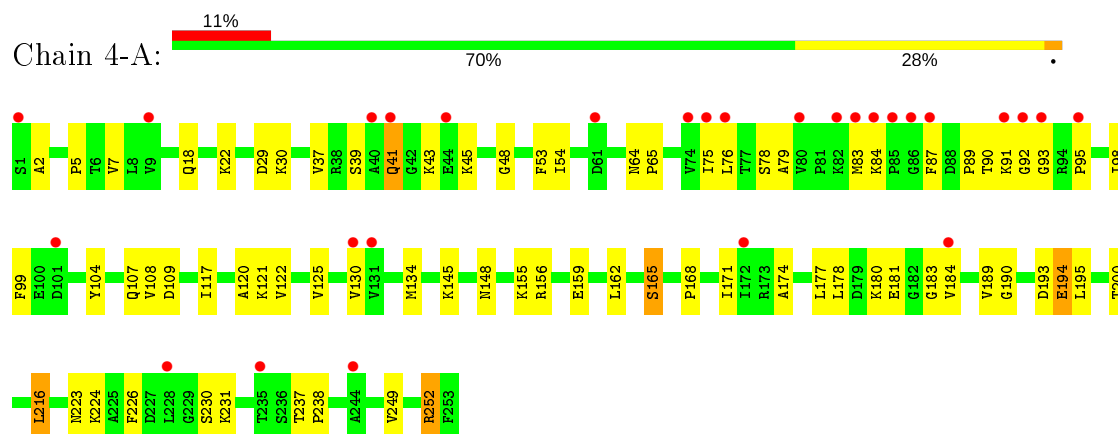
● Molecule 1: Protein At5g02240



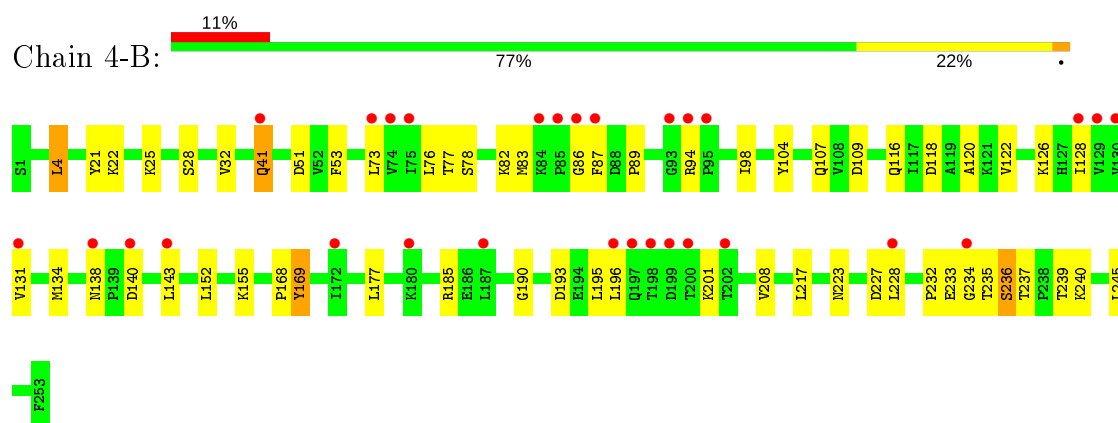
● Molecule 1: Protein At5g02240



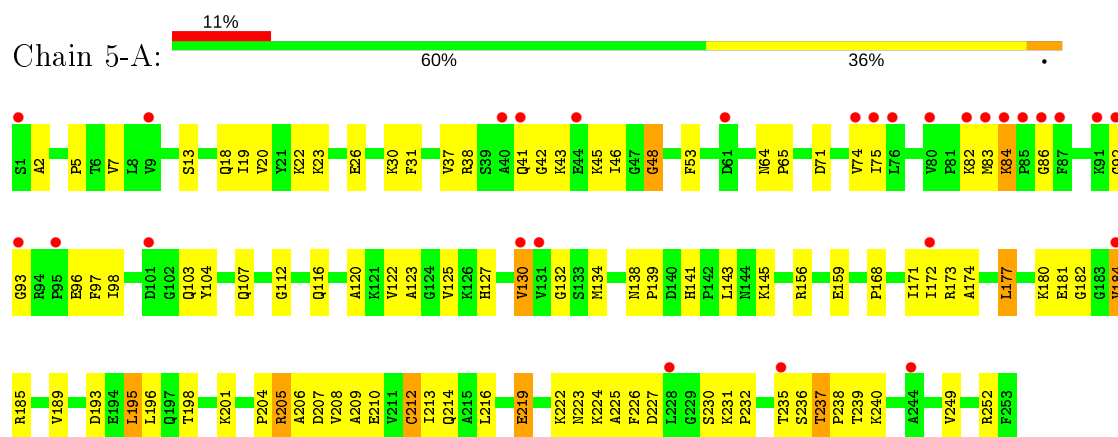
- Molecule 1: Protein At5g02240



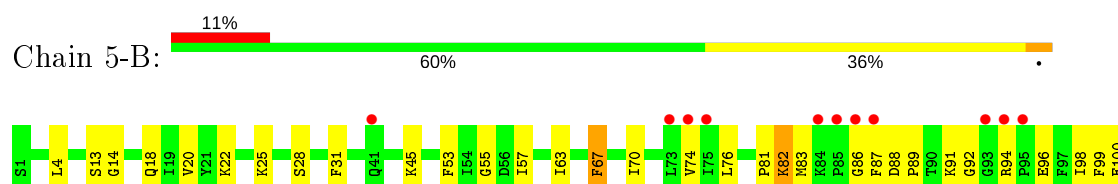
- Molecule 1: Protein At5g02240

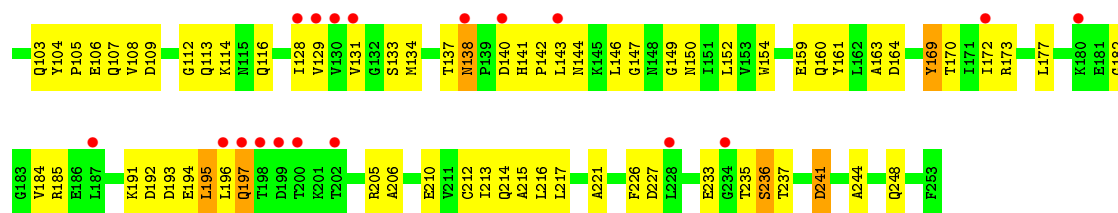


- Molecule 1: Protein At5g02240

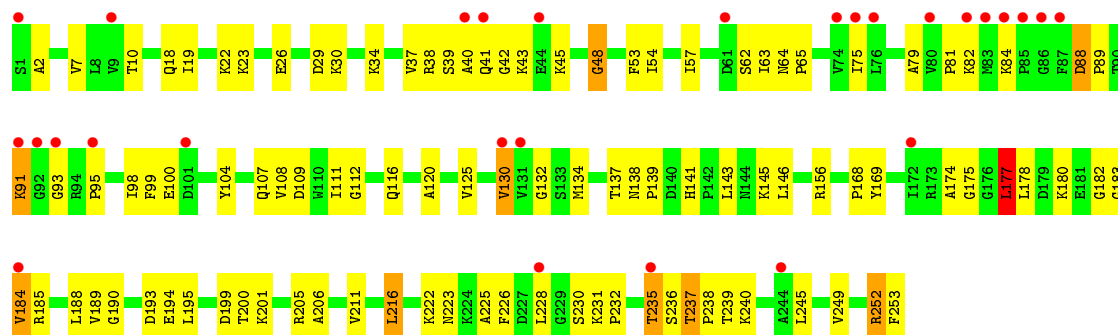


- Molecule 1: Protein At5g02240

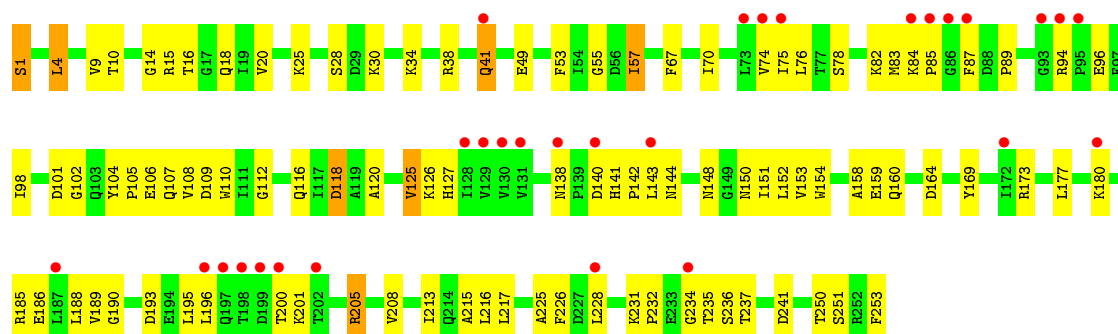




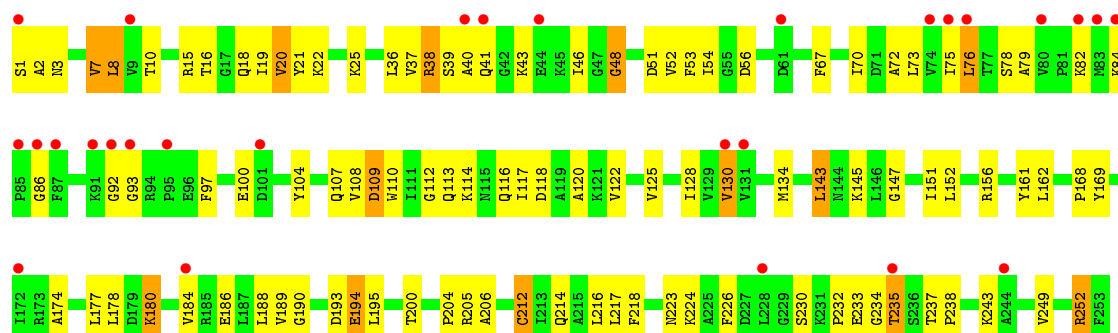
• Molecule 1: Protein At5g02240



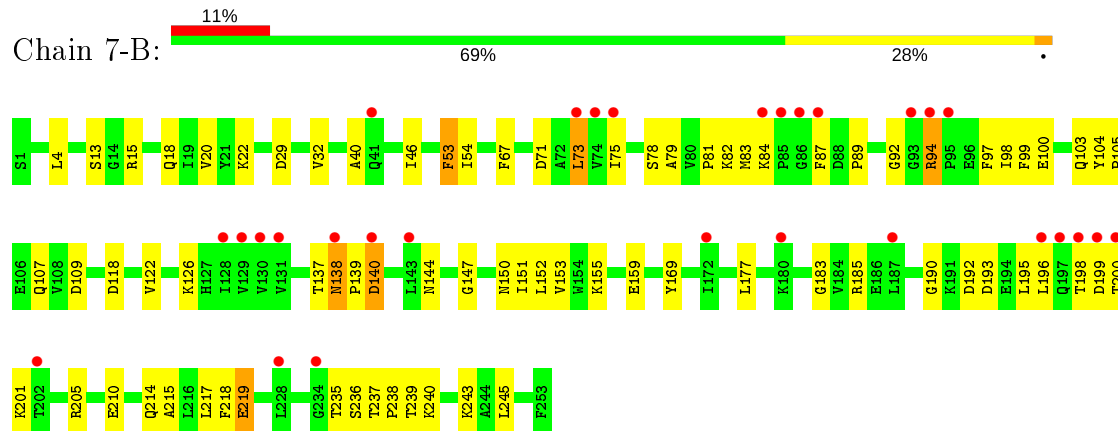
• Molecule 1: Protein At5g02240



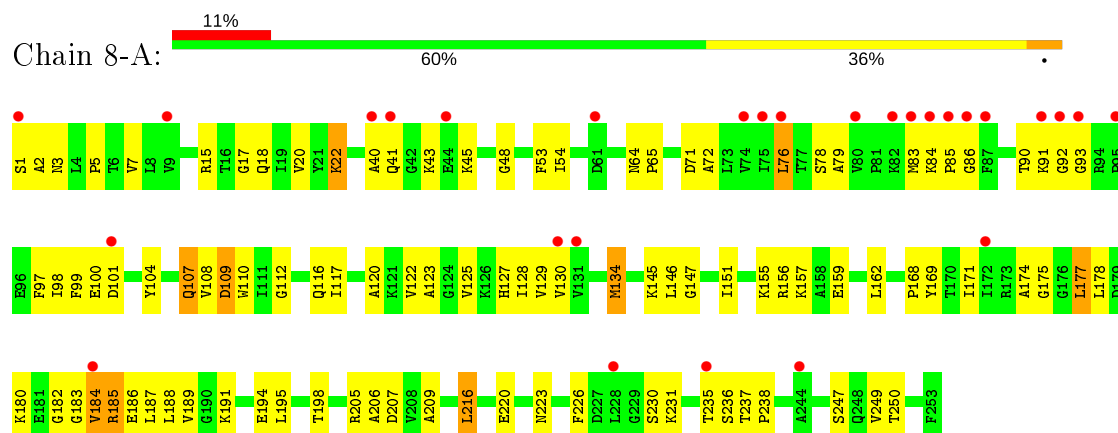
• Molecule 1: Protein At5g02240



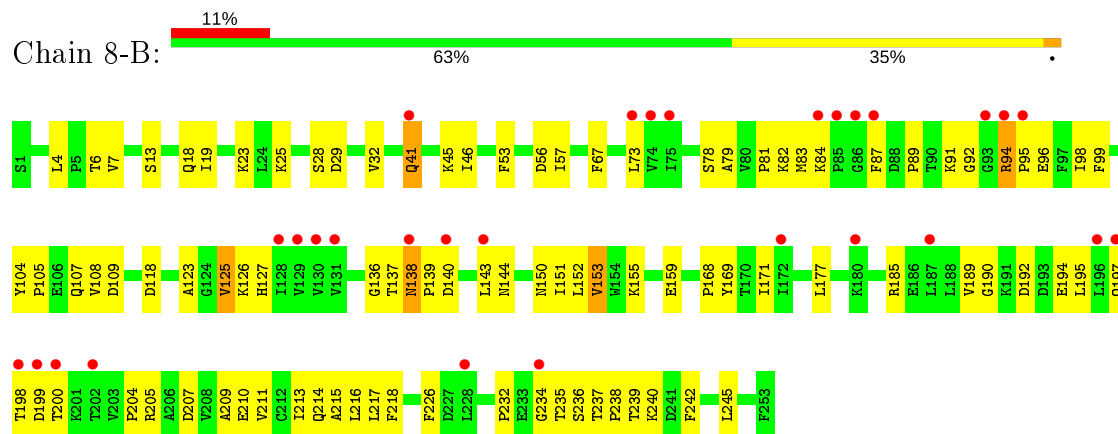
- Molecule 1: Protein At5g02240



- Molecule 1: Protein At5g02240



- Molecule 1: Protein At5g02240



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.75Å 69.80Å 83.83Å 90.00° 96.01° 90.00°	Depositor
Resolution (Å)	23.57 – 1.80 23.57 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.0 (23.57-1.80) 95.2 (23.57-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 1.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.267 0.210 , 0.268	Depositor DCC
R_{free} test set	2445 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34496	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.07	1/1941 (0.1%)	1.03	4/2621 (0.2%)
1	1-B	1.03	2/1941 (0.1%)	1.02	1/2621 (0.0%)
1	2-A	1.07	1/1941 (0.1%)	1.07	8/2621 (0.3%)
1	2-B	1.04	4/1941 (0.2%)	1.02	1/2621 (0.0%)
1	3-A	1.08	3/1941 (0.2%)	1.04	3/2621 (0.1%)
1	3-B	1.02	1/1941 (0.1%)	1.04	3/2621 (0.1%)
1	4-A	1.09	3/1941 (0.2%)	1.02	4/2621 (0.2%)
1	4-B	1.03	2/1941 (0.1%)	1.01	1/2621 (0.0%)
1	5-A	1.20	6/1941 (0.3%)	1.08	6/2621 (0.2%)
1	5-B	1.10	4/1941 (0.2%)	1.05	4/2621 (0.2%)
1	6-A	1.15	3/1941 (0.2%)	1.08	6/2621 (0.2%)
1	6-B	1.12	4/1941 (0.2%)	1.08	3/2621 (0.1%)
1	7-A	1.18	5/1941 (0.3%)	1.08	4/2621 (0.2%)
1	7-B	1.13	6/1941 (0.3%)	1.07	3/2621 (0.1%)
1	8-A	1.18	6/1941 (0.3%)	1.09	8/2621 (0.3%)
1	8-B	1.15	8/1941 (0.4%)	1.09	2/2621 (0.1%)
All	All	1.10	59/31056 (0.2%)	1.05	61/41936 (0.1%)

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5-A	212	CYS	CB-SG	-11.67	1.62	1.82
1	5-B	20	VAL	CB-CG1	8.21	1.70	1.52
1	8-A	134	MET	CG-SD	7.89	2.01	1.81
1	7-A	20	VAL	CB-CG2	7.38	1.68	1.52
1	8-B	123	ALA	CA-CB	6.94	1.67	1.52

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2-A	173	ARG	NE-CZ-NH1	-9.84	115.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6-A	156	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	8-A	156	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	5-A	156	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	2-A	156	ARG	NE-CZ-NH1	7.27	123.93	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	1908	0	1935	67	0
1	1-B	1908	0	1935	70	0
1	2-A	1908	0	1935	65	0
1	2-B	1908	0	1935	79	0
1	3-A	1908	0	1935	70	0
1	3-B	1908	0	1935	68	0
1	4-A	1908	0	1935	56	0
1	4-B	1908	0	1935	59	0
1	5-A	1908	0	1935	73	0
1	5-B	1908	0	1935	82	0
1	6-A	1908	0	1935	85	0
1	6-B	1908	0	1935	84	0
1	7-A	1908	0	1935	90	0
1	7-B	1908	0	1935	63	0
1	8-A	1908	0	1935	85	0
1	8-B	1908	0	1935	83	0
2	1-A	48	0	24	5	0
2	1-B	48	0	24	4	0
2	2-A	48	0	24	4	0
2	2-B	48	0	23	1	0
2	3-A	48	0	24	2	0
2	3-B	48	0	23	3	0
2	4-A	48	0	23	9	0
2	4-B	48	0	24	2	0
2	5-A	48	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5-B	48	0	23	1	0
2	6-A	48	0	24	3	0
2	6-B	48	0	23	8	0
2	7-A	48	0	24	2	0
2	7-B	48	0	23	3	0
2	8-A	48	0	23	4	0
2	8-B	48	0	23	2	0
3	1-A	204	0	0	4	0
3	1-B	196	0	0	7	0
3	2-A	205	0	0	7	0
3	2-B	195	0	0	9	0
3	3-A	205	0	0	7	0
3	3-B	195	0	0	13	0
3	4-A	205	0	0	7	0
3	4-B	195	0	0	9	0
3	5-A	205	0	0	10	0
3	5-B	195	0	0	15	0
3	6-A	205	0	0	11	0
3	6-B	195	0	0	10	0
3	7-A	205	0	0	3	0
3	7-B	195	0	0	12	0
3	8-A	204	0	0	9	0
3	8-B	196	0	0	13	0
All	All	34496	0	31336	1188	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 19.

The worst 5 of 1188 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:MET:CG	1:A:134:MET:SD	2.01	1.46
2:A:800:NAP:C3B	2:A:800:NAP:O3B	1.69	1.39
2:A:800:NAP:O4B	2:A:800:NAP:C5B	1.98	1.11
2:A:800:NAP:O3B	2:A:800:NAP:C4B	2.07	1.02
1:A:79:ALA:HB2	1:A:108:VAL:HG21	1.43	1.01

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	251/253 (99%)	238 (95%)	11 (4%)	2 (1%)	19	7
1	1-B	251/253 (99%)	234 (93%)	15 (6%)	2 (1%)	19	7
1	2-A	251/253 (99%)	237 (94%)	11 (4%)	3 (1%)	13	3
1	2-B	251/253 (99%)	228 (91%)	20 (8%)	3 (1%)	13	3
1	3-A	251/253 (99%)	232 (92%)	16 (6%)	3 (1%)	13	3
1	3-B	251/253 (99%)	233 (93%)	17 (7%)	1 (0%)	34	21
1	4-A	251/253 (99%)	241 (96%)	7 (3%)	3 (1%)	13	3
1	4-B	251/253 (99%)	235 (94%)	14 (6%)	2 (1%)	19	7
1	5-A	251/253 (99%)	236 (94%)	13 (5%)	2 (1%)	19	7
1	5-B	251/253 (99%)	233 (93%)	15 (6%)	3 (1%)	13	3
1	6-A	251/253 (99%)	236 (94%)	11 (4%)	4 (2%)	9	2
1	6-B	251/253 (99%)	233 (93%)	15 (6%)	3 (1%)	13	3
1	7-A	251/253 (99%)	237 (94%)	12 (5%)	2 (1%)	19	7
1	7-B	251/253 (99%)	233 (93%)	17 (7%)	1 (0%)	34	21
1	8-A	251/253 (99%)	240 (96%)	10 (4%)	1 (0%)	34	21
1	8-B	251/253 (99%)	236 (94%)	11 (4%)	4 (2%)	9	2
All	All	4016/4048 (99%)	3762 (94%)	215 (5%)	39 (1%)	15	5

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	92	GLY
1	2-A	174	ALA
1	2-B	83	MET
1	3-A	48	GLY
1	4-A	92	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	203/203 (100%)	193 (95%)	10 (5%)	25	11
1	1-B	203/203 (100%)	202 (100%)	1 (0%)	88	87
1	2-A	203/203 (100%)	194 (96%)	9 (4%)	28	14
1	2-B	203/203 (100%)	190 (94%)	13 (6%)	17	6
1	3-A	203/203 (100%)	196 (97%)	7 (3%)	37	22
1	3-B	203/203 (100%)	196 (97%)	7 (3%)	37	22
1	4-A	203/203 (100%)	197 (97%)	6 (3%)	41	27
1	4-B	203/203 (100%)	200 (98%)	3 (2%)	65	56
1	5-A	203/203 (100%)	196 (97%)	7 (3%)	37	22
1	5-B	203/203 (100%)	198 (98%)	5 (2%)	47	34
1	6-A	203/203 (100%)	195 (96%)	8 (4%)	32	17
1	6-B	203/203 (100%)	197 (97%)	6 (3%)	41	27
1	7-A	203/203 (100%)	192 (95%)	11 (5%)	22	9
1	7-B	203/203 (100%)	195 (96%)	8 (4%)	32	17
1	8-A	203/203 (100%)	196 (97%)	7 (3%)	37	22
1	8-B	203/203 (100%)	192 (95%)	11 (5%)	22	9
All	All	3248/3248 (100%)	3129 (96%)	119 (4%)	34	19

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	4-B	4	LEU
1	5-B	195	LEU
1	8-B	25	LYS
1	4-B	217	LEU
1	5-A	219	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	4-A	223	ASN
1	5-A	214	GLN
1	8-B	18	GLN
1	4-B	41	GLN
1	4-B	148	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	4-A	800	-	45,52,52	5.11	18 (40%)	56,80,80	4.61	15 (26%)
2	NAP	7-B	801	-	45,52,52	2.52	21 (46%)	56,80,80	2.38	10 (17%)
2	NAP	2-B	801	-	45,52,52	2.21	18 (40%)	56,80,80	2.81	9 (16%)
2	NAP	2-A	800	-	45,52,52	2.43	10 (22%)	56,80,80	3.17	12 (21%)
2	NAP	3-B	801	-	45,52,52	2.34	14 (31%)	56,80,80	2.89	10 (17%)
2	NAP	5-A	800	-	45,52,52	2.31	13 (28%)	56,80,80	2.97	12 (21%)
2	NAP	6-B	801	-	45,52,52	2.37	16 (35%)	56,80,80	2.05	11 (19%)
2	NAP	5-B	801	-	45,52,52	2.03	16 (35%)	56,80,80	2.85	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	1-A	800	-	45,52,52	2.58	13 (28%)	56,80,80	3.25	12 (21%)
2	NAP	1-B	801	-	45,52,52	2.14	16 (35%)	56,80,80	2.85	11 (19%)
2	NAP	6-A	800	-	45,52,52	2.45	13 (28%)	56,80,80	3.11	13 (23%)
2	NAP	7-A	800	-	45,52,52	2.40	13 (28%)	56,80,80	3.10	10 (17%)
2	NAP	4-B	801	-	45,52,52	2.14	16 (35%)	56,80,80	2.88	11 (19%)
2	NAP	3-A	800	-	45,52,52	2.43	13 (28%)	56,80,80	3.18	15 (26%)
2	NAP	8-A	800	-	45,52,52	2.51	13 (28%)	56,80,80	3.24	14 (25%)
2	NAP	8-B	801	-	45,52,52	2.52	19 (42%)	56,80,80	2.47	11 (19%)

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	2-B	801	-	1/1/12/12	7/31/67/67	0/5/5/5
2	NAP	7-B	801	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	2-A	800	-	1/1/12/12	13/31/67/67	0/5/5/5
2	NAP	3-B	801	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	5-A	800	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	6-B	801	-	1/1/12/12	8/31/67/67	0/5/5/5
2	NAP	5-B	801	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	1-A	800	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	1-B	801	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	6-A	800	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	7-A	800	-	1/1/12/12	10/31/67/67	0/5/5/5
2	NAP	4-B	801	-	1/1/12/12	13/31/67/67	0/5/5/5
2	NAP	4-A	800	-	-	10/31/67/67	0/5/5/5
2	NAP	3-A	800	-	1/1/12/12	11/31/67/67	0/5/5/5
2	NAP	8-A	800	-	1/1/12/12	14/31/67/67	0/5/5/5
2	NAP	8-B	801	-	1/1/12/12	10/31/67/67	0/5/5/5

The worst 5 of 242 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4-A	800	NAP	O4B-C4B	24.24	1.99	1.45
2	4-A	800	NAP	C3B-C2B	-15.39	1.18	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4-A	800	NAP	O3B-C3B	11.18	1.69	1.43
2	8-A	800	NAP	O4B-C1B	10.99	1.56	1.41
2	2-A	800	NAP	O4B-C1B	10.09	1.55	1.41

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-A	800	NAP	C2B-C3B-C4B	18.26	141.66	101.99
2	4-A	800	NAP	O4B-C4B-C3B	-17.71	70.07	105.11
2	2-A	800	NAP	C5B-C4B-C3B	15.62	173.71	115.18
2	8-A	800	NAP	C5B-C4B-C3B	15.60	173.66	115.18
2	4-B	801	NAP	C5B-C4B-C3B	15.58	173.57	115.18

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	7-B	801	NAP	C4B
2	2-B	801	NAP	C4B
2	2-A	800	NAP	C4B
2	3-B	801	NAP	C4B
2	5-A	800	NAP	C4B

5 of 166 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	4-A	800	NAP	C5B-O5B-PA-O2A
2	4-A	800	NAP	C5B-O5B-PA-O3
2	4-A	800	NAP	O4D-C1D-N1N-C2N
2	4-A	800	NAP	O4D-C1D-N1N-C6N
2	4-A	800	NAP	C2D-C1D-N1N-C2N

There are no ring outliers.

16 monomers are involved in 55 short contacts:

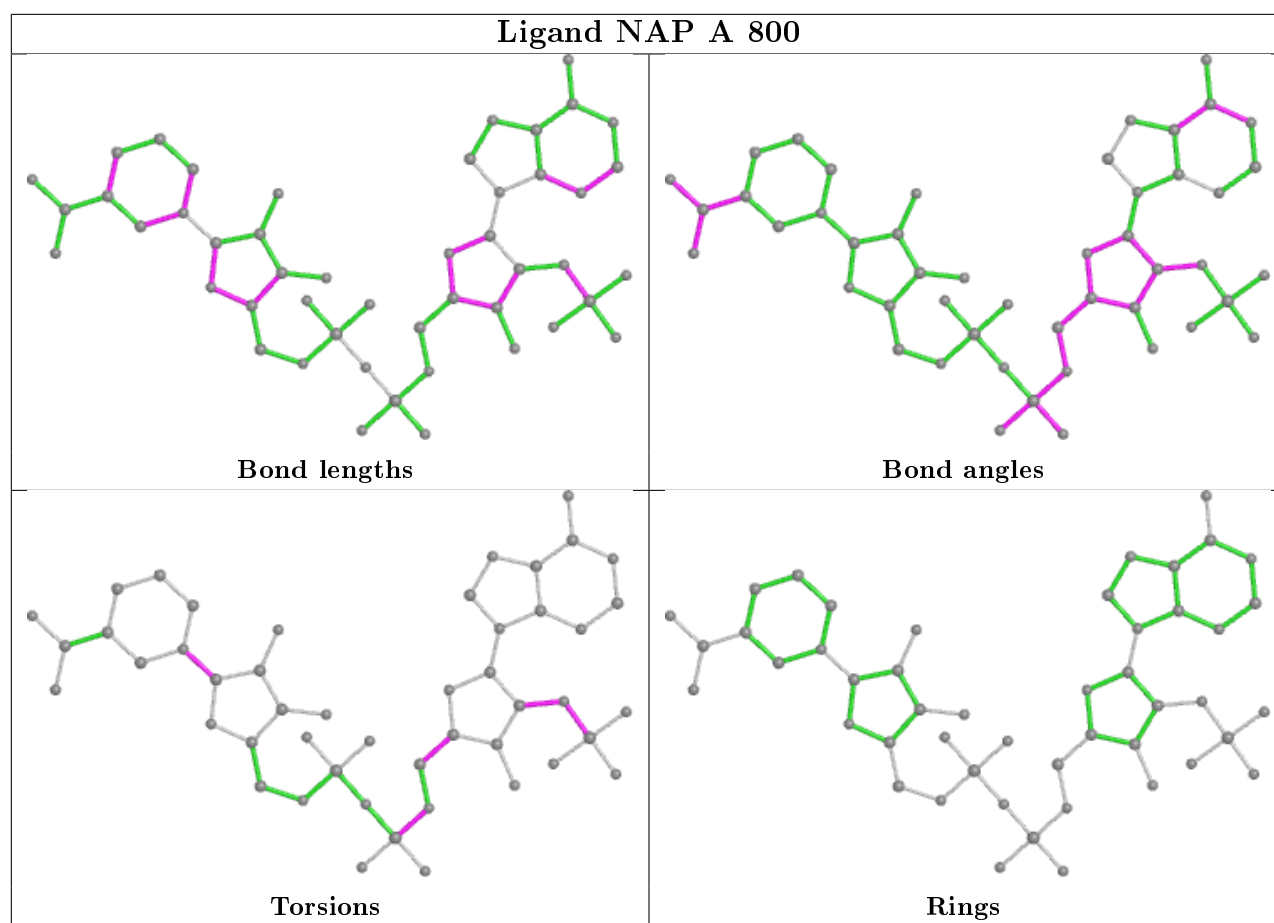
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	4-A	800	NAP	9	0
2	7-B	801	NAP	3	0
2	2-B	801	NAP	1	0
2	2-A	800	NAP	4	0
2	3-B	801	NAP	3	0
2	5-A	800	NAP	2	0

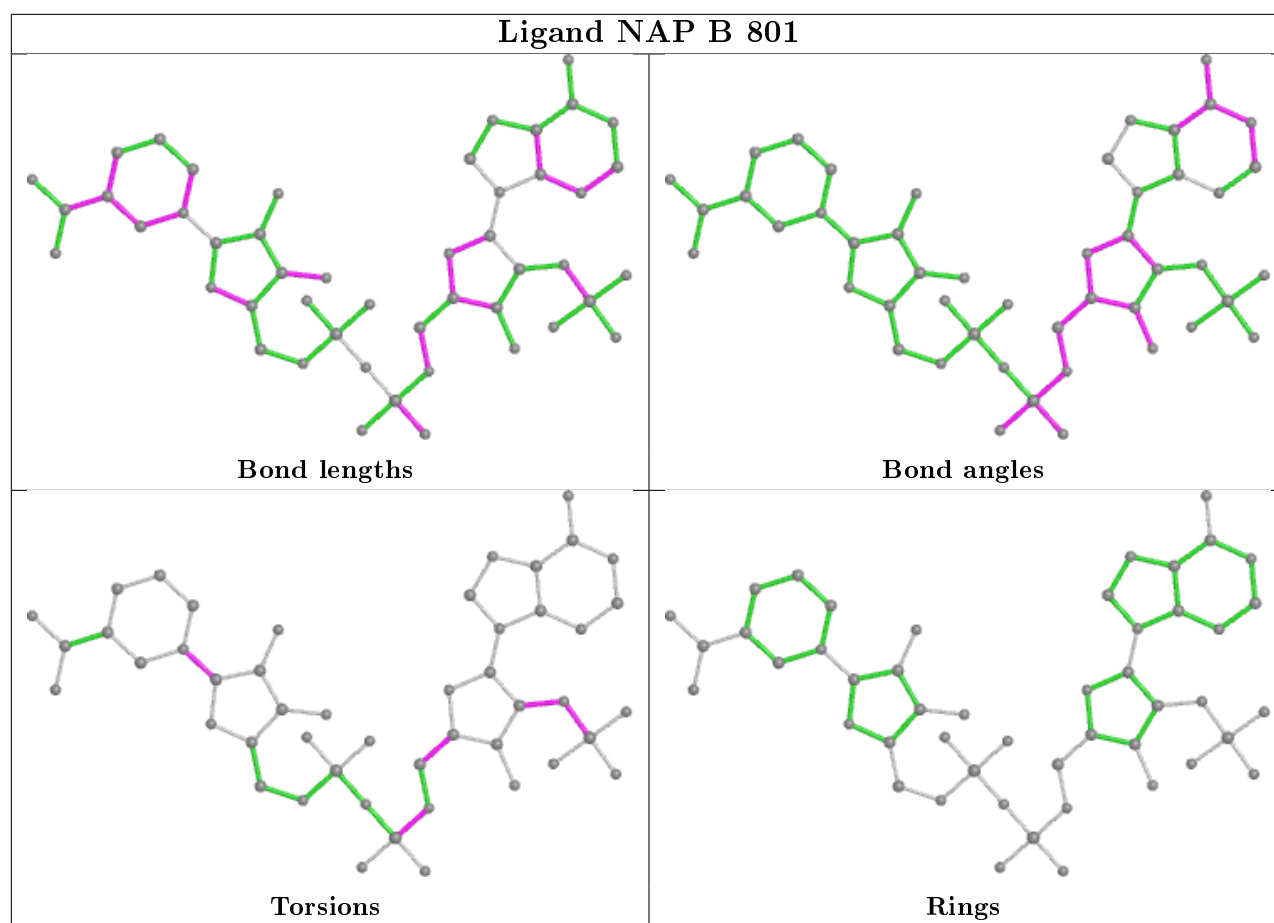
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	6-B	801	NAP	8	0
2	5-B	801	NAP	1	0
2	1-A	800	NAP	5	0
2	1-B	801	NAP	4	0
2	6-A	800	NAP	3	0
2	7-A	800	NAP	2	0
2	4-B	801	NAP	2	0
2	3-A	800	NAP	2	0
2	8-A	800	NAP	4	0
2	8-B	801	NAP	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	1-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	2-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	2-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	3-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	3-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	4-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	4-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	5-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	5-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	6-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	6-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	7-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	7-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
1	8-A	253/253 (100%)	0.67	28 (11%) 5 4	10, 21, 42, 58	253 (100%)
1	8-B	253/253 (100%)	0.71	29 (11%) 4 3	8, 21, 43, 62	253 (100%)
All	All	4048/4048 (100%)	0.69	456 (11%) 5 3	8, 21, 45, 62	4048 (100%)

The worst 5 of 456 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-B	86	GLY	6.9
1	2-B	86	GLY	6.9
1	3-B	86	GLY	6.9
1	4-B	86	GLY	6.9
1	5-B	86	GLY	6.9

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

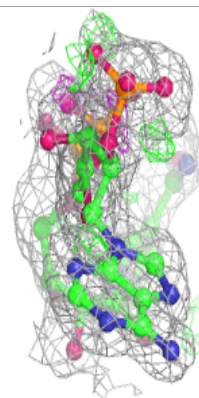
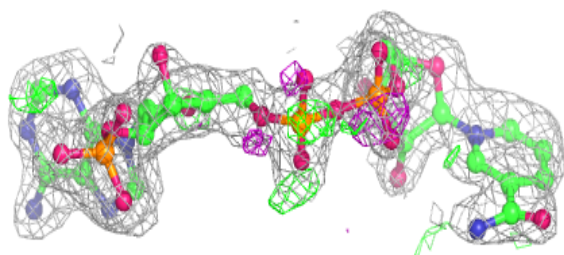
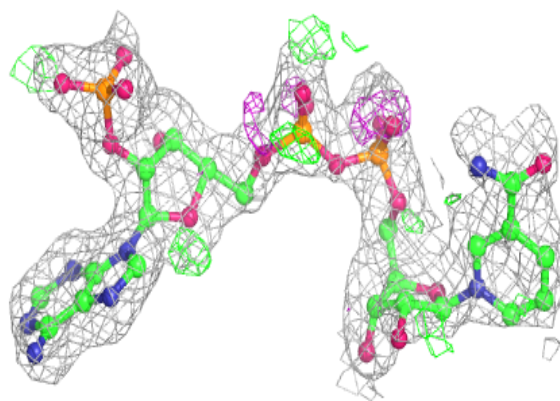
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAP	7-B	801	48/48	0.91	0.15	15,24,29,30	48
2	NAP	2-B	801	48/48	0.91	0.15	18,25,29,29	48
2	NAP	3-B	801	48/48	0.91	0.15	17,24,29,30	48
2	NAP	6-B	801	48/48	0.91	0.15	19,24,29,31	48
2	NAP	5-B	801	48/48	0.91	0.15	18,24,28,30	48
2	NAP	1-B	801	48/48	0.91	0.15	20,25,30,31	48
2	NAP	4-B	801	48/48	0.91	0.15	19,25,30,32	48
2	NAP	8-B	801	48/48	0.91	0.15	14,24,28,30	48
2	NAP	1-A	800	48/48	0.93	0.12	17,23,30,33	48
2	NAP	5-A	800	48/48	0.93	0.12	18,23,28,30	48
2	NAP	6-A	800	48/48	0.93	0.12	16,22,30,32	48
2	NAP	7-A	800	48/48	0.93	0.12	17,23,29,30	48
2	NAP	2-A	800	48/48	0.93	0.12	17,22,29,32	48
2	NAP	3-A	800	48/48	0.93	0.12	15,22,29,31	48
2	NAP	8-A	800	48/48	0.93	0.12	13,23,29,31	48
2	NAP	4-A	800	48/48	0.93	0.12	17,23,28,30	48

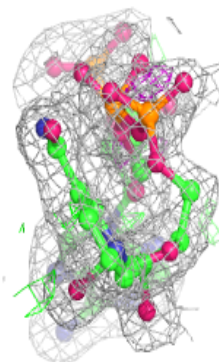
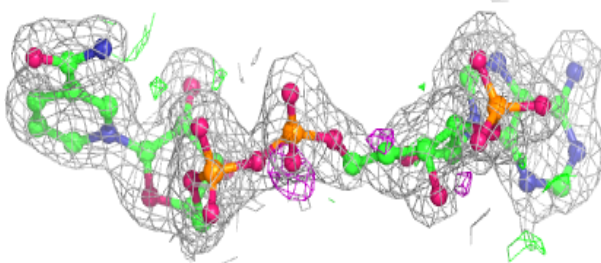
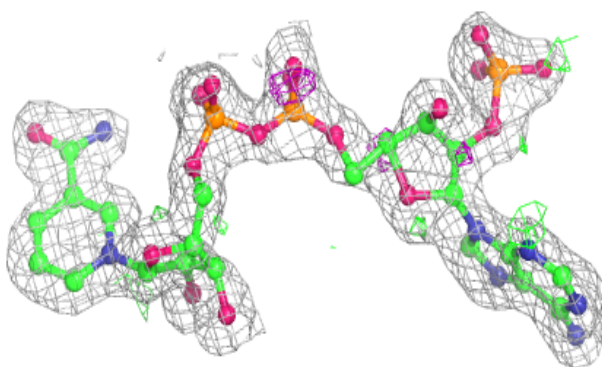
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP B 801:

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

**Electron density around NAP A 800:**

$2mF_o-DF_c$ (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.