wwPDB X-ray Structure Validation Summary Report (i)

Aug 21, 2023 – 11:56 AM EDT

PDB ID	:	2Q49
Title	:	Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At2g19940
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	:	2.19 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

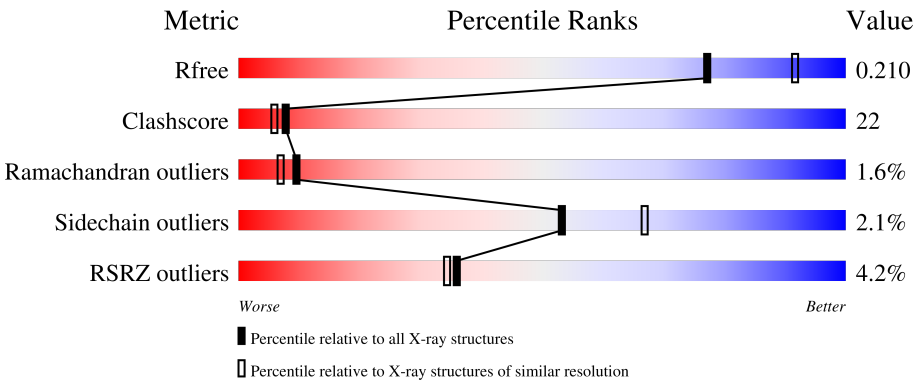
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	1-A	359	2%, 61%, 34%, • •
1	1-B	359	6%, 57%, 38%, • •
1	1-C	359	7%, 53%, 42%, • •
1	1-D	359	3%, 64%, 30%, • •
1	2-A	359	2%, 65%, 30%, • •

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Mol	Chain	Length	Quality of chain
1	2-B	359	6% 61% 33%
1	2-C	359	7% 52% 41%
1	2-D	359	3% 62% 31%
1	3-A	359	2% 58% 37%
1	3-B	359	6% 56% 36%
1	3-C	359	7% 55% 38%
1	3-D	359	3% 60% 35%
1	4-A	359	2% 58% 37%
1	4-B	359	6% 51% 42%
1	4-C	359	7% 53% 39%
1	4-D	359	3% 63% 32%
1	5-A	359	2% 63% 31%
1	5-B	359	6% 53% 41%
1	5-C	359	7% 59% 35%
1	5-D	359	3% 60% 35%
1	6-A	359	2% 62% 32%
1	6-B	359	6% 56% 37%
1	6-C	359	7% 56% 36%
1	6-D	359	3% 64% 31%
1	7-A	359	2% 60% 35%
1	7-B	359	6% 56% 38%
1	7-C	359	7% 57% 37%
1	7-D	359	3% 60% 35%
1	8-A	359	2% 63% 32%
1	8-B	359	6% 55% 37%

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Mol	Chain	Length	Quality of chain
1	8-C	359	7% 60% 34%
1	8-D	359	3% 61% 33%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 93408 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 Probable N-acetyl-gamma-glutamyl-phosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1-A	345	2680	1700	467	501	12	0	0	0
1	2-A	345	2680	1700	467	501	12	0	0	0
1	3-A	345	2680	1700	467	501	12	0	0	0
1	4-A	345	2680	1700	467	501	12	0	0	0
1	5-A	345	2680	1700	467	501	12	0	0	0
1	6-A	345	2680	1700	467	501	12	0	0	0
1	7-A	345	2680	1700	467	501	12	0	0	0
1	8-A	345	2680	1700	467	501	12	0	0	0
1	1-B	345	2680	1700	467	501	12	0	0	0
1	2-B	345	2680	1700	467	501	12	0	0	0
1	3-B	345	2680	1700	467	501	12	0	0	0
1	4-B	345	2680	1700	467	501	12	0	0	0
1	5-B	345	2680	1700	467	501	12	0	0	0
1	6-B	345	2680	1700	467	501	12	0	0	0
1	7-B	345	2680	1700	467	501	12	0	0	0
1	8-B	345	2680	1700	467	501	12	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1-C	345	2680	1700	467	501	12	0	0	0
1	2-C	345	2680	1700	467	501	12	0	0	0
1	3-C	345	2680	1700	467	501	12	0	0	0
1	4-C	345	2680	1700	467	501	12	0	0	0
1	5-C	345	2680	1700	467	501	12	0	0	0
1	6-C	345	2680	1700	467	501	12	0	0	0
1	7-C	345	2680	1700	467	501	12	0	0	0
1	8-C	345	2680	1700	467	501	12	0	0	0
1	1-D	345	2680	1700	467	501	12	0	0	0
1	2-D	345	2680	1700	467	501	12	0	0	0
1	3-D	345	2680	1700	467	501	12	0	0	0
1	4-D	345	2680	1700	467	501	12	0	0	0
1	5-D	345	2680	1700	467	501	12	0	0	0
1	6-D	345	2680	1700	467	501	12	0	0	0
1	7-D	345	2680	1700	467	501	12	0	0	0
1	8-D	345	2680	1700	467	501	12	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	1-A	270	270	270	0	0
2	2-A	263	263	263	0	0
2	3-A	268	268	268	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	4-A	267	Total O 267 267	0	0
2	5-A	262	Total O 262 262	0	0
2	6-A	267	Total O 267 267	0	0
2	7-A	269	Total O 269 269	0	0
2	8-A	267	Total O 267 267	0	0
2	1-B	225	Total O 225 225	0	0
2	2-B	227	Total O 227 227	0	0
2	3-B	216	Total O 216 216	0	0
2	4-B	224	Total O 224 224	0	0
2	5-B	223	Total O 223 223	0	0
2	6-B	225	Total O 225 225	0	0
2	7-B	223	Total O 223 223	0	0
2	8-B	222	Total O 222 222	0	0
2	1-C	220	Total O 220 220	0	0
2	2-C	231	Total O 231 231	0	0
2	3-C	228	Total O 228 228	0	0
2	4-C	223	Total O 223 223	0	0
2	5-C	229	Total O 229 229	0	0
2	6-C	224	Total O 224 224	0	0
2	7-C	224	Total O 224 224	0	0
2	8-C	231	Total O 231 231	0	0

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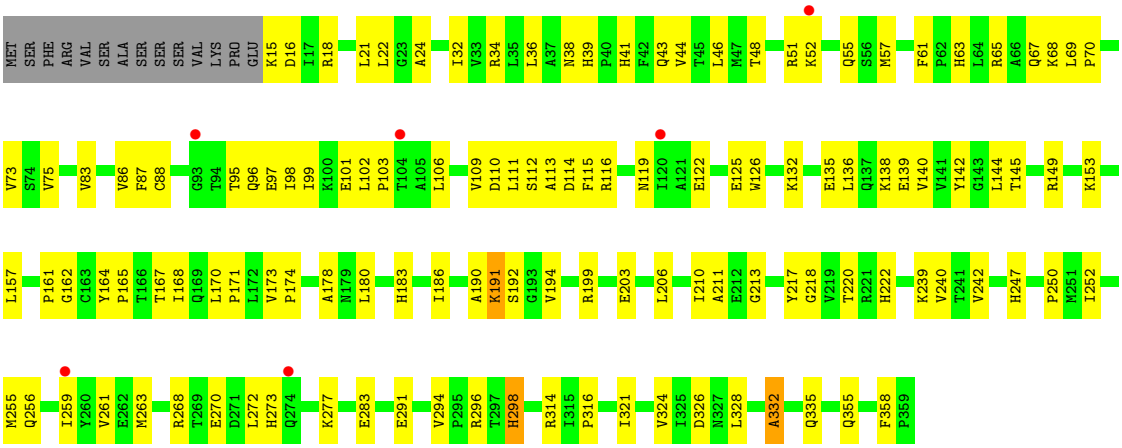
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	1-D	241	241	241	0	0
			Total	O		
2	2-D	235	235	235	0	0
			Total	O		
2	3-D	244	244	244	0	0
			Total	O		
2	4-D	242	242	242	0	0
			Total	O		
2	5-D	242	242	242	0	0
			Total	O		
2	6-D	240	240	240	0	0
			Total	O		
2	7-D	240	240	240	0	0
			Total	O		
2	8-D	236	236	236	0	0

3 Residue-property plots (i)

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

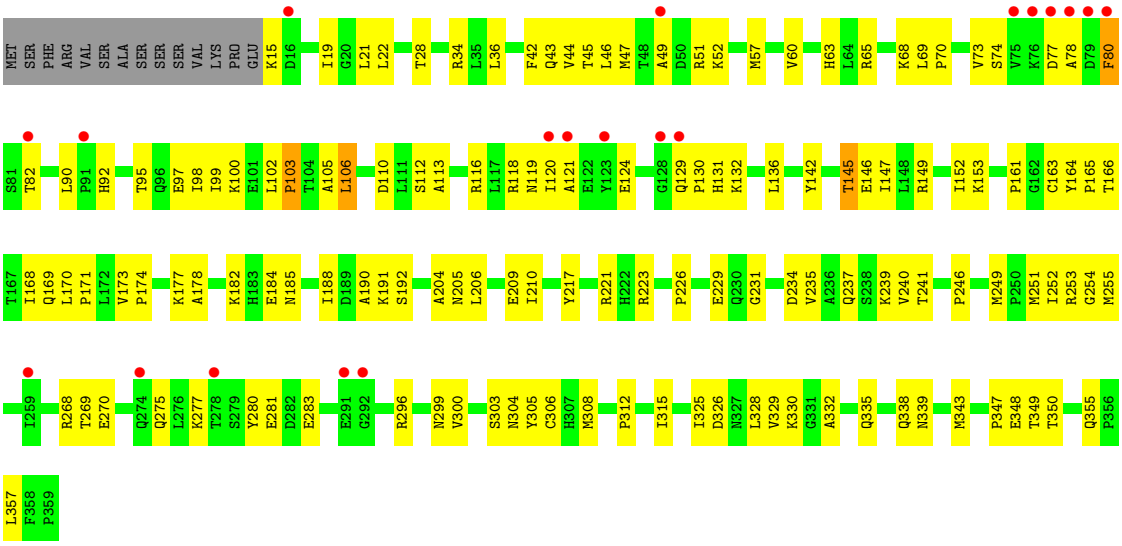
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 1-A:



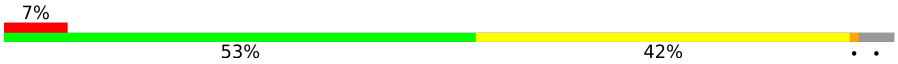
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

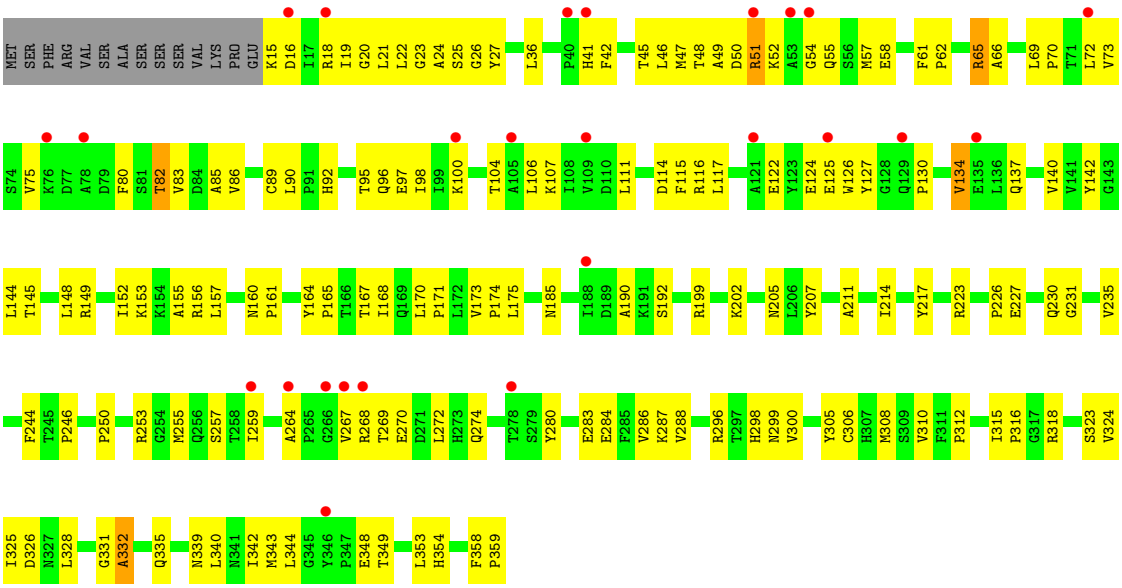
Chain 1-B:



• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

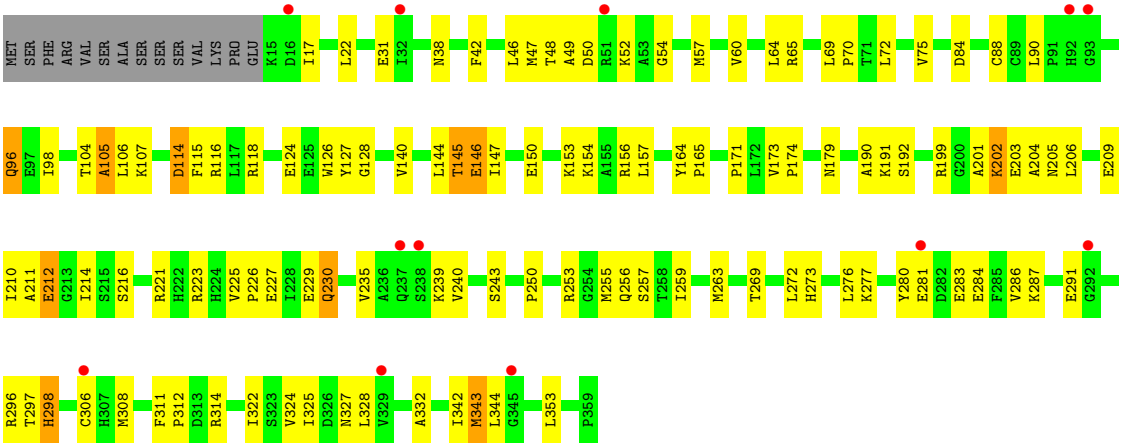
Chain 1-C:





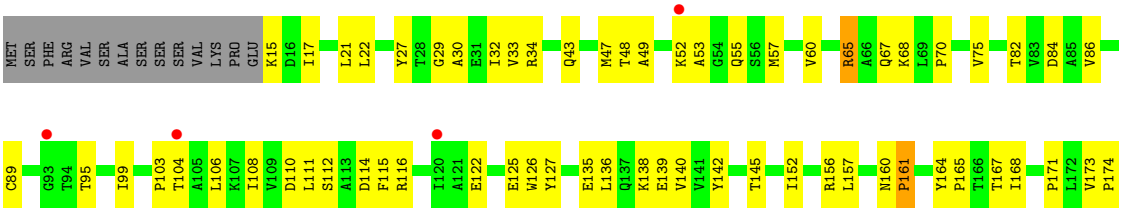
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

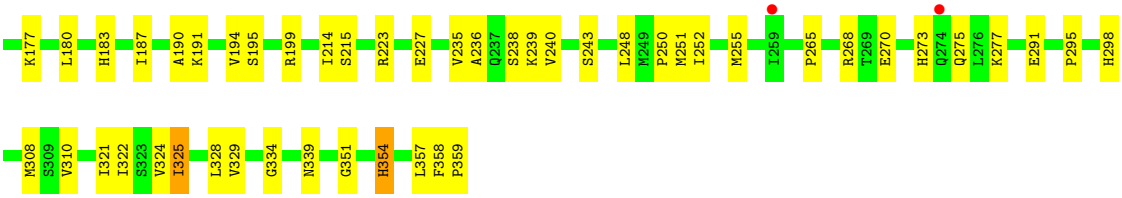
Chain 1-D:



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

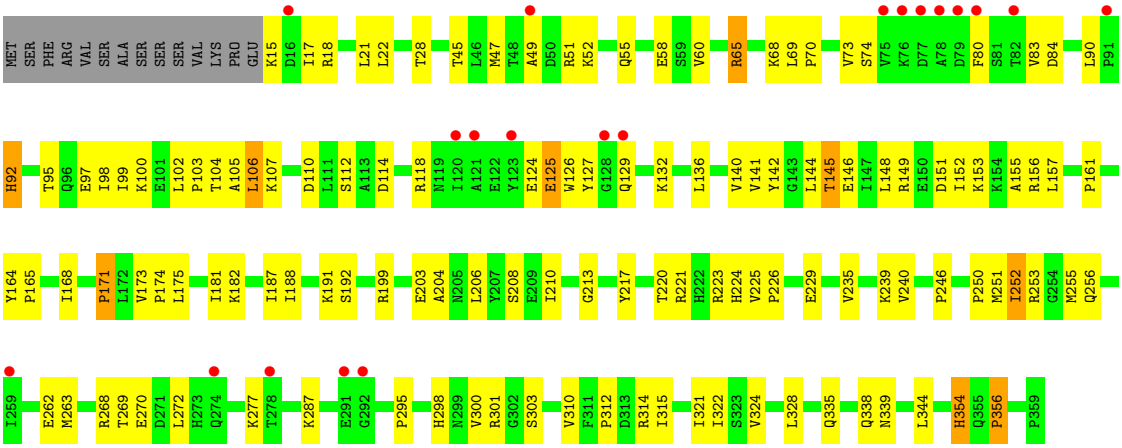
Chain 2-A:





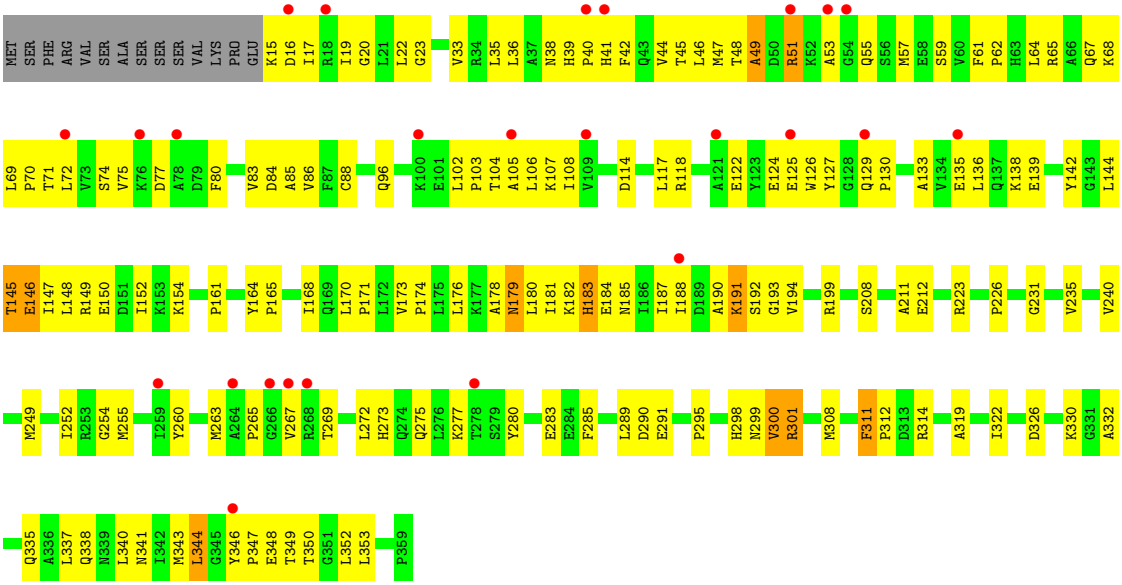
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 2-B:



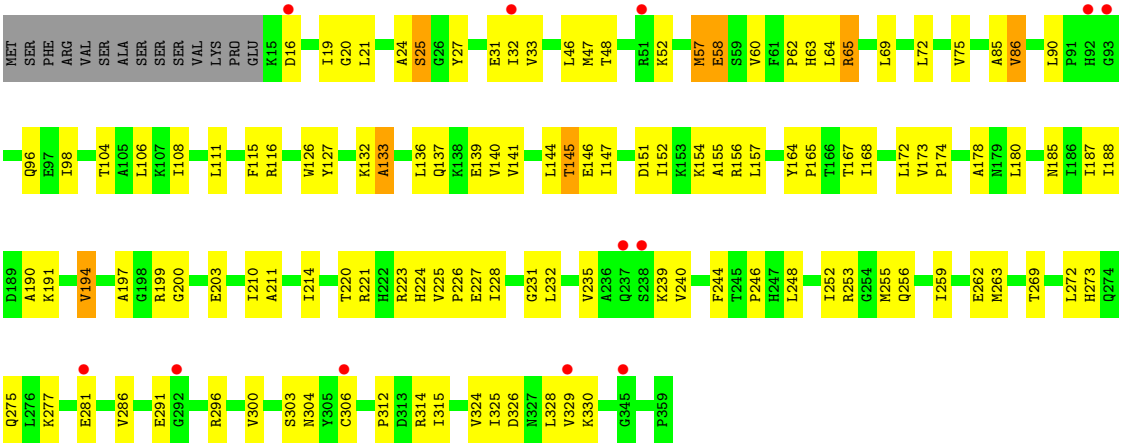
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 2-C:



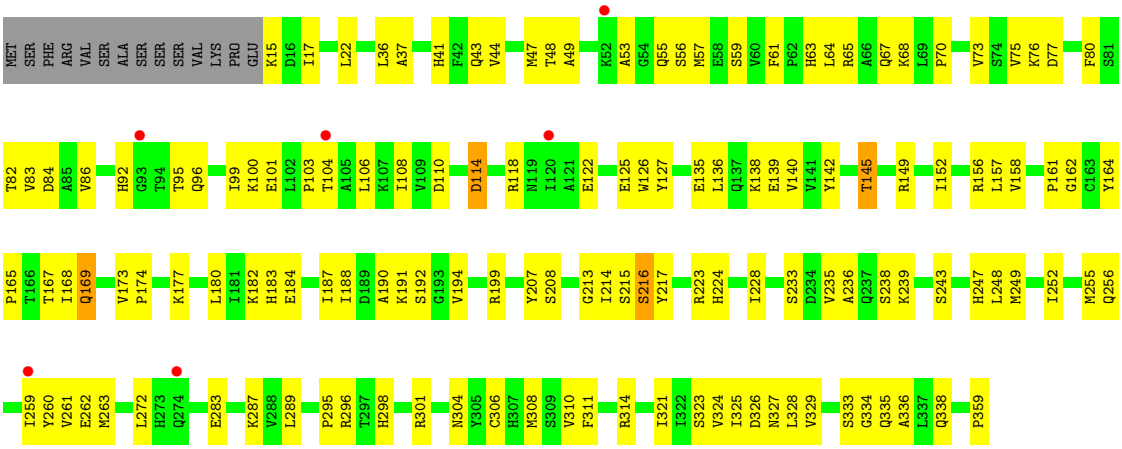
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 2-D:



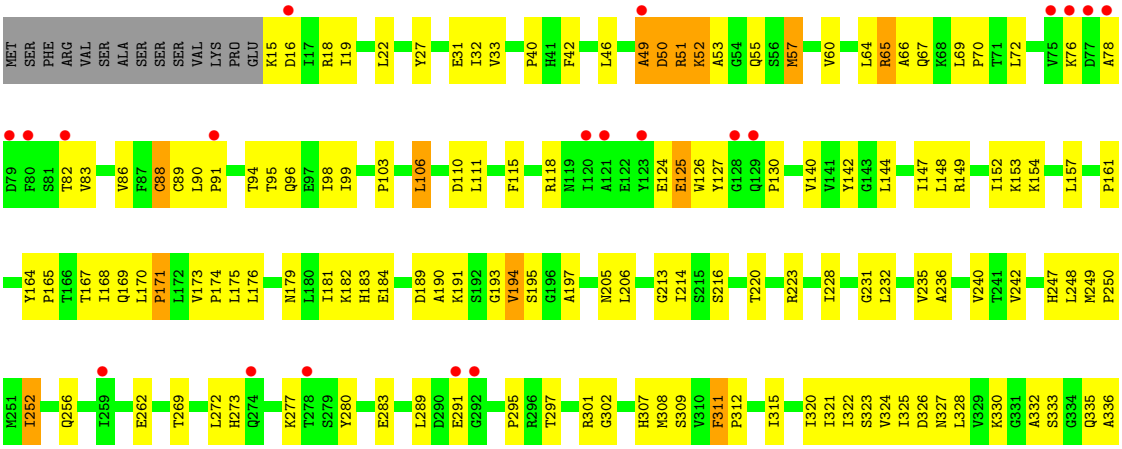
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

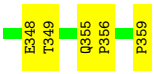
Chain 3-A:



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

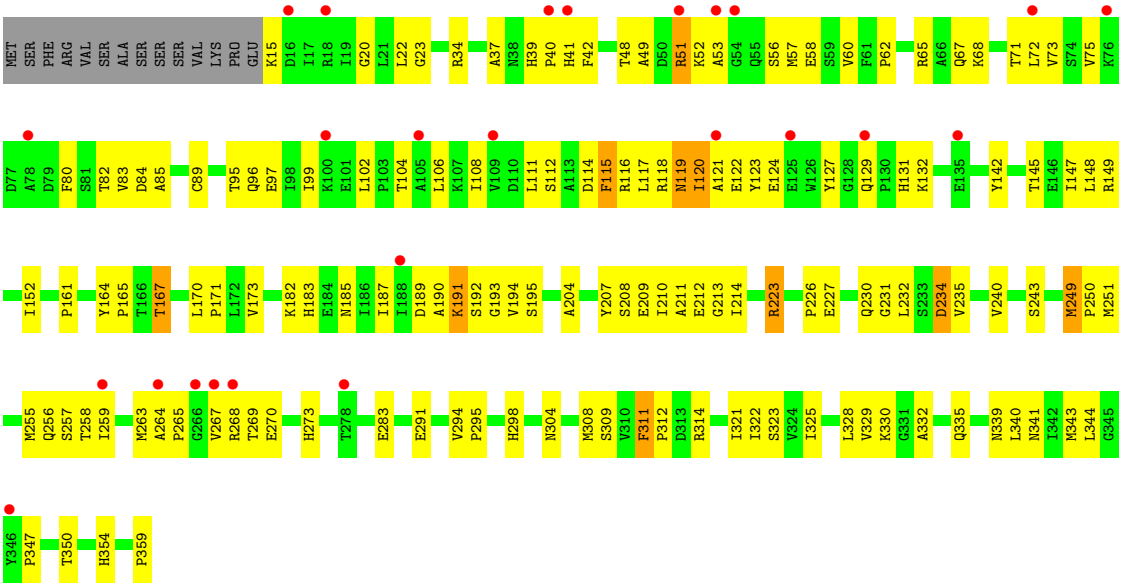
Chain 3-B:





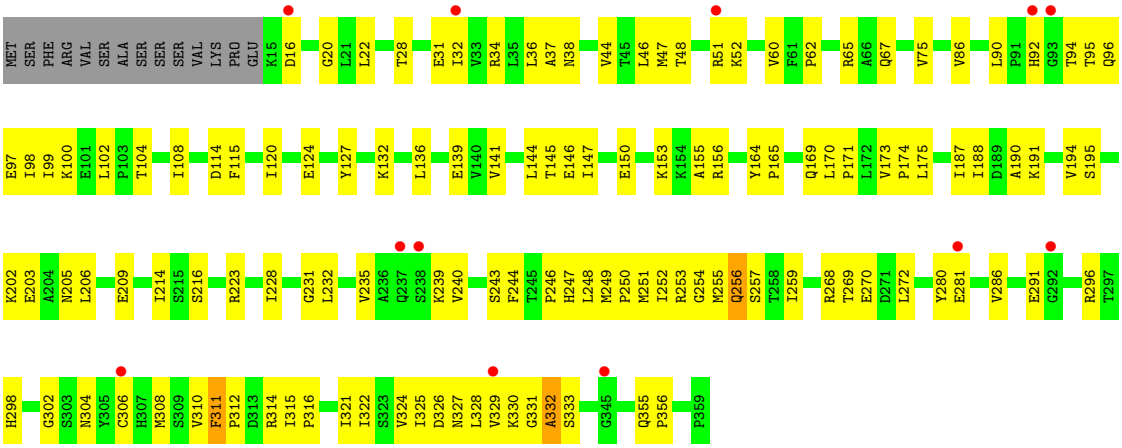
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 3-C:



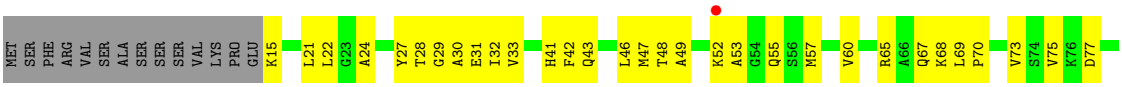
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

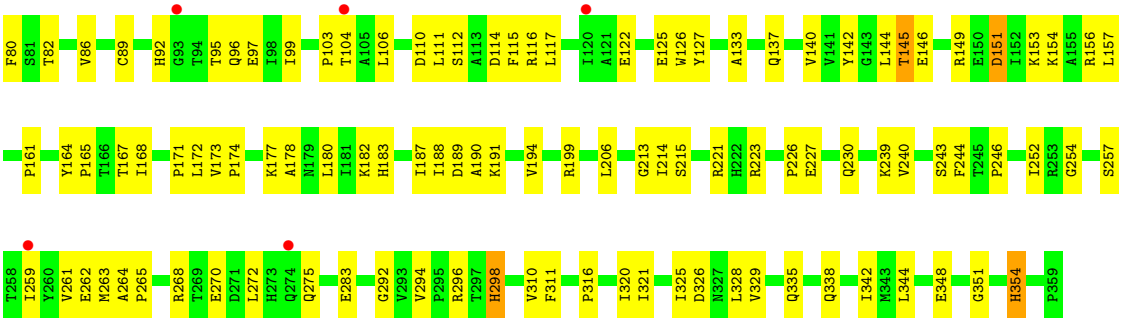
Chain 3-D:



• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

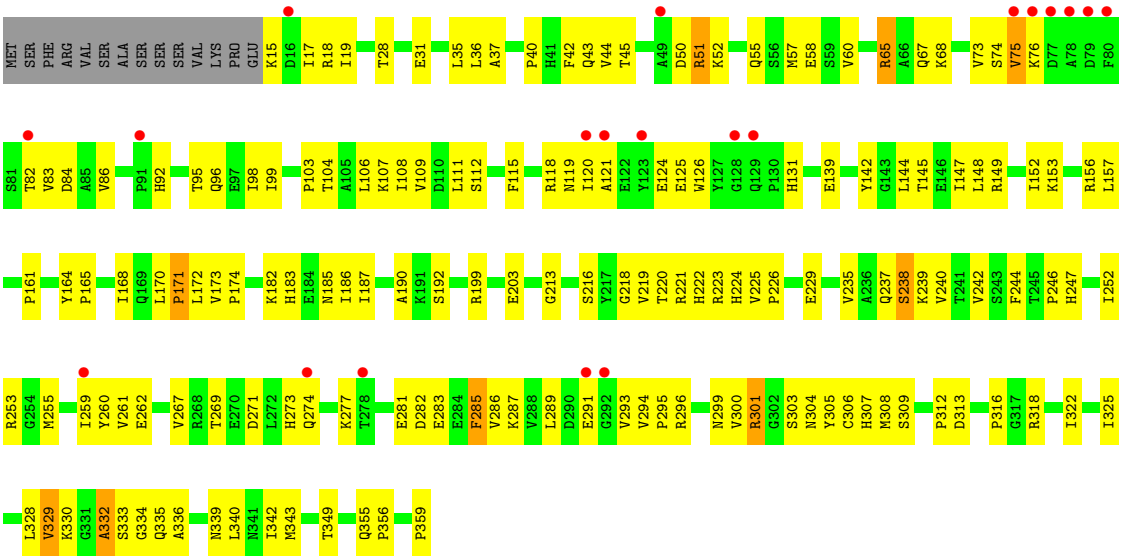
Chain 4-A:





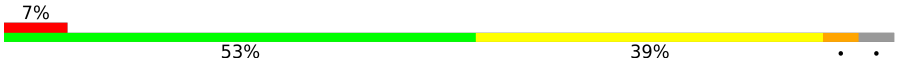
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

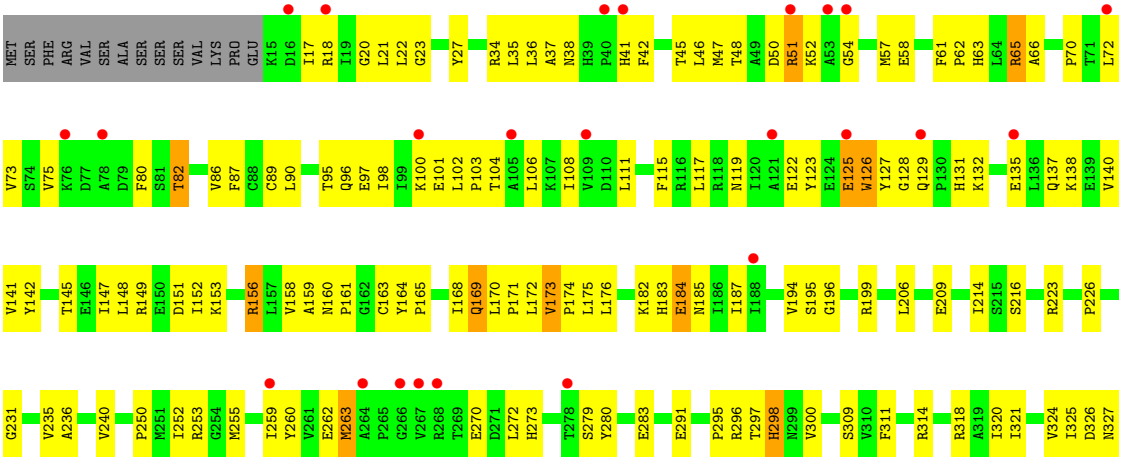
Chain 4-B:

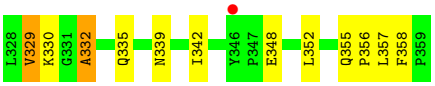


- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 4-C:

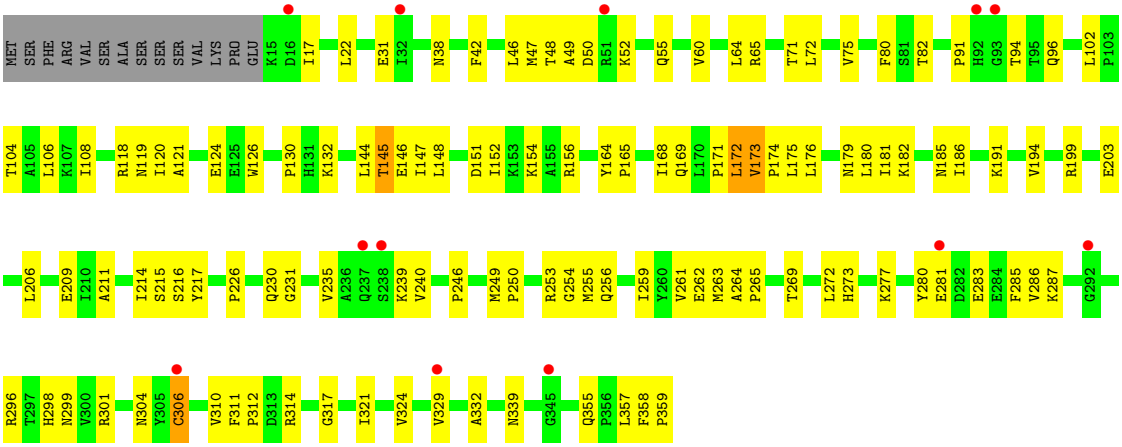






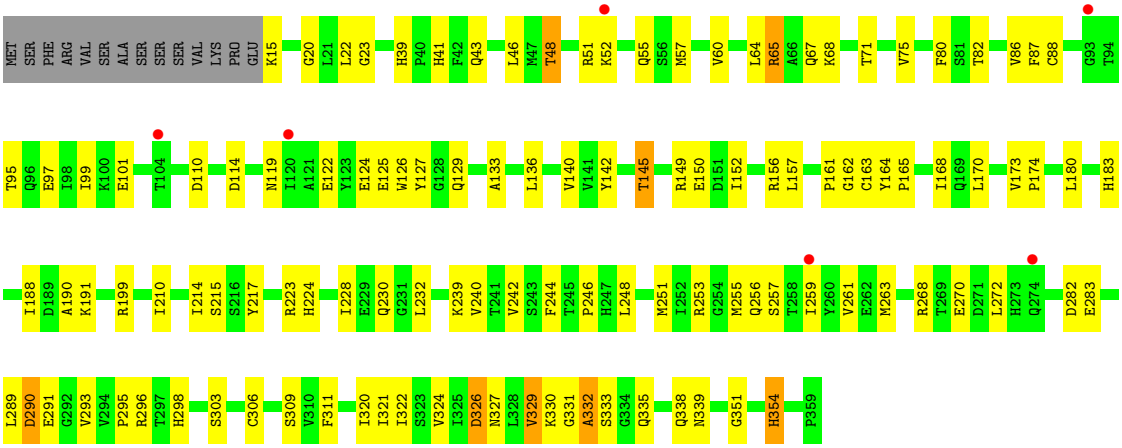
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 4-D:



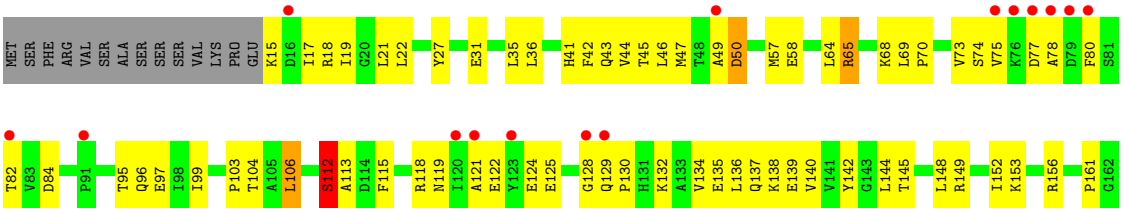
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

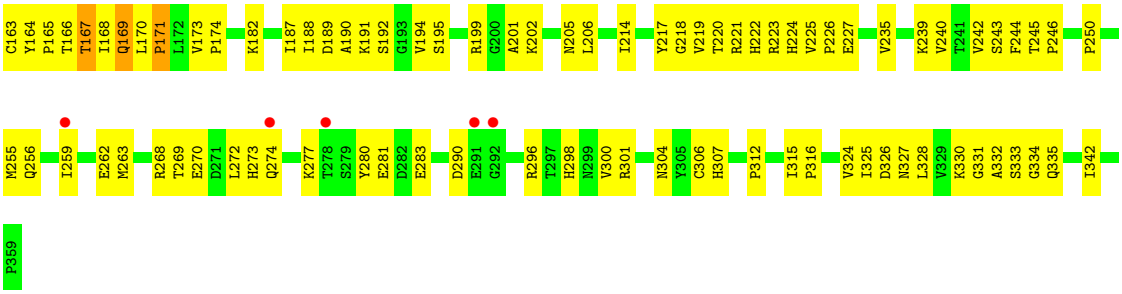
Chain 5-A:



• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

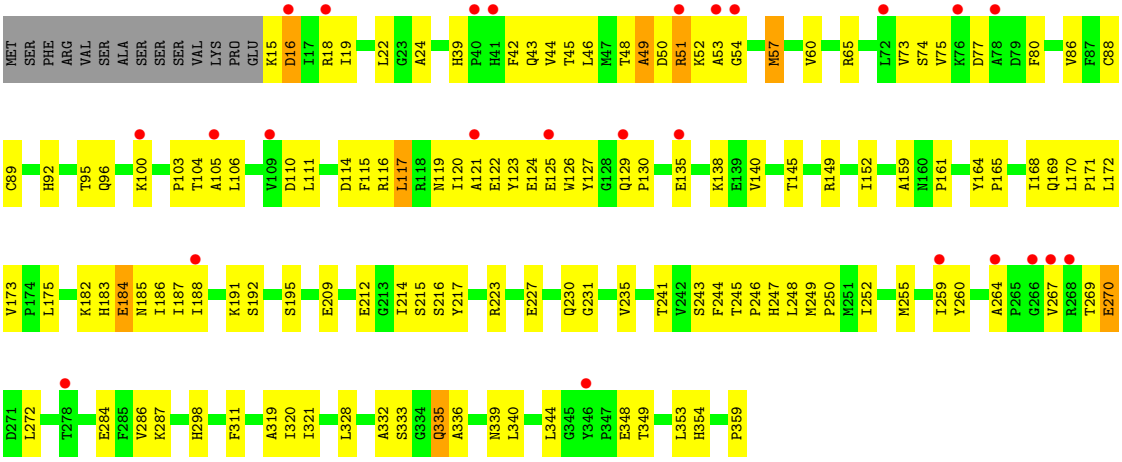
Chain 5-B:





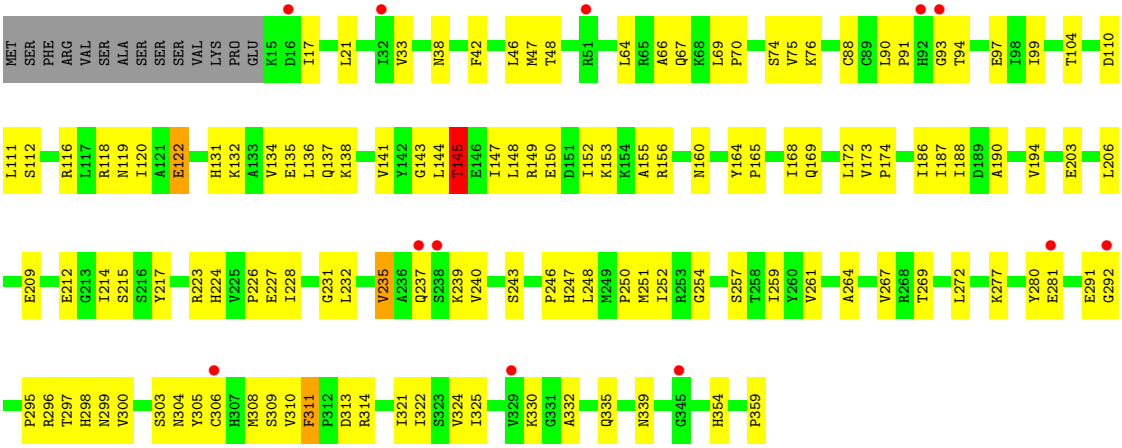
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 5-C:



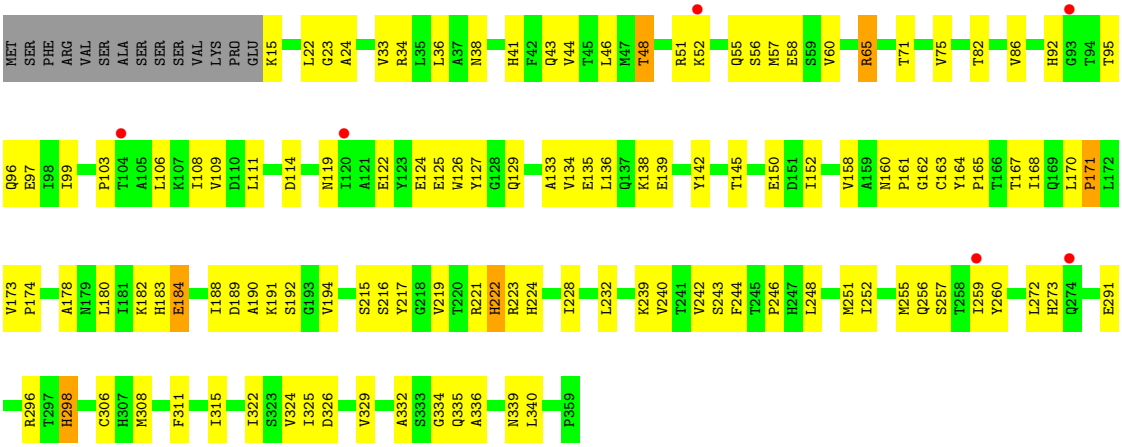
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 5-D:



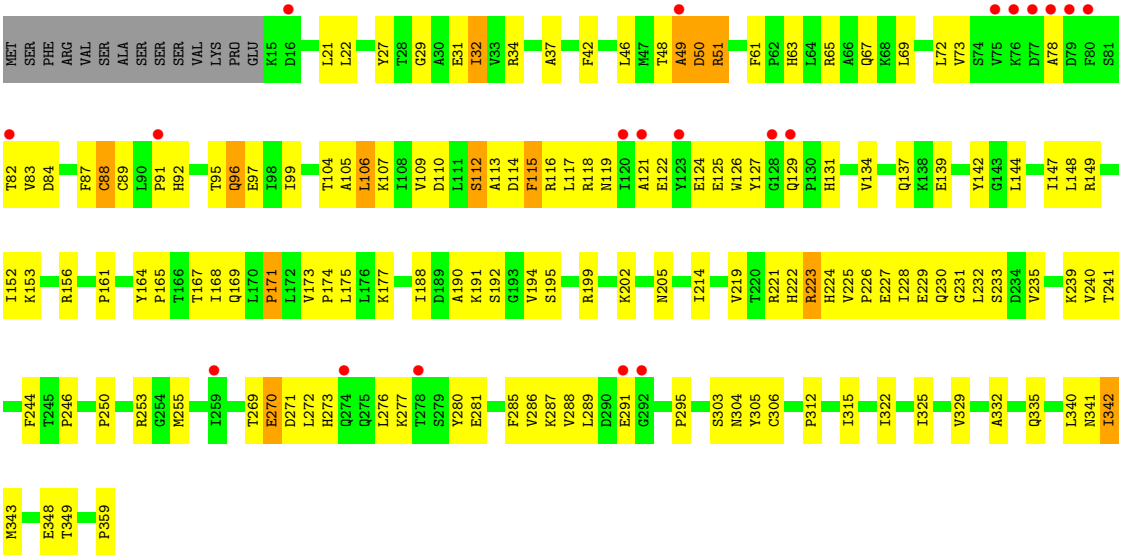
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 6-A:



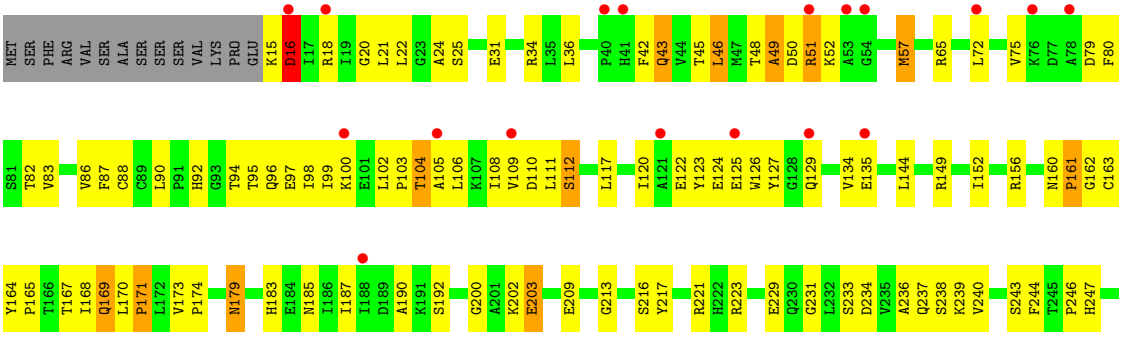
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

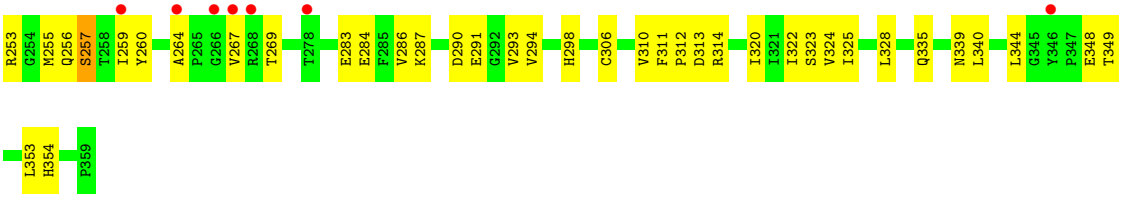
Chain 6-B:



• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

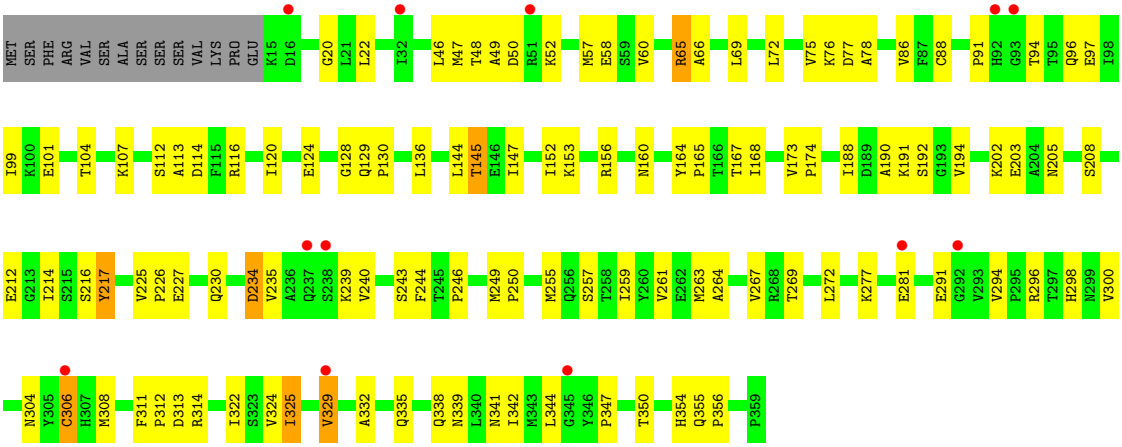
Chain 6-C:





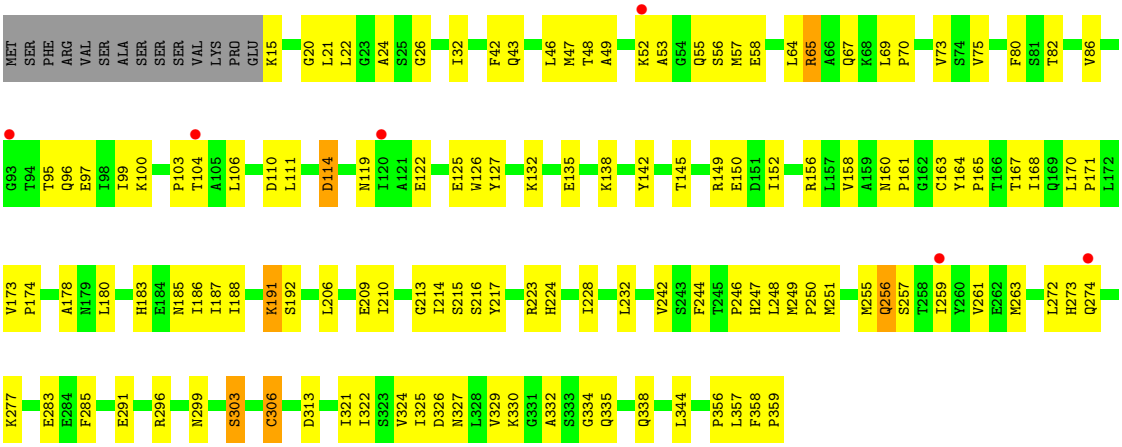
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 6-D:



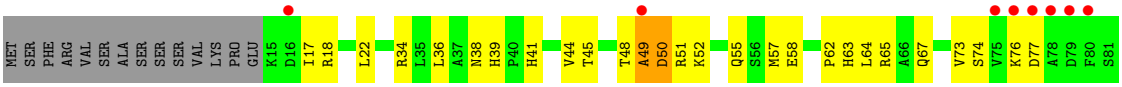
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

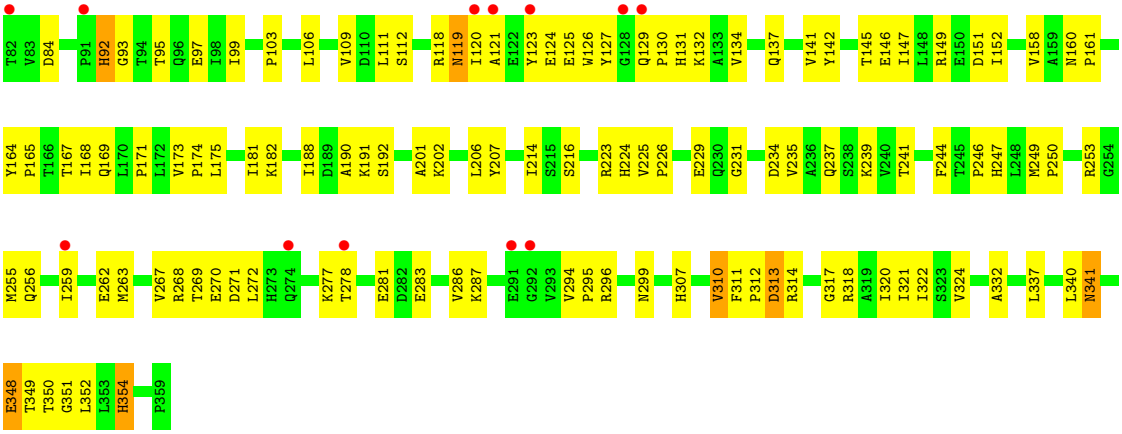
Chain 7-A:



• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

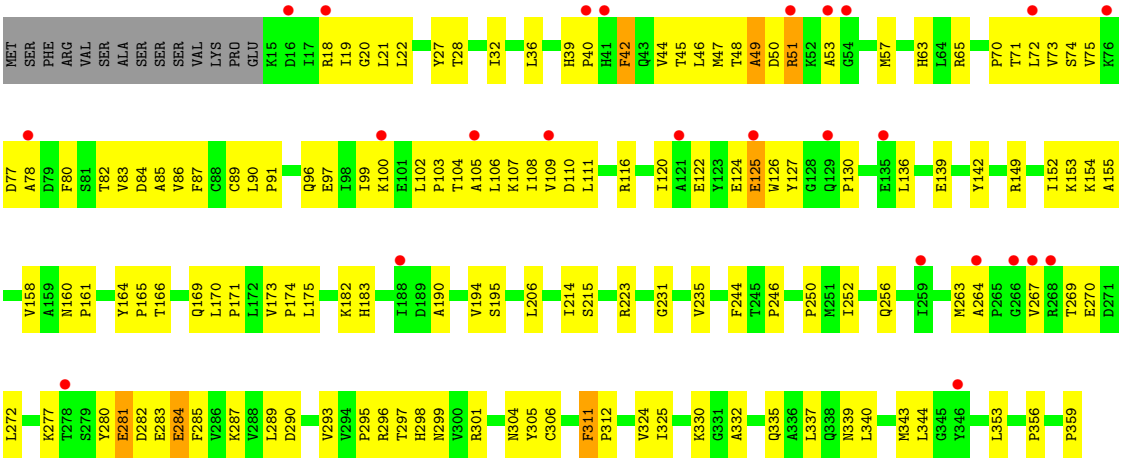
Chain 7-B:





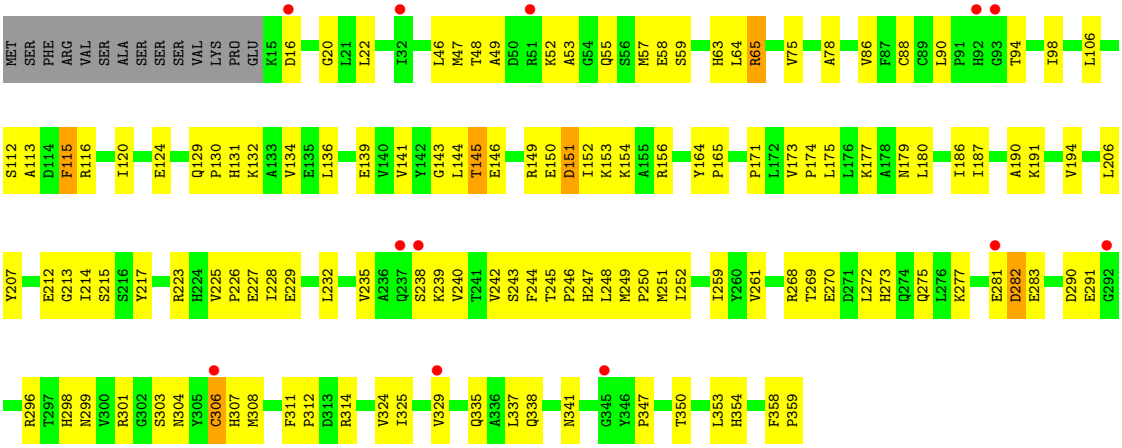
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 7-C:



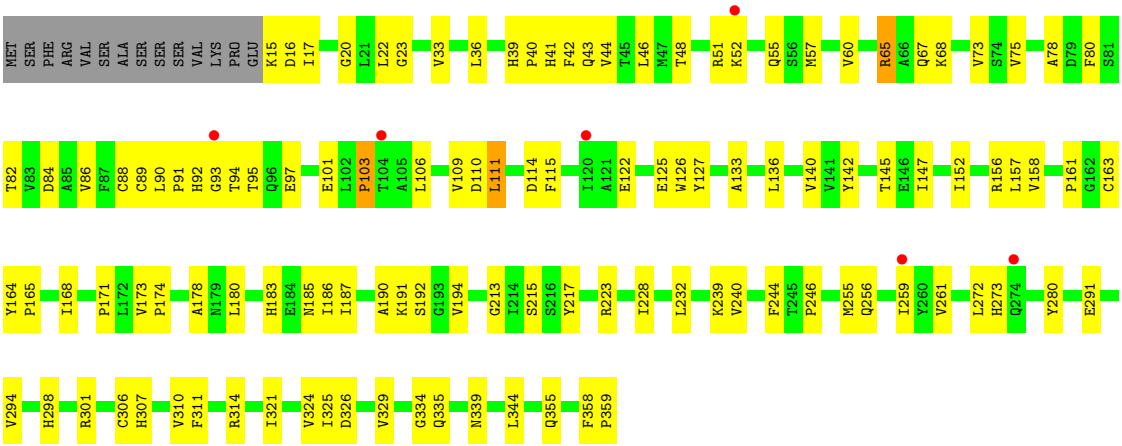
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 7-D:



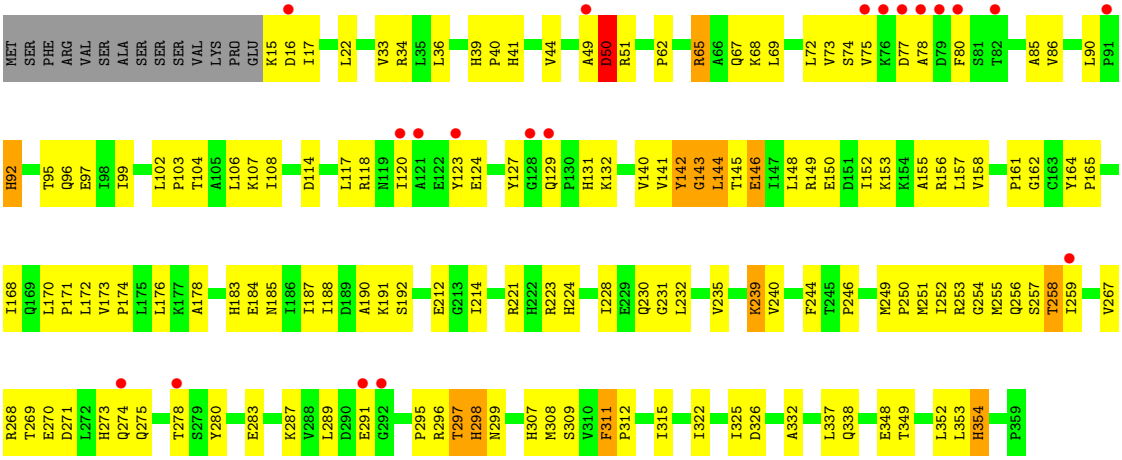
• Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 8-A:



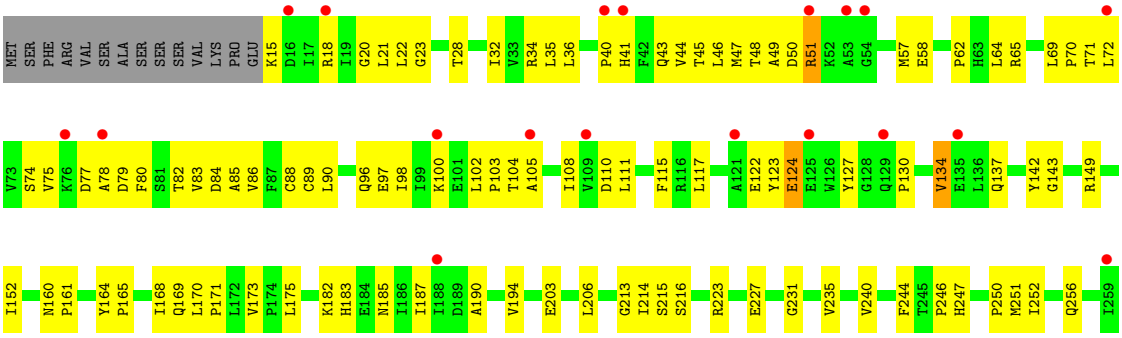
- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

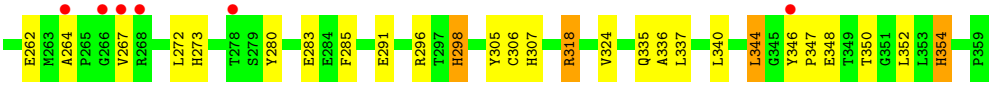
Chain 8-B:



- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

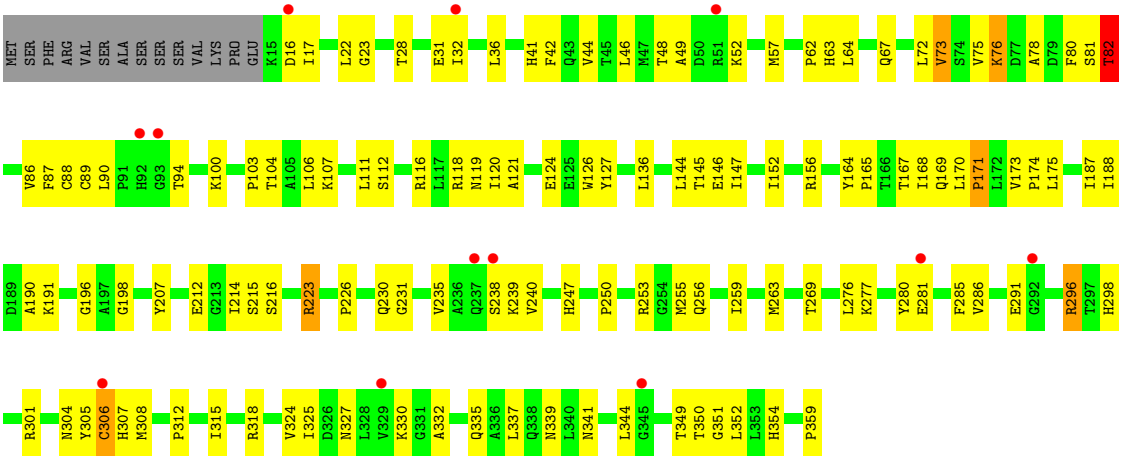
Chain 8-C:





- Molecule 1: Probable N-acetyl-gamma-glutamyl-phosphate reductase

Chain 8-D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.60Å 107.07Å 85.75Å 90.00° 118.88° 90.00°	Depositor
Resolution (Å)	27.31 – 2.19 27.54 – 2.19	Depositor EDS
% Data completeness (in resolution range)	92.9 (27.31-2.19) 92.9 (27.54-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.152 , 0.212 0.154 , 0.210	Depositor DCC
R_{free} test set	3240 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 73.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h-l,k,h 0.002 for l,k,-h-l 0.018 for h,-k,-h-l 0.017 for -h-l,-k,l 0.016 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	93408	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.45	0/2734	0.68	1/3709 (0.0%)
1	1-B	0.45	0/2734	0.66	0/3709
1	1-C	0.44	0/2734	0.66	0/3709
1	1-D	0.45	0/2734	0.67	0/3709
1	2-A	0.46	0/2734	0.68	0/3709
1	2-B	0.45	0/2734	0.66	0/3709
1	2-C	0.44	0/2734	0.66	0/3709
1	2-D	0.47	0/2734	0.67	0/3709
1	3-A	0.45	0/2734	0.67	0/3709
1	3-B	0.46	0/2734	0.67	0/3709
1	3-C	0.44	0/2734	0.66	0/3709
1	3-D	0.47	0/2734	0.68	0/3709
1	4-A	0.45	0/2734	0.68	0/3709
1	4-B	0.46	0/2734	0.67	0/3709
1	4-C	0.43	0/2734	0.66	0/3709
1	4-D	0.47	0/2734	0.68	0/3709
1	5-A	0.47	0/2734	0.71	1/3709 (0.0%)
1	5-B	0.47	0/2734	0.70	0/3709
1	5-C	0.46	0/2734	0.70	0/3709
1	5-D	0.49	0/2734	0.69	0/3709
1	6-A	0.48	0/2734	0.70	1/3709 (0.0%)
1	6-B	0.48	1/2734 (0.0%)	0.71	0/3709
1	6-C	0.46	0/2734	0.70	0/3709
1	6-D	0.50	1/2734 (0.0%)	0.70	0/3709
1	7-A	0.47	0/2734	0.72	2/3709 (0.1%)
1	7-B	0.48	0/2734	0.70	0/3709
1	7-C	0.46	0/2734	0.68	0/3709
1	7-D	0.49	0/2734	0.73	0/3709
1	8-A	0.47	0/2734	0.71	1/3709 (0.0%)
1	8-B	0.47	0/2734	0.69	0/3709
1	8-C	0.46	0/2734	0.69	0/3709
1	8-D	0.53	1/2734 (0.0%)	0.72	0/3709
All	All	0.46	3/87488 (0.0%)	0.69	6/118688 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	8-D	306	CYS	CB-SG	-8.15	1.68	1.82
1	6-B	88	CYS	CB-SG	6.15	1.92	1.82
1	6-D	306	CYS	CB-SG	-5.67	1.72	1.81

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	7-A	326	ASP	N-CA-C	-5.49	96.17	111.00
1	1-A	326	ASP	N-CA-C	-5.36	96.52	111.00
1	8-A	326	ASP	N-CA-C	-5.33	96.61	111.00
1	7-A	285	PHE	N-CA-C	5.11	124.78	111.00
1	6-A	326	ASP	N-CA-C	-5.05	97.36	111.00

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	1-A	2680	0	2718	104	0
1	1-B	2680	0	2718	113	0
1	1-C	2680	0	2718	135	0
1	1-D	2680	0	2718	101	0
1	2-A	2680	0	2718	104	0
1	2-B	2680	0	2718	101	0
1	2-C	2680	0	2718	155	0
1	2-D	2680	0	2718	104	0
1	3-A	2680	0	2718	158	0
1	3-B	2680	0	2718	147	0
1	3-C	2680	0	2718	154	0
1	3-D	2680	0	2718	115	0
1	4-A	2680	0	2718	113	0
1	4-B	2680	0	2718	169	0
1	4-C	2680	0	2718	145	0
1	4-D	2680	0	2718	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5-A	2680	0	2718	109	0
1	5-B	2680	0	2718	144	0
1	5-C	2680	0	2718	119	0
1	5-D	2680	0	2718	124	0
1	6-A	2680	0	2718	100	0
1	6-B	2680	0	2718	134	0
1	6-C	2680	0	2718	127	0
1	6-D	2680	0	2718	100	0
1	7-A	2680	0	2718	128	0
1	7-B	2680	0	2718	126	0
1	7-C	2680	0	2718	137	0
1	7-D	2680	0	2718	131	0
1	8-A	2680	0	2718	100	0
1	8-B	2680	0	2718	141	0
1	8-C	2680	0	2718	108	0
1	8-D	2680	0	2718	113	0
2	1-A	270	0	0	10	0
2	1-B	225	0	0	17	0
2	1-C	220	0	0	11	0
2	1-D	241	0	0	11	0
2	2-A	263	0	0	10	0
2	2-B	227	0	0	15	0
2	2-C	231	0	0	16	0
2	2-D	235	0	0	12	0
2	3-A	268	0	0	11	0
2	3-B	216	0	0	8	0
2	3-C	228	0	0	14	0
2	3-D	244	0	0	13	0
2	4-A	267	0	0	12	0
2	4-B	224	0	0	21	0
2	4-C	223	0	0	13	0
2	4-D	242	0	0	16	0
2	5-A	262	0	0	17	0
2	5-B	223	0	0	14	0
2	5-C	229	0	0	15	0
2	5-D	242	0	0	20	0
2	6-A	267	0	0	16	0
2	6-B	225	0	0	13	0
2	6-C	224	0	0	10	0
2	6-D	240	0	0	13	0
2	7-A	269	0	0	10	0
2	7-B	223	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	7-C	224	0	0	11	0
2	7-D	240	0	0	13	0
2	8-A	267	0	0	11	0
2	8-B	222	0	0	12	0
2	8-C	231	0	0	11	0
2	8-D	236	0	0	11	0
All	All	93408	0	86976	3764	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 22.

The worst 5 of 3764 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:151:ASP:HA	1:A:154:LYS:HE2	1.37	1.06
1:C:67:GLN:HE21	1:C:69:LEU:HD21	1.21	1.04
1:B:15:LYS:HD2	1:B:43:GLN:HB2	1.38	1.03
1:B:306:CYS:HA	1:B:325:ILE:HG22	1.42	1.01
1:D:306:CYS:HB3	1:D:325:ILE:HG22	1.42	1.01

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	343/359 (96%)	318 (93%)	22 (6%)	3 (1%)	17 16
1	1-B	343/359 (96%)	311 (91%)	25 (7%)	7 (2%)	7 4
1	1-C	343/359 (96%)	317 (92%)	24 (7%)	2 (1%)	25 26
1	1-D	343/359 (96%)	316 (92%)	19 (6%)	8 (2%)	6 3
1	2-A	343/359 (96%)	316 (92%)	24 (7%)	3 (1%)	17 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2-B	343/359 (96%)	318 (93%)	16 (5%)	9 (3%)	5	3
1	2-C	343/359 (96%)	305 (89%)	30 (9%)	8 (2%)	6	3
1	2-D	343/359 (96%)	315 (92%)	21 (6%)	7 (2%)	7	4
1	3-A	343/359 (96%)	310 (90%)	29 (8%)	4 (1%)	13	10
1	3-B	343/359 (96%)	308 (90%)	26 (8%)	9 (3%)	5	3
1	3-C	343/359 (96%)	304 (89%)	33 (10%)	6 (2%)	9	6
1	3-D	343/359 (96%)	316 (92%)	25 (7%)	2 (1%)	25	26
1	4-A	343/359 (96%)	317 (92%)	22 (6%)	4 (1%)	13	10
1	4-B	343/359 (96%)	299 (87%)	34 (10%)	10 (3%)	4	2
1	4-C	343/359 (96%)	310 (90%)	24 (7%)	9 (3%)	5	3
1	4-D	343/359 (96%)	312 (91%)	28 (8%)	3 (1%)	17	16
1	5-A	343/359 (96%)	318 (93%)	21 (6%)	4 (1%)	13	10
1	5-B	343/359 (96%)	313 (91%)	22 (6%)	8 (2%)	6	3
1	5-C	343/359 (96%)	311 (91%)	29 (8%)	3 (1%)	17	16
1	5-D	343/359 (96%)	310 (90%)	31 (9%)	2 (1%)	25	26
1	6-A	343/359 (96%)	320 (93%)	18 (5%)	5 (2%)	10	8
1	6-B	343/359 (96%)	301 (88%)	32 (9%)	10 (3%)	4	2
1	6-C	343/359 (96%)	310 (90%)	25 (7%)	8 (2%)	6	3
1	6-D	343/359 (96%)	312 (91%)	29 (8%)	2 (1%)	25	26
1	7-A	343/359 (96%)	316 (92%)	24 (7%)	3 (1%)	17	16
1	7-B	343/359 (96%)	304 (89%)	31 (9%)	8 (2%)	6	3
1	7-C	343/359 (96%)	311 (91%)	28 (8%)	4 (1%)	13	10
1	7-D	343/359 (96%)	309 (90%)	30 (9%)	4 (1%)	13	10
1	8-A	343/359 (96%)	317 (92%)	24 (7%)	2 (1%)	25	26
1	8-B	343/359 (96%)	310 (90%)	25 (7%)	8 (2%)	6	3
1	8-C	343/359 (96%)	308 (90%)	28 (8%)	7 (2%)	7	4
1	8-D	343/359 (96%)	309 (90%)	27 (8%)	7 (2%)	7	4
All	All	10976/11488 (96%)	9971 (91%)	826 (8%)	179 (2%)	9	7

5 of 179 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-C	332	ALA

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Mol	Chain	Res	Type
1	1-D	105	ALA
1	1-D	212	GLU
1	2-A	161	PRO
1	2-C	145	THR

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	295/308 (96%)	291 (99%)	4 (1%)	67	80
1	1-B	295/308 (96%)	292 (99%)	3 (1%)	76	86
1	1-C	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	1-D	295/308 (96%)	288 (98%)	7 (2%)	49	62
1	2-A	295/308 (96%)	292 (99%)	3 (1%)	76	86
1	2-B	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	2-C	295/308 (96%)	287 (97%)	8 (3%)	44	57
1	2-D	295/308 (96%)	289 (98%)	6 (2%)	55	69
1	3-A	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	3-B	295/308 (96%)	288 (98%)	7 (2%)	49	62
1	3-C	295/308 (96%)	286 (97%)	9 (3%)	40	51
1	3-D	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	4-A	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	4-B	295/308 (96%)	291 (99%)	4 (1%)	67	80
1	4-C	295/308 (96%)	287 (97%)	8 (3%)	44	57
1	4-D	295/308 (96%)	291 (99%)	4 (1%)	67	80
1	5-A	295/308 (96%)	287 (97%)	8 (3%)	44	57
1	5-B	295/308 (96%)	289 (98%)	6 (2%)	55	69
1	5-C	295/308 (96%)	286 (97%)	9 (3%)	40	51
1	5-D	295/308 (96%)	290 (98%)	5 (2%)	60	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	6-A	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	6-B	295/308 (96%)	290 (98%)	5 (2%)	60	74
1	6-C	295/308 (96%)	282 (96%)	13 (4%)	28	35
1	6-D	295/308 (96%)	286 (97%)	9 (3%)	40	51
1	7-A	295/308 (96%)	289 (98%)	6 (2%)	55	69
1	7-B	295/308 (96%)	287 (97%)	8 (3%)	44	57
1	7-C	295/308 (96%)	289 (98%)	6 (2%)	55	69
1	7-D	295/308 (96%)	287 (97%)	8 (3%)	44	57
1	8-A	295/308 (96%)	292 (99%)	3 (1%)	76	86
1	8-B	295/308 (96%)	286 (97%)	9 (3%)	40	51
1	8-C	295/308 (96%)	291 (99%)	4 (1%)	67	80
1	8-D	295/308 (96%)	286 (97%)	9 (3%)	40	51
All	All	9440/9856 (96%)	9239 (98%)	201 (2%)	53	67

5 of 201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5-D	311	PHE
1	6-D	145	THR
1	8-D	223	ARG
1	6-A	184	GLU
1	6-C	79	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
1	7-A	237	GLN
1	8-C	43	GLN
1	7-B	67	GLN
1	7-D	275	GLN
1	8-D	169	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)

There are no ligands in this entry.

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	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	1-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	1-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	1-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
1	2-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	2-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	2-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	2-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
1	3-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	3-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	3-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	3-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
1	4-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	4-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	4-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	4-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
1	5-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	5-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	5-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	5-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
1	6-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	6-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	6-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	6-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	7-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	7-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	7-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	7-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
1	8-A	345/359 (96%)	-0.06	6 (1%)	70	68	17, 30, 56, 67	345 (100%)
1	8-B	345/359 (96%)	0.18	20 (5%)	23	22	14, 31, 60, 98	345 (100%)
1	8-C	345/359 (96%)	0.27	25 (7%)	15	14	16, 31, 65, 88	345 (100%)
1	8-D	345/359 (96%)	0.02	12 (3%)	44	42	16, 30, 57, 94	345 (100%)
All	All	11040/11488 (96%)	0.10	504 (4%)	36	31	14, 30, 60, 98	11040 (100%)

The worst 5 of 504 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	93	GLY	6.6
1	2-A	93	GLY	6.6
1	3-A	93	GLY	6.6
1	4-A	93	GLY	6.6
1	5-A	93	GLY	6.6

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.