wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:00 PM GMT

PDB ID	:	1HTO
Title	:	CRYSTALLOGRAPHIC STRUCTURE OF A RELAXED GLUTAMINE SYNTHETASE FROM MYCOBACTERIUM TUBERCULOSIS
Authors	:	Gill, H.S.; Eisenberg, D.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2001-01-01
Resolution	:	2.40 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

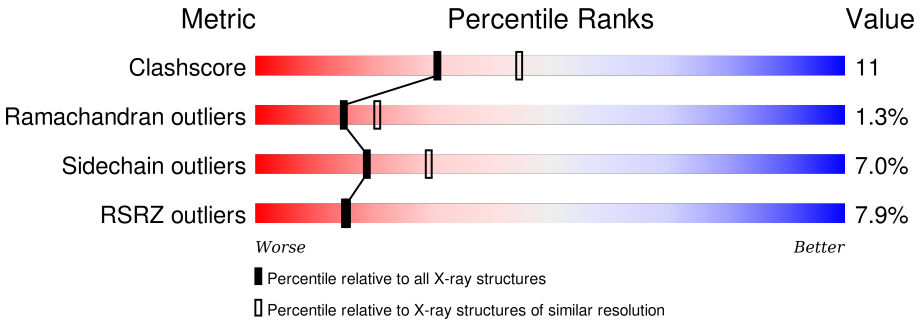
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.40 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))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	A	477	7% 76% 21%
1	B	477	9% 78% 20%
1	C	477	9% 78% 19%
1	D	477	7% 76% 21%
1	E	477	9% 77% 21%
1	F	477	8% 77% 21%
1	G	477	9% 76% 21%

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Mol	Chain	Length	Quality of chain
1	H	477	8% 77% 20%
1	I	477	11% 78% 19%
1	J	477	6% 78% 20%
1	K	477	9% 78% 19%
1	L	477	8% 77% 21%
1	M	477	7% 78% 20%
1	N	477	7% 77% 20%
1	O	477	7% 78% 20%
1	P	477	8% 76% 21%
1	Q	477	8% 76% 21%
1	R	477	7% 77% 21%
1	S	477	8% 77% 20%
1	T	477	8% 77% 20%
1	U	477	8% 78% 19%
1	V	477	7% 78% 19%
1	W	477	6% 78% 20%
1	X	477	9% 77% 21%

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	MN	A	470	-	-	-	X
2	MN	C	470	-	-	-	X
2	MN	E	470	-	-	-	X
2	MN	H	470	-	-	-	X
2	MN	I	470	-	-	-	X
2	MN	L	470	-	-	-	X
2	MN	M	470	-	-	-	X
2	MN	O	470	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MN	Q	470	-	-	-	X
2	MN	R	470	-	-	-	X
2	MN	T	470	-	-	-	X
2	MN	X	470	-	-	-	X
3	AMP	A	7475	-	-	X	X
3	AMP	B	7477	-	-	X	X
3	AMP	C	7479	-	-	X	X
3	AMP	D	7481	-	-	X	X
3	AMP	E	7483	-	-	X	X
3	AMP	F	7485	-	-	X	X
3	AMP	G	7487	-	-	X	X
3	AMP	H	7489	-	-	X	X
3	AMP	I	7491	-	-	X	X
3	AMP	J	7493	-	-	X	X
3	AMP	K	7495	-	-	X	X
3	AMP	L	7497	-	-	X	X
3	AMP	M	7499	-	-	X	X
3	AMP	N	7501	-	-	X	X
3	AMP	O	7503	-	-	X	X
3	AMP	P	7505	-	-	X	X
3	AMP	Q	7507	-	-	X	X
3	AMP	R	7509	-	-	X	X
3	AMP	S	7511	-	-	X	X
3	AMP	T	7513	-	-	X	X
3	AMP	U	7515	-	-	X	X
3	AMP	V	7517	-	-	X	X
3	AMP	W	7519	-	-	X	X
3	AMP	X	7521	-	-	X	X
4	CIT	A	7476	-	-	X	-
4	CIT	B	7478	-	-	X	-
4	CIT	D	7482	-	-	X	-
4	CIT	E	7484	-	-	-	X
4	CIT	F	7486	-	-	X	X
4	CIT	G	7488	-	-	X	X
4	CIT	H	7490	-	-	X	-
4	CIT	I	7492	-	-	X	-
4	CIT	K	7496	-	-	X	X
4	CIT	L	7498	-	-	X	X
4	CIT	M	7500	-	-	X	-
4	CIT	N	7502	-	-	X	-
4	CIT	P	7506	-	-	X	-
4	CIT	Q	7508	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	R	7510	-	-	X	X
4	CIT	S	7512	-	-	X	-
4	CIT	T	7514	-	-	X	X
4	CIT	U	7516	-	-	X	-
4	CIT	W	7520	-	-	X	-
4	CIT	X	7522	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 97872 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 GLUTAMINE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	B	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	C	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	G	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	H	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	I	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	J	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	K	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	L	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	M	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	N	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total	Mn	0	0
			1	1		
2	K	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	W	1	Total	Mn	0	0
			1	1		
2	N	1	Total	Mn	0	0
			1	1		
2	X	1	Total	Mn	0	0
			1	1		
2	S	1	Total	Mn	0	0
			1	1		
2	J	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	V	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

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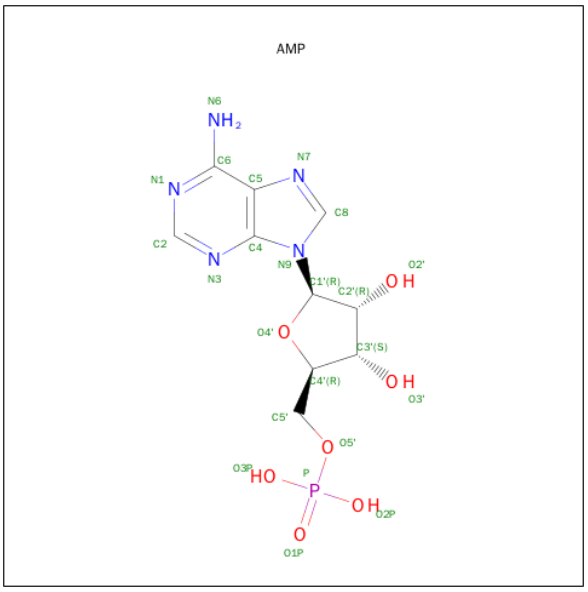
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	R	1	Total Mn 1 1	0	0
2	M	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	I	1	Total Mn 1 1	0	0
2	U	1	Total Mn 1 1	0	0
2	L	1	Total Mn 1 1	0	0
2	G	1	Total Mn 1 1	0	0
2	Q	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	T	1	Total Mn 1 1	0	0
2	O	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	I	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	J	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	K	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	L	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	N	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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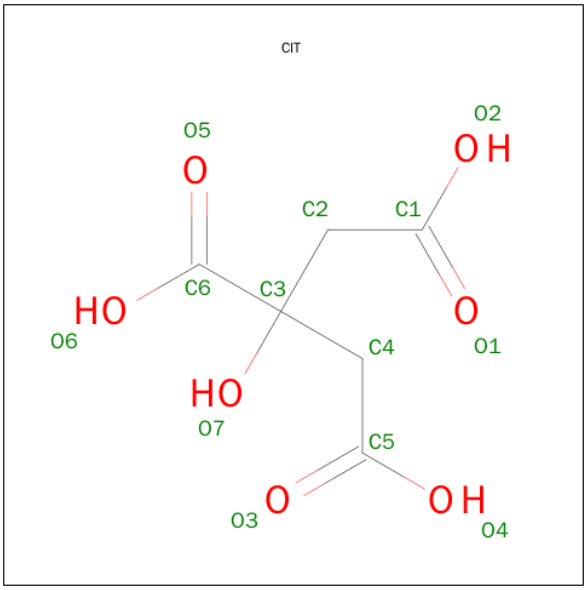
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	P	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	T	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	U	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	V	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	W	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	X	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			13	6	7			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 13 6 7	0	0
4	C	1	Total C O 13 6 7	0	0
4	D	1	Total C O 13 6 7	0	0
4	E	1	Total C O 13 6 7	0	0
4	F	1	Total C O 13 6 7	0	0
4	G	1	Total C O 13 6 7	0	0
4	H	1	Total C O 13 6 7	0	0
4	I	1	Total C O 13 6 7	0	0
4	J	1	Total C O 13 6 7	0	0
4	K	1	Total C O 13 6 7	0	0
4	L	1	Total C O 13 6 7	0	0
4	M	1	Total C O 13 6 7	0	0
4	N	1	Total C O 13 6 7	0	0
4	O	1	Total C O 13 6 7	0	0
4	P	1	Total C O 13 6 7	0	0
4	Q	1	Total C O 13 6 7	0	0
4	R	1	Total C O 13 6 7	0	0
4	S	1	Total C O 13 6 7	0	0
4	T	1	Total C O 13 6 7	0	0
4	U	1	Total C O 13 6 7	0	0
4	V	1	Total C O 13 6 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	W	1	Total C O 13 6 7	0	0
4	X	1	Total C O 13 6 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	261	Total O 261 261	0	0
5	B	262	Total O 262 262	0	0
5	C	264	Total O 264 264	0	0
5	D	262	Total O 262 262	0	0
5	E	261	Total O 261 261	0	0
5	F	267	Total O 267 267	0	0
5	G	262	Total O 262 262	0	0
5	H	263	Total O 263 263	0	0
5	I	263	Total O 263 263	0	0
5	J	262	Total O 262 262	0	0
5	K	267	Total O 267 267	0	0
5	L	262	Total O 262 262	0	0
5	M	263	Total O 263 263	0	0
5	N	262	Total O 262 262	0	0
5	O	265	Total O 265 265	0	0
5	P	265	Total O 265 265	0	0
5	Q	259	Total O 259 259	0	0

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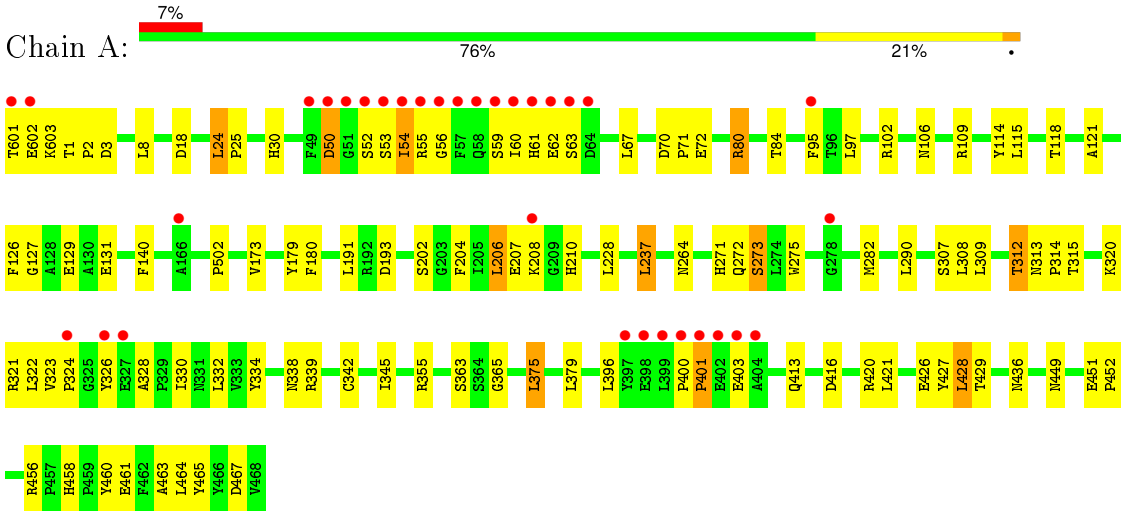
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	R	269	Total O 269 269	0	0
5	S	262	Total O 262 262	0	0
5	T	258	Total O 258 258	0	0
5	U	265	Total O 265 265	0	0
5	V	263	Total O 263 263	0	0
5	W	263	Total O 263 263	0	0
5	X	262	Total O 262 262	0	0

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 errors 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.

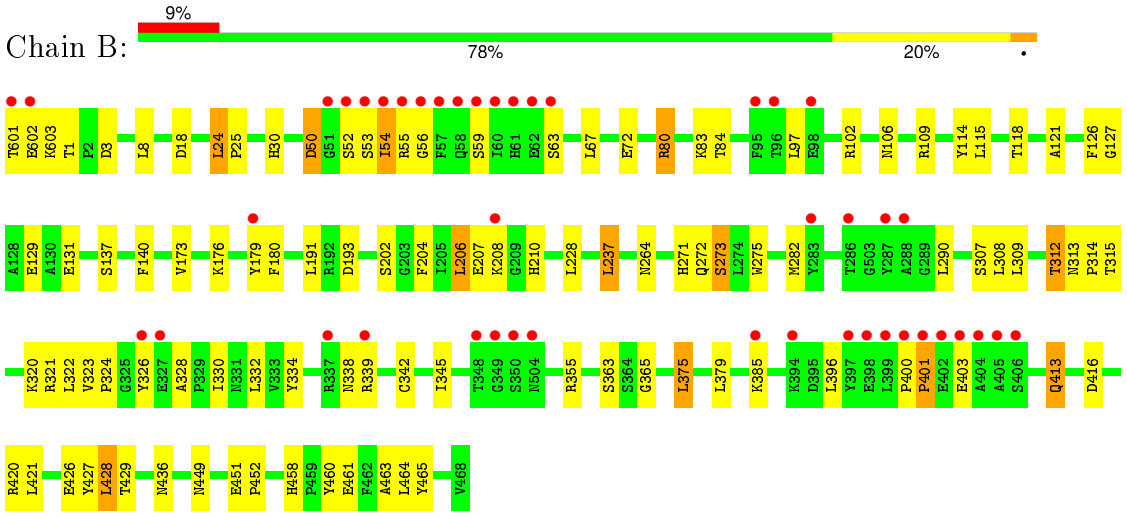
- Molecule 1: GLUTAMINE SYNTHETASE

Chain A:



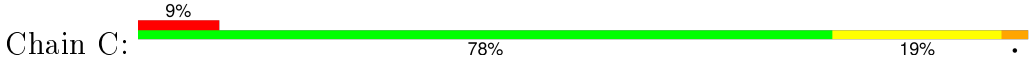
- Molecule 1: GLUTAMINE SYNTHETASE

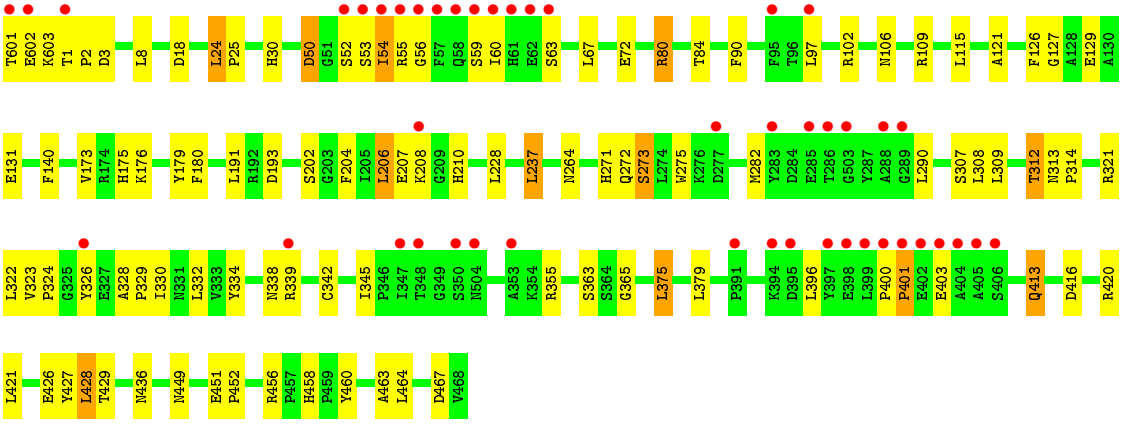
Chain B:



- Molecule 1: GLUTAMINE SYNTHETASE

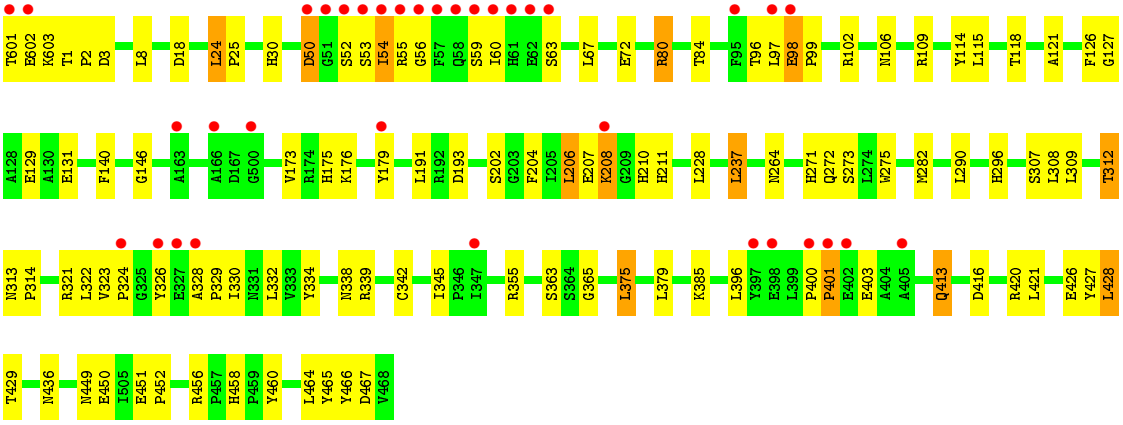
Chain C:





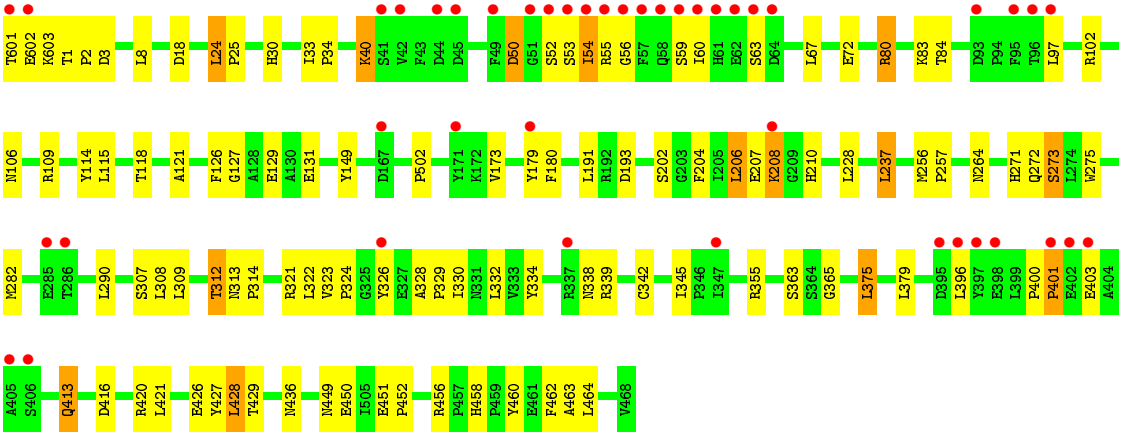
• Molecule 1: GLUTAMINE SYNTHETASE

Chain D:



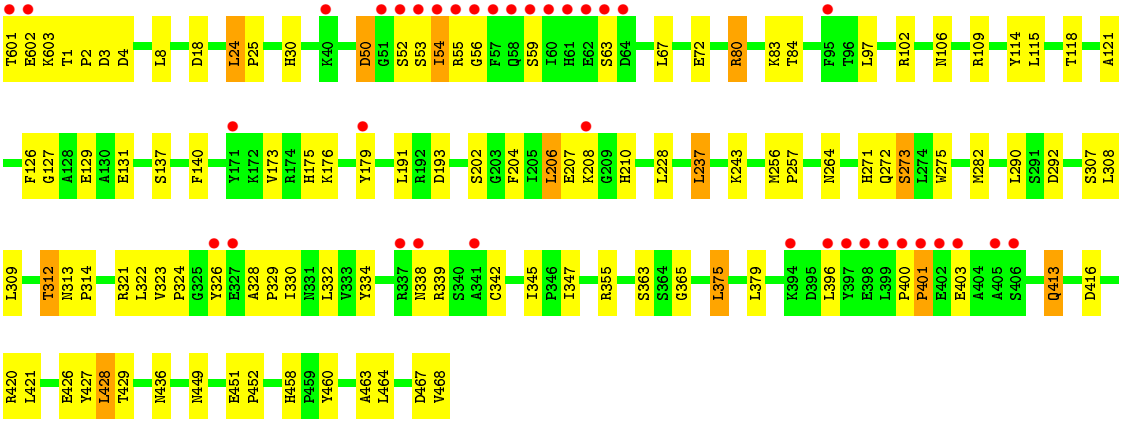
• Molecule 1: GLUTAMINE SYNTHETASE

Chain E:



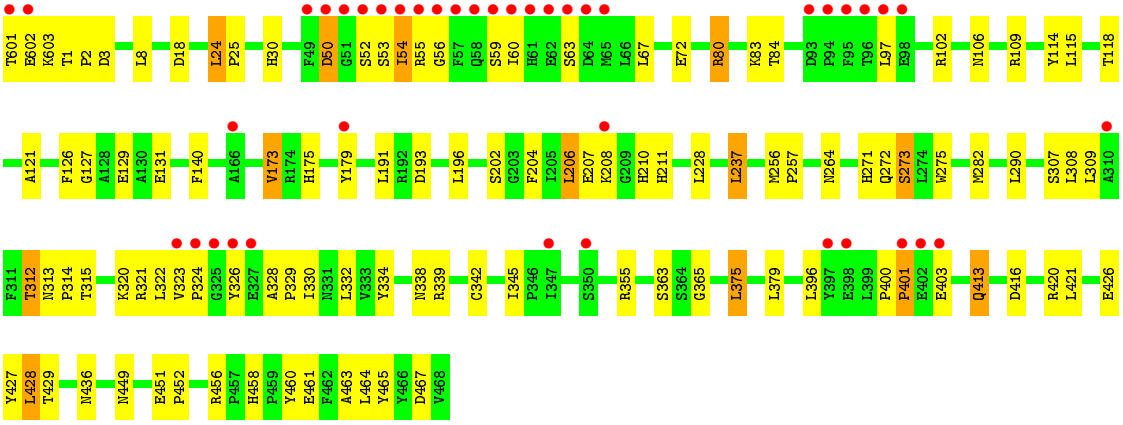
• Molecule 1: GLUTAMINE SYNTHETASE

Chain F:



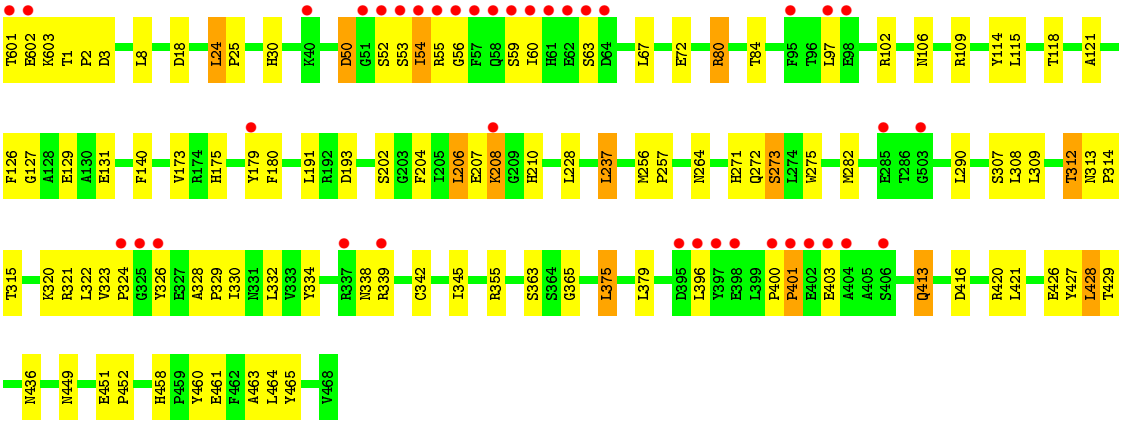
• Molecule 1: GLUTAMINE SYNTHETASE

Chain G:



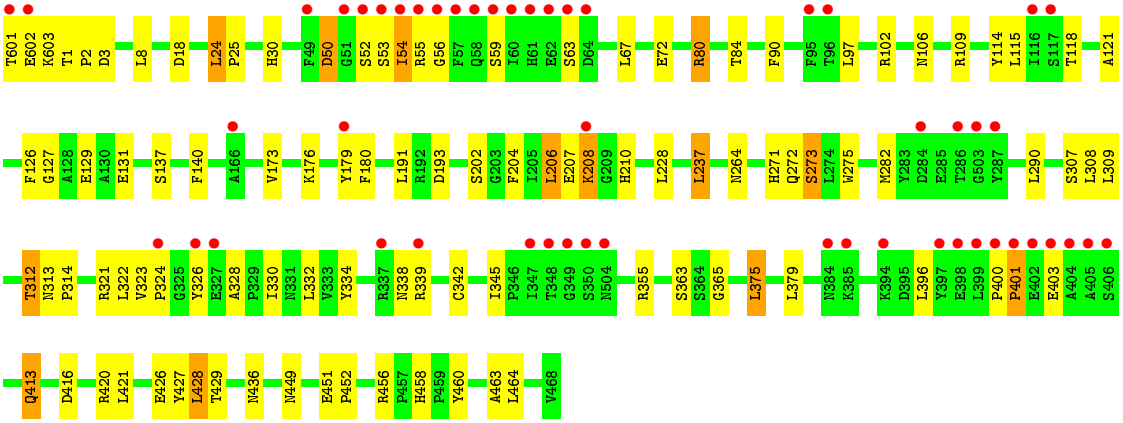
• Molecule 1: GLUTAMINE SYNTHETASE

Chain H:



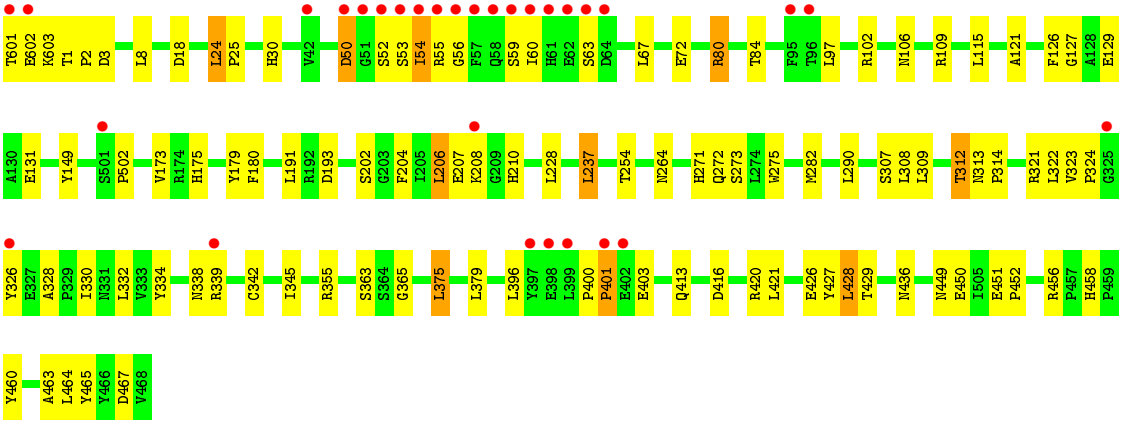
• Molecule 1: GLUTAMINE SYNTHETASE

Chain I:



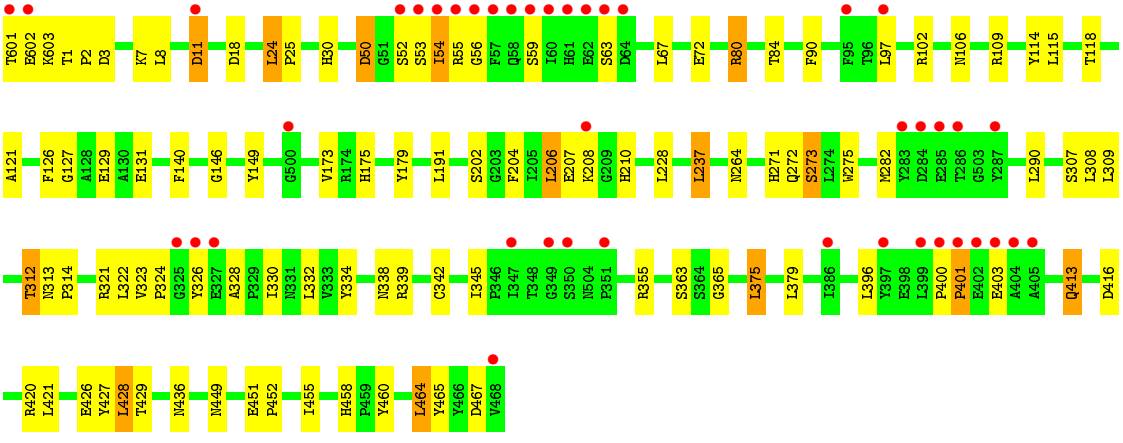
• Molecule 1: GLUTAMINE SYNTHETASE

Chain J:



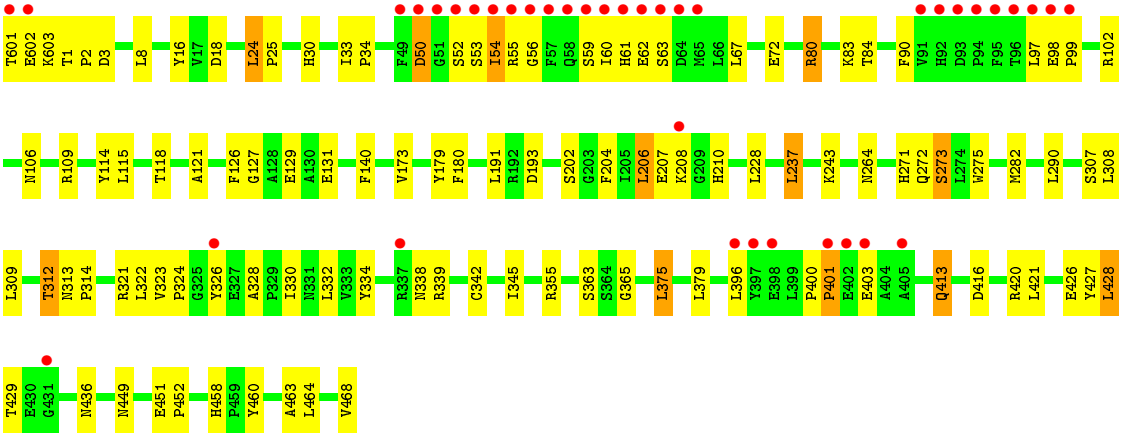
• Molecule 1: GLUTAMINE SYNTHETASE

Chain K:



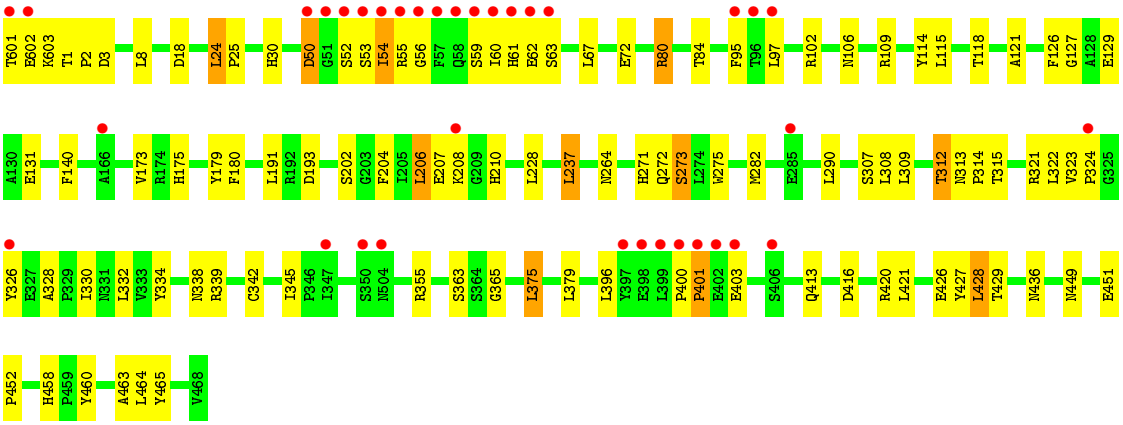
• Molecule 1: GLUTAMINE SYNTHETASE

Chain L:



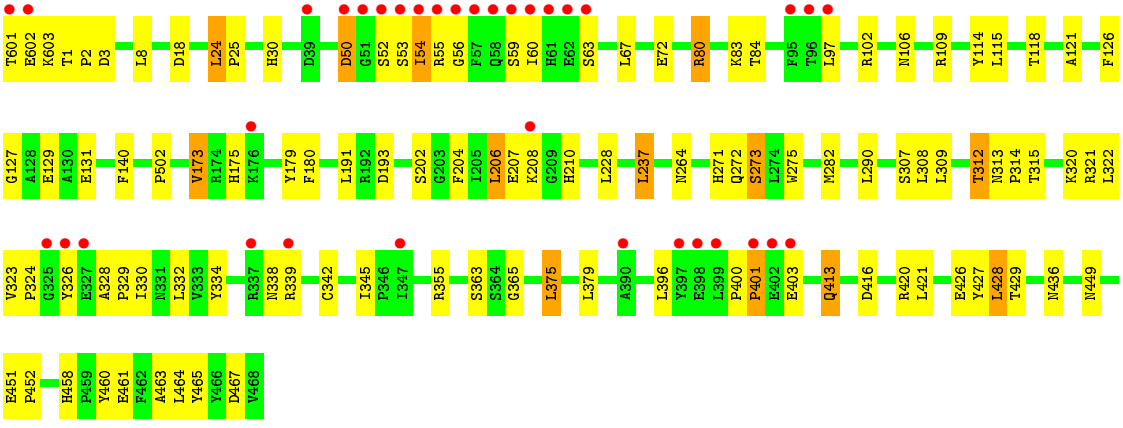
• Molecule 1: GLUTAMINE SYNTHETASE

Chain M:



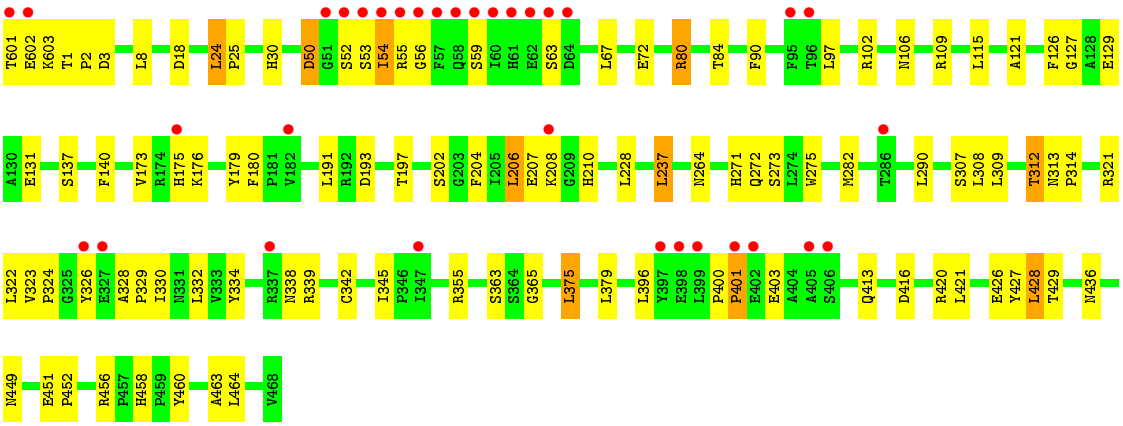
• Molecule 1: GLUTAMINE SYNTHETASE

Chain N:



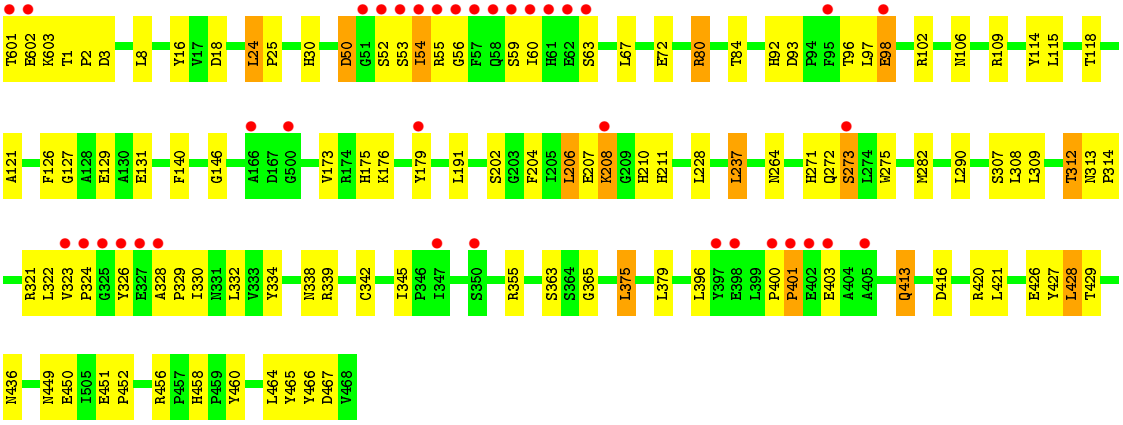
• Molecule 1: GLUTAMINE SYNTHETASE

Chain O:



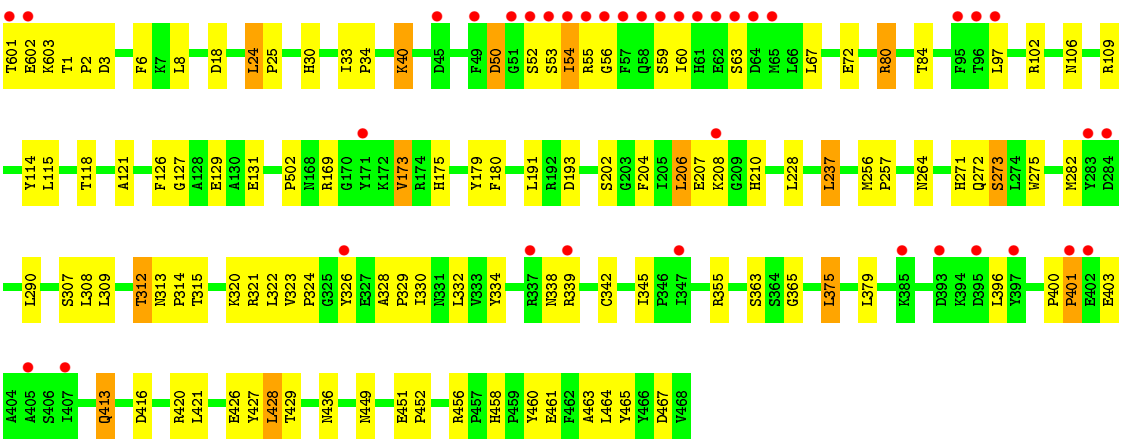
• Molecule 1: GLUTAMINE SYNTHETASE

Chain P:



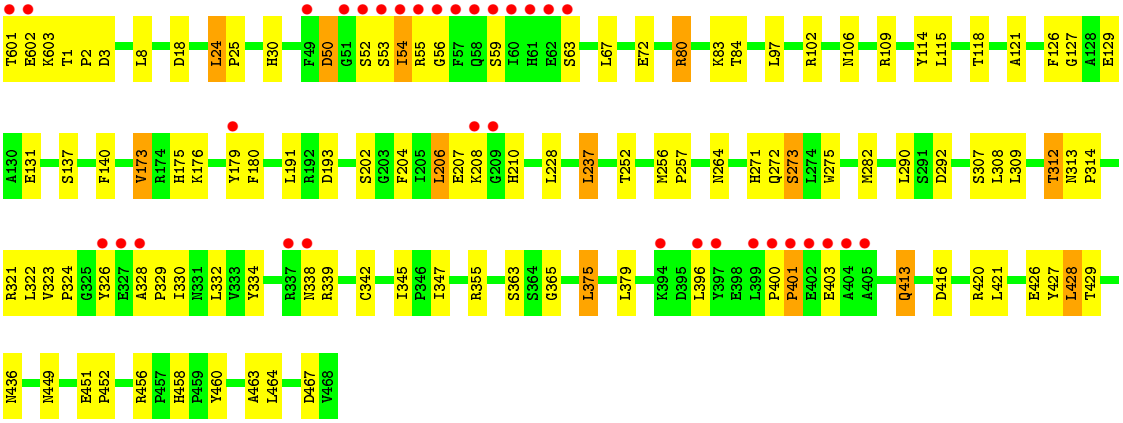
• Molecule 1: GLUTAMINE SYNTHETASE

Chain Q:



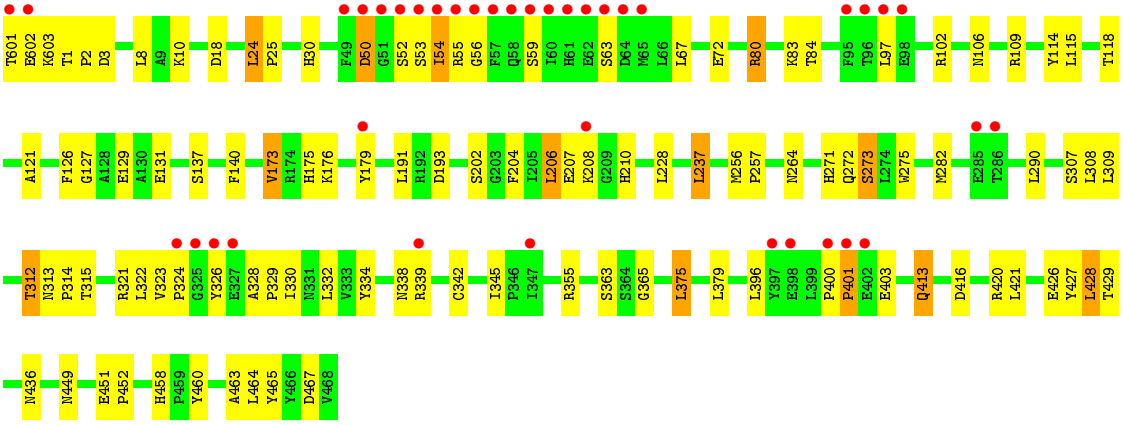
• Molecule 1: GLUTAMINE SYNTHETASE

Chain R:



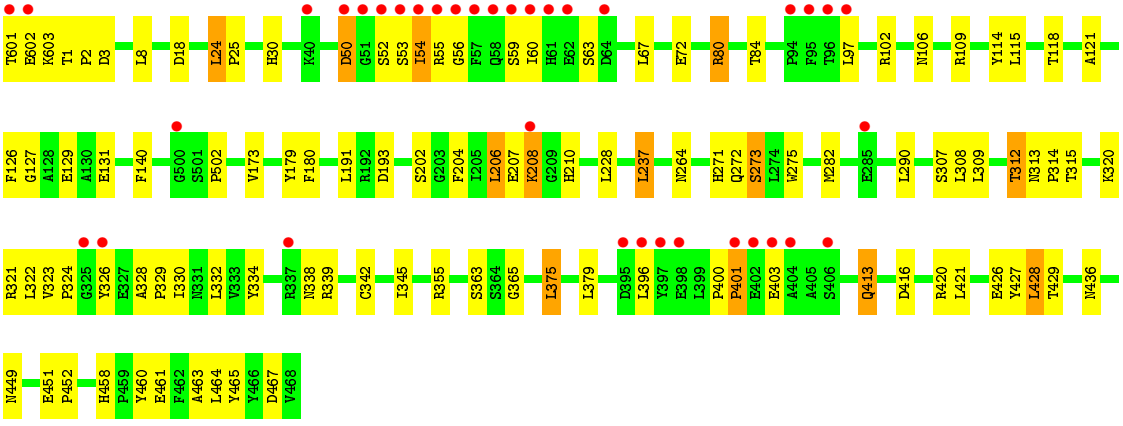
• Molecule 1: GLUTAMINE SYNTHETASE

Chain S:



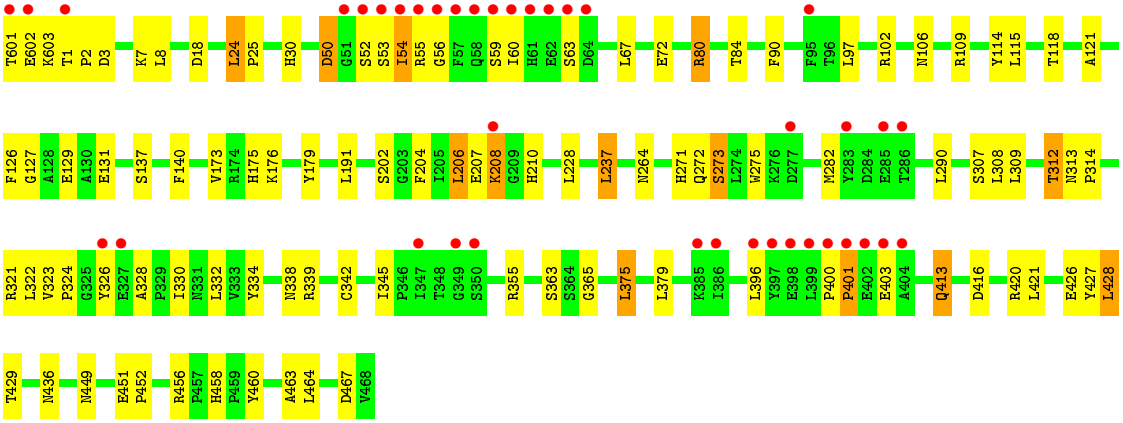
• Molecule 1: GLUTAMINE SYNTHETASE

Chain T:



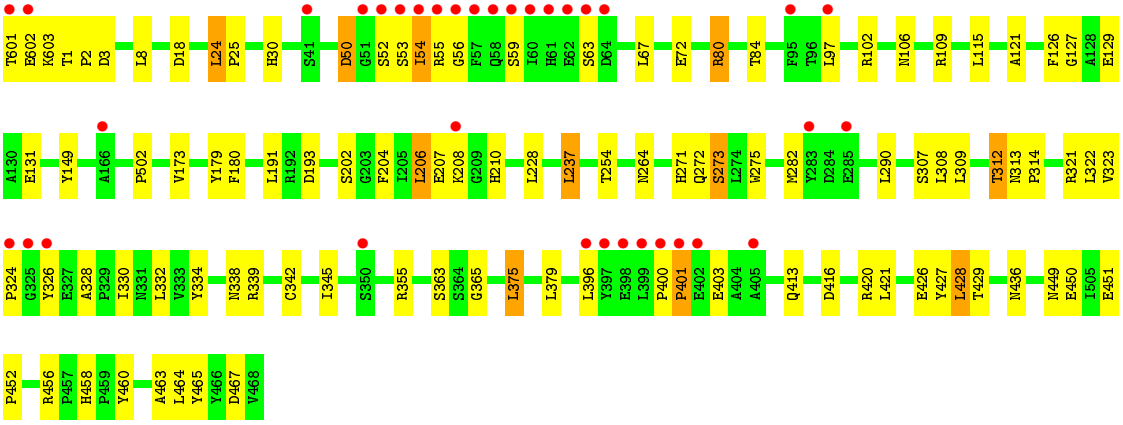
• Molecule 1: GLUTAMINE SYNTHETASE

Chain U:



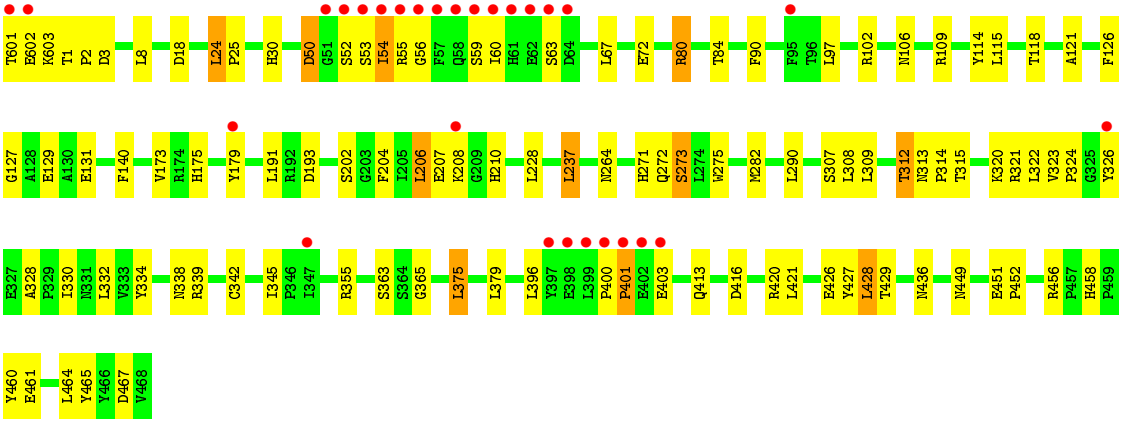
• Molecule 1: GLUTAMINE SYNTHETASE

Chain V:



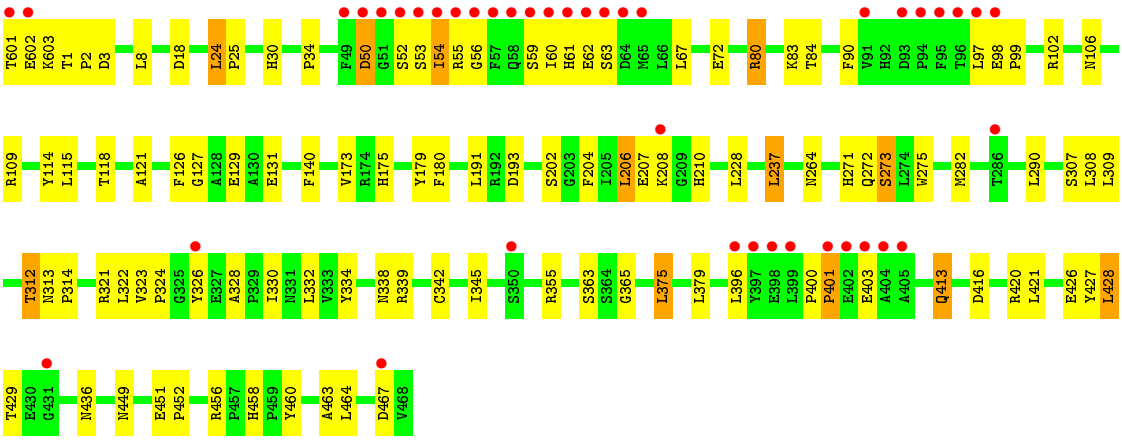
• Molecule 1: GLUTAMINE SYNTHETASE

Chain W:



• Molecule 1: GLUTAMINE SYNTHETASE

Chain X:


T601 E602 K603 T1 P2 D3 L8 D18 L24 P25 H30 P34 F49 D50 G51 S52 S53 I54 R55 G56 F57 Q58 S59 I60 H61 E62 S63 D64 N65 I66 I67 E72 R80 K83 T84 F90 V91 H92 D93 P94 F95 T96 L97 E98 P99 R102 N106
R109 Y114 L115 T118 A121 F126 G127 A128 E129 A130 E131 F140 V173 R174 H175 Y179 F180 L191 R192 D193 S202 G203 F204 I205 L206 E207 K208 G209 H210 L228 L237 N264 H271 Q272 S273 L274 W275 M282 T286 L290 S307 L308 L309
T312 N313 P314 R321 L322 V323 P324 G325 Y326 E327 A328 P329 I330 N331 L332 V333 Y334 N338 R339 C342 I345 S350 R355 S363 S364 G365 L375 L379 L396 Y397 E398 L399 P400 P401 E402 E403 A404 A405 Q413 D416 R420 L421 E426 Y427 L428
T429 E430 G431 N436 N449 E451 P452 R456 P457 H458 P459 Y460 A463 L464 D467 V468

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	207.72Å 257.69Å 274.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.40) 99.7 (20.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.38 (at 2.41Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.227 , 0.255 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	13 of 566314 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	97872	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.31 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.0949e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: AMP, MN, CIT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/3884	0.68	0/5279
1	B	0.35	0/3884	0.68	0/5279
1	C	0.35	0/3884	0.68	0/5279
1	D	0.35	0/3884	0.69	0/5279
1	E	0.35	0/3884	0.68	0/5279
1	F	0.35	0/3884	0.68	0/5279
1	G	0.35	0/3884	0.68	0/5279
1	H	0.35	0/3884	0.68	0/5279
1	I	0.35	0/3884	0.68	0/5279
1	J	0.35	0/3884	0.68	0/5279
1	K	0.35	0/3884	0.68	0/5279
1	L	0.35	0/3884	0.68	0/5279
1	M	0.35	0/3884	0.68	0/5279
1	N	0.35	0/3884	0.68	0/5279
1	O	0.35	0/3884	0.68	0/5279
1	P	0.35	0/3884	0.69	0/5279
1	Q	0.35	0/3884	0.68	0/5279
1	R	0.35	0/3884	0.68	0/5279
1	S	0.35	0/3884	0.68	0/5279
1	T	0.35	0/3884	0.68	0/5279
1	U	0.35	0/3884	0.68	0/5279
1	V	0.35	0/3884	0.68	0/5279
1	W	0.35	0/3884	0.68	0/5279
1	X	0.35	0/3884	0.68	0/5279
All	All	0.35	0/93216	0.68	0/126696

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3778	0	3604	94	0
1	B	3778	0	3604	93	0
1	C	3778	0	3604	88	0
1	D	3778	0	3604	103	0
1	E	3778	0	3604	99	0
1	F	3778	0	3604	99	0
1	G	3778	0	3604	103	0
1	H	3778	0	3604	96	0
1	I	3778	0	3604	90	0
1	J	3778	0	3604	85	0
1	K	3778	0	3604	100	0
1	L	3778	0	3604	90	0
1	M	3778	0	3604	92	0
1	N	3778	0	3604	99	0
1	O	3778	0	3604	90	0
1	P	3778	0	3604	106	0
1	Q	3778	0	3604	93	0
1	R	3778	0	3604	99	0
1	S	3778	0	3604	94	0
1	T	3778	0	3604	90	0
1	U	3778	0	3604	95	0
1	V	3778	0	3604	88	0
1	W	3778	0	3604	96	0
1	X	3778	0	3604	89	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
3	A	23	0	10	7	0
3	B	23	0	10	7	0
3	C	23	0	10	7	0
3	D	23	0	10	7	0
3	E	23	0	10	7	0
3	F	23	0	10	7	0
3	G	23	0	10	7	0
3	H	23	0	10	7	0
3	I	23	0	10	7	0
3	J	23	0	10	7	0
3	K	23	0	10	8	0
3	L	23	0	10	7	0
3	M	23	0	10	7	0
3	N	23	0	10	7	0
3	O	23	0	10	7	0
3	P	23	0	10	7	0
3	Q	23	0	10	7	0
3	R	23	0	10	7	0
3	S	23	0	10	7	0
3	T	23	0	10	7	0
3	U	23	0	10	7	0
3	V	23	0	10	7	0
3	W	23	0	10	7	0
3	X	23	0	10	7	0
4	A	13	0	5	6	0
4	B	13	0	5	6	0
4	C	13	0	5	5	0
4	D	13	0	5	6	0
4	E	13	0	5	5	0
4	F	13	0	5	6	0
4	G	13	0	5	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	13	0	5	6	0
4	I	13	0	5	6	0
4	J	13	0	5	5	0
4	K	13	0	5	6	0
4	L	13	0	5	6	0
4	M	13	0	5	6	0
4	N	13	0	5	6	0
4	O	13	0	5	5	0
4	P	13	0	5	6	0
4	Q	13	0	5	5	0
4	R	13	0	5	6	0
4	S	13	0	5	6	0
4	T	13	0	5	6	0
4	U	13	0	5	6	0
4	V	13	0	5	5	0
4	W	13	0	5	6	0
4	X	13	0	5	6	0
5	A	261	0	0	4	0
5	B	262	0	0	5	0
5	C	264	0	0	4	0
5	D	262	0	0	7	0
5	E	261	0	0	4	0
5	F	267	0	0	6	0
5	G	262	0	0	4	0
5	H	263	0	0	4	0
5	I	263	0	0	4	0
5	J	262	0	0	3	0
5	K	267	0	0	5	0
5	L	262	0	0	3	0
5	M	263	0	0	4	0
5	N	262	0	0	4	0
5	O	265	0	0	3	0
5	P	265	0	0	7	0
5	Q	259	0	0	4	0
5	R	269	0	0	6	0
5	S	262	0	0	5	0
5	T	258	0	0	5	0
5	U	265	0	0	5	0
5	V	263	0	0	3	0
5	W	263	0	0	3	0
5	X	262	0	0	5	0
All	All	97872	0	86856	1941	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 11.

The worst 5 of 1941 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)
3:X:7521:AMP:N9	3:X:7521:AMP:C1'	1.76	1.49
3:L:7497:AMP:C1'	3:L:7497:AMP:N9	1.76	1.49
3:S:7511:AMP:N9	3:S:7511:AMP:C1'	1.76	1.49
3:M:7499:AMP:C1'	3:M:7499:AMP:N9	1.76	1.49
3:T:7513:AMP:N9	3:T:7513:AMP:C1'	1.76	1.49

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	A	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	B	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	C	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	15	21
1	D	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	E	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	15	21
1	F	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	15	21
1	G	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	H	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	I	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	15	21
1	J	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	K	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	L	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	15	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	N	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	O	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	P	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	15	21
1	Q	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	R	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	S	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	T	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	U	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	15	21
1	V	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	15	21
1	W	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	15	21
1	X	475/477 (100%)	445 (94%)	24 (5%)	6 (1%)	15	21
All	All	11400/11448 (100%)	10718 (94%)	538 (5%)	144 (1%)	15	21

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	SER
1	A	208	LYS
1	B	63	SER
1	B	208	LYS
1	C	63	SER

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	A	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	B	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	C	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	D	404/404 (100%)	376 (93%)	28 (7%)	19	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	404/404 (100%)	375 (93%)	29 (7%)	18	28
1	F	404/404 (100%)	375 (93%)	29 (7%)	18	28
1	G	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	H	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	I	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	J	404/404 (100%)	377 (93%)	27 (7%)	20	31
1	K	404/404 (100%)	375 (93%)	29 (7%)	18	28
1	L	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	M	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	N	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	O	404/404 (100%)	377 (93%)	27 (7%)	20	31
1	P	404/404 (100%)	375 (93%)	29 (7%)	18	28
1	Q	404/404 (100%)	375 (93%)	29 (7%)	18	28
1	R	404/404 (100%)	375 (93%)	29 (7%)	18	28
1	S	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	T	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	U	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	V	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	W	404/404 (100%)	376 (93%)	28 (7%)	19	30
1	X	404/404 (100%)	376 (93%)	28 (7%)	19	30
All	All	9696/9696 (100%)	9020 (93%)	676 (7%)	19	29

5 of 676 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	401	PRO
1	N	202	SER
1	W	50	ASP
1	L	50	ASP
1	M	54	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 416 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	458	HIS
1	N	244	ASN
1	W	113	ASN
1	L	175	HIS
1	M	187	GLN

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

Of 72 ligands modelled in this entry, 24 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AMP	A	7475	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	A	7476	-	3,12,12	2.87	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	B	7477	-	20,25,25	3.66	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	B	7478	-	3,12,12	2.87	2 (66%)	3,17,17	1.67	1 (33%)
3	AMP	C	7479	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	C	7480	-	3,12,12	2.90	2 (66%)	3,17,17	1.65	1 (33%)
3	AMP	D	7481	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	D	7482	-	3,12,12	2.88	2 (66%)	3,17,17	1.66	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	AMP	E	7483	-	20,25,25	3.64	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	E	7484	-	3,12,12	2.88	2 (66%)	3,17,17	1.67	1 (33%)
3	AMP	F	7485	-	20,25,25	3.65	12 (60%)	22,38,38	3.31	11 (50%)
4	CIT	F	7486	-	3,12,12	2.88	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	G	7487	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	G	7488	-	3,12,12	2.86	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	H	7489	-	20,25,25	3.64	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	H	7490	-	3,12,12	2.87	2 (66%)	3,17,17	1.65	1 (33%)
3	AMP	I	7491	-	20,25,25	3.64	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	I	7492	-	3,12,12	2.88	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	J	7493	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	J	7494	-	3,12,12	2.86	2 (66%)	3,17,17	1.65	1 (33%)
3	AMP	K	7495	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	K	7496	-	3,12,12	2.85	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	L	7497	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	L	7498	-	3,12,12	2.90	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	M	7499	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	M	7500	-	3,12,12	2.85	2 (66%)	3,17,17	1.67	1 (33%)
3	AMP	N	7501	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	N	7502	-	3,12,12	2.88	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	O	7503	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	O	7504	-	3,12,12	2.86	2 (66%)	3,17,17	1.67	1 (33%)
3	AMP	P	7505	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	P	7506	-	3,12,12	2.87	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	Q	7507	-	20,25,25	3.64	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	Q	7508	-	3,12,12	2.87	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	R	7509	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	R	7510	-	3,12,12	2.87	2 (66%)	3,17,17	1.65	1 (33%)
3	AMP	S	7511	-	20,25,25	3.64	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	S	7512	-	3,12,12	2.88	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	T	7513	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	T	7514	-	3,12,12	2.86	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	U	7515	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	U	7516	-	3,12,12	2.86	2 (66%)	3,17,17	1.65	1 (33%)
3	AMP	V	7517	-	20,25,25	3.64	12 (60%)	22,38,38	3.32	11 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CIT	V	7518	-	3,12,12	2.90	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	W	7519	-	20,25,25	3.65	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	W	7520	-	3,12,12	2.88	2 (66%)	3,17,17	1.67	1 (33%)
3	AMP	X	7521	-	20,25,25	3.66	12 (60%)	22,38,38	3.32	11 (50%)
4	CIT	X	7522	-	3,12,12	2.85	2 (66%)	3,17,17	1.66	1 (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
3	AMP	A	7475	-	-	0/6/26/26	0/3/3/3
4	CIT	A	7476	-	-	0/6/16/16	0/0/0/0
3	AMP	B	7477	-	-	0/6/26/26	0/3/3/3
4	CIT	B	7478	-	-	0/6/16/16	0/0/0/0
3	AMP	C	7479	-	-	0/6/26/26	0/3/3/3
4	CIT	C	7480	-	-	0/6/16/16	0/0/0/0
3	AMP	D	7481	-	-	0/6/26/26	0/3/3/3
4	CIT	D	7482	-	-	0/6/16/16	0/0/0/0
3	AMP	E	7483	-	-	0/6/26/26	0/3/3/3
4	CIT	E	7484	-	-	0/6/16/16	0/0/0/0
3	AMP	F	7485	-	-	0/6/26/26	0/3/3/3
4	CIT	F	7486	-	-	0/6/16/16	0/0/0/0
3	AMP	G	7487	-	-	0/6/26/26	0/3/3/3
4	CIT	G	7488	-	-	0/6/16/16	0/0/0/0
3	AMP	H	7489	-	-	0/6/26/26	0/3/3/3
4	CIT	H	7490	-	-	0/6/16/16	0/0/0/0
3	AMP	I	7491	-	-	0/6/26/26	0/3/3/3
4	CIT	I	7492	-	-	0/6/16/16	0/0/0/0
3	AMP	J	7493	-	-	0/6/26/26	0/3/3/3
4	CIT	J	7494	-	-	0/6/16/16	0/0/0/0
3	AMP	K	7495	-	-	0/6/26/26	0/3/3/3
4	CIT	K	7496	-	-	0/6/16/16	0/0/0/0
3	AMP	L	7497	-	-	0/6/26/26	0/3/3/3
4	CIT	L	7498	-	-	0/6/16/16	0/0/0/0
3	AMP	M	7499	-	-	0/6/26/26	0/3/3/3
4	CIT	M	7500	-	-	0/6/16/16	0/0/0/0
3	AMP	N	7501	-	-	0/6/26/26	0/3/3/3
4	CIT	N	7502	-	-	0/6/16/16	0/0/0/0
3	AMP	O	7503	-	-	0/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	O	7504	-	-	0/6/16/16	0/0/0/0
3	AMP	P	7505	-	-	0/6/26/26	0/3/3/3
4	CIT	P	7506	-	-	0/6/16/16	0/0/0/0
3	AMP	Q	7507	-	-	0/6/26/26	0/3/3/3
4	CIT	Q	7508	-	-	0/6/16/16	0/0/0/0
3	AMP	R	7509	-	-	0/6/26/26	0/3/3/3
4	CIT	R	7510	-	-	0/6/16/16	0/0/0/0
3	AMP	S	7511	-	-	0/6/26/26	0/3/3/3
4	CIT	S	7512	-	-	0/6/16/16	0/0/0/0
3	AMP	T	7513	-	-	0/6/26/26	0/3/3/3
4	CIT	T	7514	-	-	0/6/16/16	0/0/0/0
3	AMP	U	7515	-	-	0/6/26/26	0/3/3/3
4	CIT	U	7516	-	-	0/6/16/16	0/0/0/0
3	AMP	V	7517	-	-	0/6/26/26	0/3/3/3
4	CIT	V	7518	-	-	0/6/16/16	0/0/0/0
3	AMP	W	7519	-	-	0/6/26/26	0/3/3/3
4	CIT	W	7520	-	-	0/6/16/16	0/0/0/0
3	AMP	X	7521	-	-	0/6/26/26	0/3/3/3
4	CIT	X	7522	-	-	0/6/16/16	0/0/0/0

The worst 5 of 336 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	7511	AMP	C6-N6	-4.06	1.22	1.34
3	L	7497	AMP	C6-N6	-4.06	1.22	1.34
3	D	7481	AMP	C6-N6	-4.06	1.22	1.34
3	K	7495	AMP	C6-N6	-4.06	1.22	1.34
3	U	7515	AMP	C6-N6	-4.05	1.22	1.34

The worst 5 of 288 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	7477	AMP	C4'-O4'-C1'	-7.38	101.61	109.72
3	K	7495	AMP	C4'-O4'-C1'	-7.37	101.62	109.72
3	H	7489	AMP	C4'-O4'-C1'	-7.35	101.64	109.72
3	Q	7507	AMP	C4'-O4'-C1'	-7.35	101.64	109.72
3	S	7511	AMP	C4'-O4'-C1'	-7.35	101.64	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

48 monomers are involved in 307 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	7475	AMP	7	0
4	A	7476	CIT	6	0
3	B	7477	AMP	7	0
4	B	7478	CIT	6	0
3	C	7479	AMP	7	0
4	C	7480	CIT	5	0
3	D	7481	AMP	7	0
4	D	7482	CIT	6	0
3	E	7483	AMP	7	0
4	E	7484	CIT	5	0
3	F	7485	AMP	7	0
4	F	7486	CIT	6	0
3	G	7487	AMP	7	0
4	G	7488	CIT	6	0
3	H	7489	AMP	7	0
4	H	7490	CIT	6	0
3	I	7491	AMP	7	0
4	I	7492	CIT	6	0
3	J	7493	AMP	7	0
4	J	7494	CIT	5	0
3	K	7495	AMP	8	0
4	K	7496	CIT	6	0
3	L	7497	AMP	7	0
4	L	7498	CIT	6	0
3	M	7499	AMP	7	0
4	M	7500	CIT	6	0
3	N	7501	AMP	7	0
4	N	7502	CIT	6	0
3	O	7503	AMP	7	0
4	O	7504	CIT	5	0
3	P	7505	AMP	7	0
4	P	7506	CIT	6	0
3	Q	7507	AMP	7	0
4	Q	7508	CIT	5	0
3	R	7509	AMP	7	0
4	R	7510	CIT	6	0
3	S	7511	AMP	7	0
4	S	7512	CIT	6	0
3	T	7513	AMP	7	0
4	T	7514	CIT	6	0
3	U	7515	AMP	7	0
4	U	7516	CIT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	V	7517	AMP	7	0
4	V	7518	CIT	5	0
3	W	7519	AMP	7	0
4	W	7520	CIT	6	0
3	X	7521	AMP	7	0
4	X	7522	CIT	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	477/477 (100%)	0.20	33 (6%)	20	19	10, 26, 90, 100	0
1	B	477/477 (100%)	0.31	44 (9%)	11	11	10, 26, 90, 100	0
1	C	477/477 (100%)	0.31	45 (9%)	11	10	10, 26, 90, 100	0
1	D	477/477 (100%)	0.21	35 (7%)	18	18	10, 26, 90, 100	0
1	E	477/477 (100%)	0.30	43 (9%)	12	11	10, 26, 90, 100	0
1	F	477/477 (100%)	0.29	37 (7%)	16	15	10, 26, 90, 100	0
1	G	477/477 (100%)	0.36	41 (8%)	13	13	10, 26, 90, 100	0
1	H	477/477 (100%)	0.20	39 (8%)	14	14	10, 26, 90, 100	0
1	I	477/477 (100%)	0.35	51 (10%)	8	8	10, 26, 90, 100	0
1	J	477/477 (100%)	0.08	30 (6%)	23	24	10, 26, 90, 100	0
1	K	477/477 (100%)	0.21	42 (8%)	12	12	10, 26, 90, 100	0
1	L	477/477 (100%)	0.42	39 (8%)	14	14	10, 26, 90, 100	0
1	M	477/477 (100%)	0.29	35 (7%)	18	18	10, 26, 90, 100	0
1	N	477/477 (100%)	0.31	35 (7%)	18	18	10, 26, 90, 100	0
1	O	477/477 (100%)	0.31	33 (6%)	20	19	10, 26, 90, 100	0
1	P	477/477 (100%)	0.42	37 (7%)	16	15	10, 26, 90, 100	0
1	Q	477/477 (100%)	0.39	38 (7%)	15	15	10, 26, 90, 100	0
1	R	477/477 (100%)	0.35	34 (7%)	19	19	10, 26, 90, 100	0
1	S	477/477 (100%)	0.33	38 (7%)	15	15	10, 26, 90, 100	0
1	T	477/477 (100%)	0.24	36 (7%)	17	17	10, 26, 90, 100	0
1	U	477/477 (100%)	0.29	39 (8%)	14	14	10, 26, 90, 100	0
1	V	477/477 (100%)	0.15	35 (7%)	18	18	10, 26, 90, 100	0
1	W	477/477 (100%)	0.13	28 (5%)	26	26	10, 26, 90, 100	0
1	X	477/477 (100%)	0.37	41 (8%)	13	13	10, 26, 90, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
All	All	11448/11448 (100%)	0.28	908 (7%)	15 15	10, 26, 92, 100	0

The worst 5 of 908 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	60	ILE	16.8
1	Q	54	ILE	16.7
1	K	61	HIS	16.6
1	E	60	ILE	16.0
1	R	53	SER	15.9

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	MN	O	470	1/1	0.26	0.41	34.04	60,60,60,60	1
3	AMP	S	7511	23/23	0.55	0.68	17.03	2,16,71,83	23
3	AMP	A	7475	23/23	0.48	0.72	16.33	2,16,71,83	23
3	AMP	L	7497	23/23	0.61	0.65	15.62	2,16,71,83	23
3	AMP	J	7493	23/23	0.60	0.63	14.50	2,16,71,83	23
3	AMP	G	7487	23/23	0.55	0.67	14.43	2,16,71,83	23
3	AMP	W	7519	23/23	0.54	0.62	14.40	2,16,71,83	23
3	AMP	F	7485	23/23	0.61	0.66	13.41	2,16,71,83	23
3	AMP	V	7517	23/23	0.59	0.62	12.79	2,16,71,83	23
3	AMP	M	7499	23/23	0.65	0.57	12.43	2,16,71,83	23

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	AMP	R	7509	23/23	0.60	0.68	12.23	2,16,71,83	23
3	AMP	X	7521	23/23	0.65	0.57	12.11	2,16,71,83	23
3	AMP	K	7495	23/23	0.62	0.62	12.07	2,16,71,83	23
3	AMP	D	7481	23/23	0.62	0.54	12.03	2,16,71,83	23
3	AMP	N	7501	23/23	0.64	0.57	11.45	2,16,71,83	23
3	AMP	H	7489	23/23	0.67	0.54	11.07	2,16,71,83	23
3	AMP	Q	7507	23/23	0.67	0.52	10.53	2,16,71,83	23
3	AMP	P	7505	23/23	0.62	0.59	10.35	2,16,71,83	23
3	AMP	E	7483	23/23	0.58	0.61	10.19	2,16,71,83	23
3	AMP	I	7491	23/23	0.63	0.56	9.53	2,16,71,83	23
3	AMP	O	7503	23/23	0.61	0.55	9.18	2,16,71,83	23
3	AMP	T	7513	23/23	0.62	0.59	8.99	2,16,71,83	23
3	AMP	U	7515	23/23	0.53	0.59	8.66	2,16,71,83	23
3	AMP	B	7477	23/23	0.60	0.56	8.38	2,16,71,83	23
2	MN	T	470	1/1	0.81	0.35	7.83	60,60,60,60	1
2	MN	L	470	1/1	0.65	0.25	6.41	60,60,60,60	1
2	MN	A	470	1/1	0.59	0.29	6.08	60,60,60,60	1
2	MN	R	470	1/1	0.47	0.33	5.83	60,60,60,60	1
2	MN	E	470	1/1	0.40	0.30	5.77	60,60,60,60	1
2	MN	M	470	1/1	0.42	0.31	5.67	60,60,60,60	1
2	MN	C	470	1/1	0.64	0.27	5.44	60,60,60,60	1
3	AMP	C	7479	23/23	0.68	0.48	5.42	2,16,71,83	23
2	MN	Q	470	1/1	0.66	0.25	4.39	60,60,60,60	1
2	MN	I	470	1/1	0.56	0.28	4.04	60,60,60,60	1
4	CIT	L	7498	13/13	0.80	0.38	3.01	41,62,79,84	0
2	MN	X	470	1/1	0.79	0.24	2.87	60,60,60,60	1
4	CIT	E	7484	13/13	0.72	0.38	2.76	41,62,79,84	0
4	CIT	Q	7508	13/13	0.71	0.39	2.69	41,62,79,84	0
4	CIT	F	7486	13/13	0.76	0.47	2.57	41,62,79,84	0
4	CIT	X	7522	13/13	0.79	0.37	2.45	41,62,79,84	0
2	MN	H	470	1/1	0.82	0.26	2.41	60,60,60,60	1
4	CIT	R	7510	13/13	0.75	0.45	2.38	41,62,79,84	0
4	CIT	T	7514	13/13	0.69	0.36	2.35	41,62,79,84	0
4	CIT	K	7496	13/13	0.77	0.36	2.04	41,62,79,84	0
4	CIT	J	7494	13/13	0.81	0.33	2.00	41,62,79,84	0
2	MN	N	470	1/1	0.39	0.23	1.99	60,60,60,60	1
2	MN	D	470	1/1	0.66	0.22	1.87	60,60,60,60	1
2	MN	F	470	1/1	0.71	0.24	1.86	60,60,60,60	1
4	CIT	W	7520	13/13	0.84	0.33	1.81	41,62,79,84	0
4	CIT	M	7500	13/13	0.86	0.30	1.74	41,62,79,84	0
2	MN	U	470	1/1	0.86	0.20	1.72	60,60,60,60	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MN	P	470	1/1	0.78	0.22	1.63	60,60,60,60	1
4	CIT	V	7518	13/13	0.79	0.33	1.62	41,62,79,84	0
4	CIT	C	7480	13/13	0.79	0.28	1.57	41,62,79,84	0
4	CIT	O	7504	13/13	0.80	0.35	1.53	41,62,79,84	0
4	CIT	S	7512	13/13	0.82	0.38	1.43	41,62,79,84	0
2	MN	J	470	1/1	0.79	0.20	1.38	60,60,60,60	1
4	CIT	H	7490	13/13	0.78	0.34	1.30	41,62,79,84	0
4	CIT	G	7488	13/13	0.77	0.42	1.27	41,62,79,84	0
2	MN	W	470	1/1	0.61	0.18	1.13	60,60,60,60	1
4	CIT	B	7478	13/13	0.80	0.29	1.03	41,62,79,84	0
4	CIT	N	7502	13/13	0.77	0.30	1.01	41,62,79,84	0
4	CIT	D	7482	13/13	0.82	0.39	0.99	41,62,79,84	0
2	MN	V	470	1/1	0.84	0.19	0.91	60,60,60,60	1
4	CIT	A	7476	13/13	0.76	0.29	0.88	41,62,79,84	0
4	CIT	I	7492	13/13	0.82	0.25	0.81	41,62,79,84	0
2	MN	S	470	1/1	0.80	0.19	0.73	60,60,60,60	1
4	CIT	P	7506	13/13	0.79	0.31	0.69	41,62,79,84	0
4	CIT	U	7516	13/13	0.80	0.28	0.60	41,62,79,84	0
2	MN	G	470	1/1	0.77	0.17	0.08	60,60,60,60	1
2	MN	B	470	1/1	0.77	0.16	-0.56	60,60,60,60	1
2	MN	K	470	1/1	0.84	0.12	-1.77	60,60,60,60	1

6.5 Other polymers (i)

There are no such residues in this entry.