



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:10 PM GMT

PDB ID : 1F52  
Title : CRYSTAL STRUCTURE OF GLUTAMINE SYNTHETASE FROM  
SALMONELLA TYPHIMURIUM CO-CRYSTALLIZED WITH ADP  
Authors : Gill, H.S.; Pfluegl, G.M.U.; Eisenberg, D.  
Deposited on : 2000-06-12  
Resolution : 2.49 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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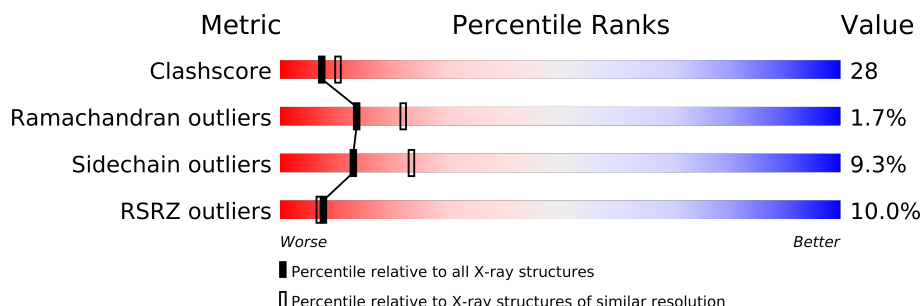
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.49 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	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	468	
1	B	468	
1	C	468	
1	D	468	
1	E	468	
1	F	468	
1	G	468	
1	H	468	
1	I	468	
1	J	468	
1	K	468	
1	L	468	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ADP	A	4471	-	X
3	ADP	B	4472	-	X
3	ADP	F	4476	-	X
3	ADP	G	4477	-	X
3	ADP	I	4479	-	X
3	ADP	J	4480	-	X
3	ADP	K	4481	-	X
3	ADP	L	4482	-	X
4	MPD	A	5472	-	X
4	MPD	A	5481	-	X
4	MPD	B	5471	-	X
4	MPD	B	5474	-	X
4	MPD	C	5473	-	X
4	MPD	C	5476	-	X
4	MPD	D	5475	-	X
4	MPD	D	5478	-	X
4	MPD	E	5477	-	X
4	MPD	E	5480	-	X
4	MPD	F	5479	-	X
4	MPD	F	5482	-	X
4	MPD	G	5484	-	X
4	MPD	G	5485	-	X
4	MPD	H	5486	-	X
4	MPD	H	5487	-	X
4	MPD	I	5488	-	X
4	MPD	I	5489	-	X
4	MPD	J	5490	-	X
4	MPD	J	5491	-	X
4	MPD	K	5492	-	X
4	MPD	K	5493	-	X
4	MPD	L	5483	-	X
4	MPD	L	5494	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 47688 atoms, of which 0 are hydrogen and 0 are deuterium.

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	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	B	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	C	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	D	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	E	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	F	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	G	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	H	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	I	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	J	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	K	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	L	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			

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

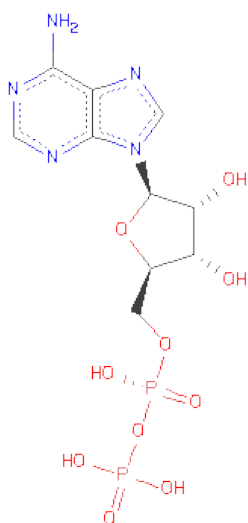
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mn	0	0
			2	2		
2	K	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	H	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	I	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	L	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



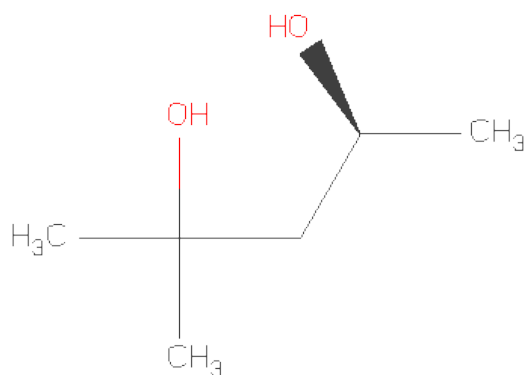
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O P	0	0
			27	10	5	10 2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	L	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	J	1	Total	C	O	0	0
			8	6	2		
4	J	1	Total	C	O	0	0
			8	6	2		
4	K	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	K	1	Total	C	O	0	0
			8	6	2		
4	L	1	Total	C	O	0	0
			8	6	2		

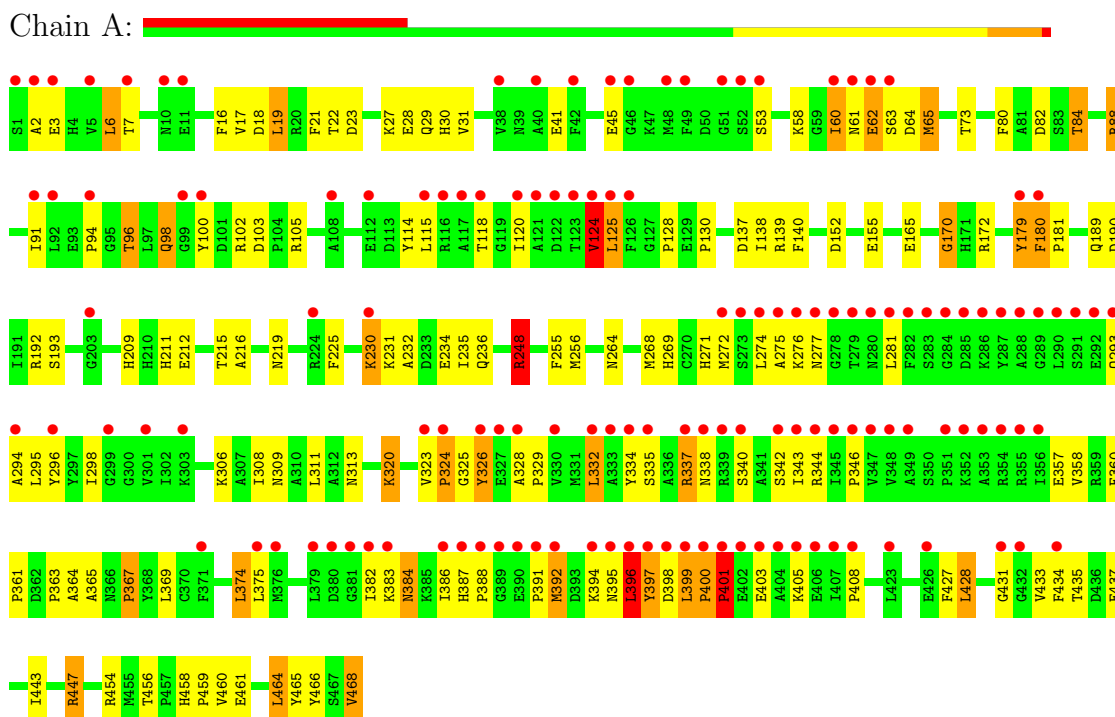
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	294	Total	O	0	0
			294	294		
5	B	297	Total	O	0	0
			297	297		
5	C	293	Total	O	0	0
			293	293		
5	D	295	Total	O	0	0
			295	295		
5	E	294	Total	O	0	0
			294	294		
5	F	293	Total	O	0	0
			293	293		
5	G	288	Total	O	0	0
			288	288		
5	H	288	Total	O	0	0
			288	288		
5	I	295	Total	O	0	0
			295	295		
5	J	287	Total	O	0	0
			287	287		
5	K	288	Total	O	0	0
			288	288		
5	L	292	Total	O	0	0
			292	292		

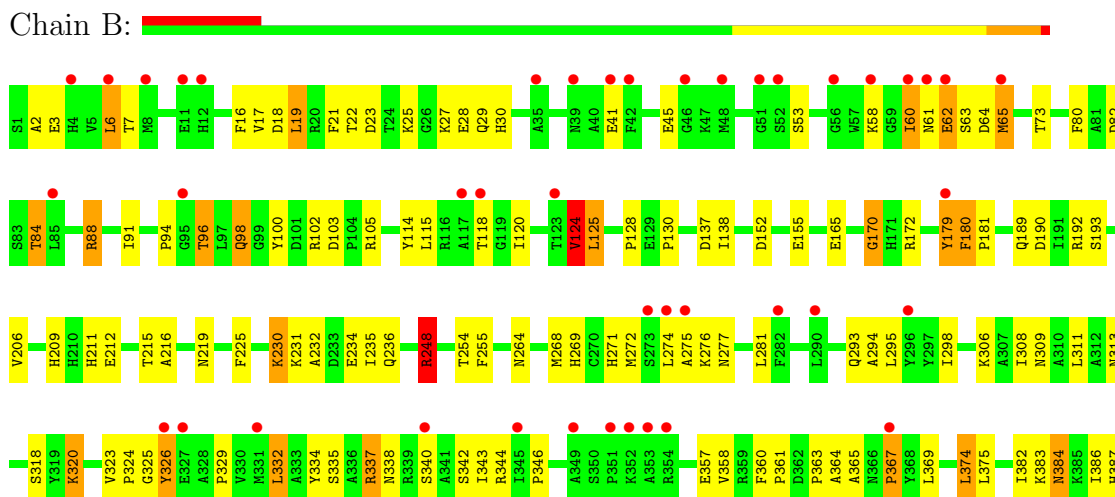
### 3 Residue-property plots

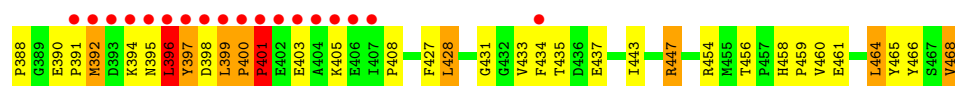
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



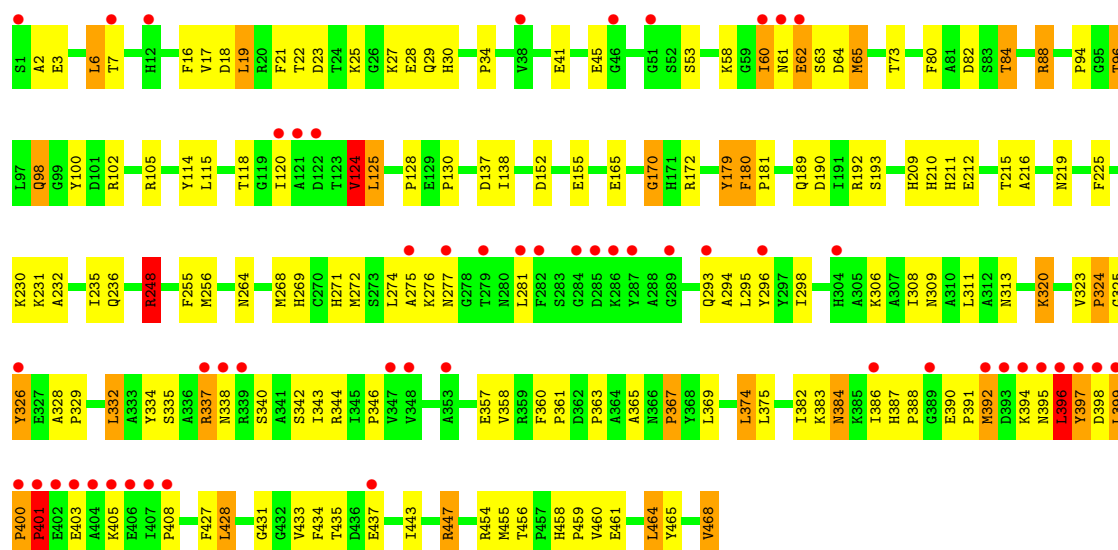
#### • Molecule 1: GLUTAMINE SYNTHETASE





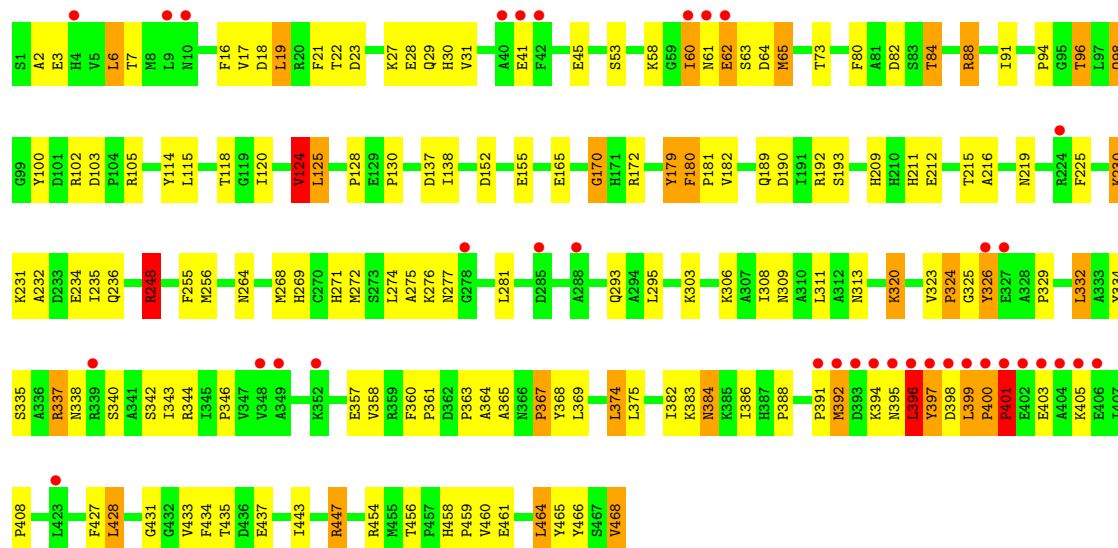
• Molecule 1: GLUTAMINE SYNTHETASE

Chain C:



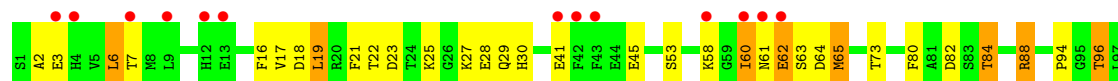
• Molecule 1: GLUTAMINE SYNTHETASE

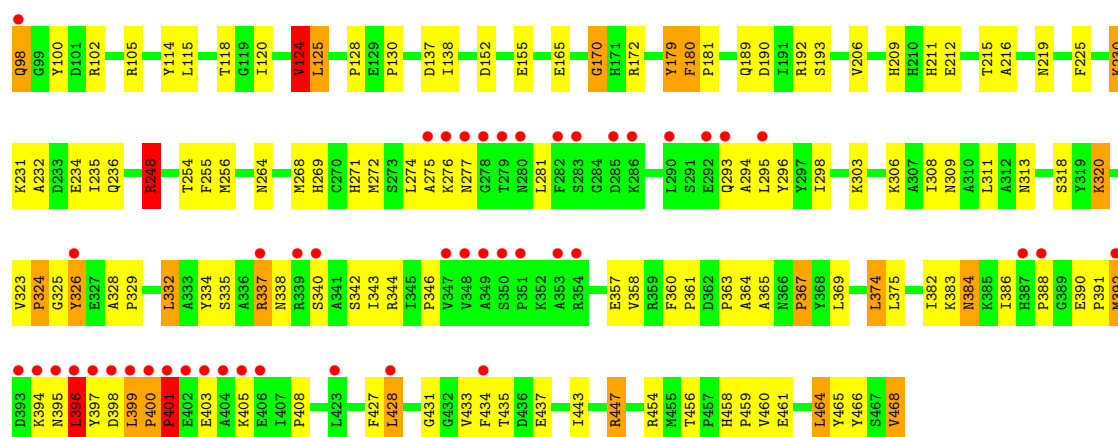
Chain D:



• Molecule 1: GLUTAMINE SYNTHETASE

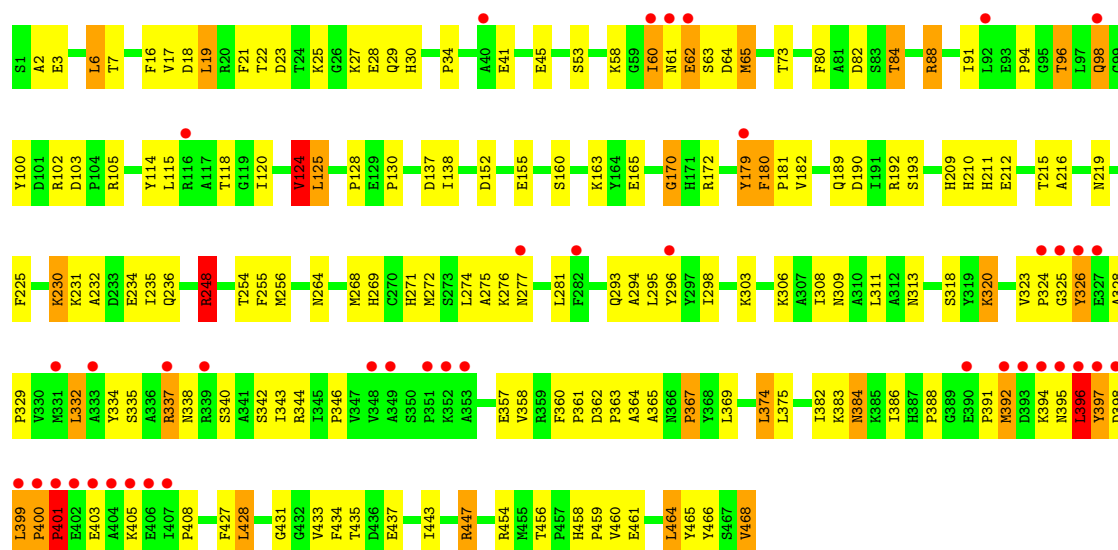
Chain E:





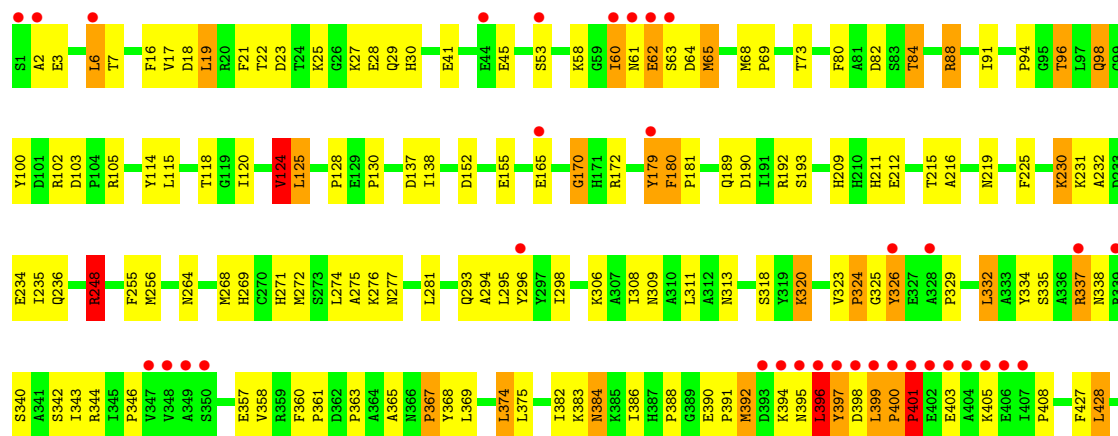
• Molecule 1: GLUTAMINE SYNTHETASE

Chain F:



• Molecule 1: GLUTAMINE SYNTHETASE

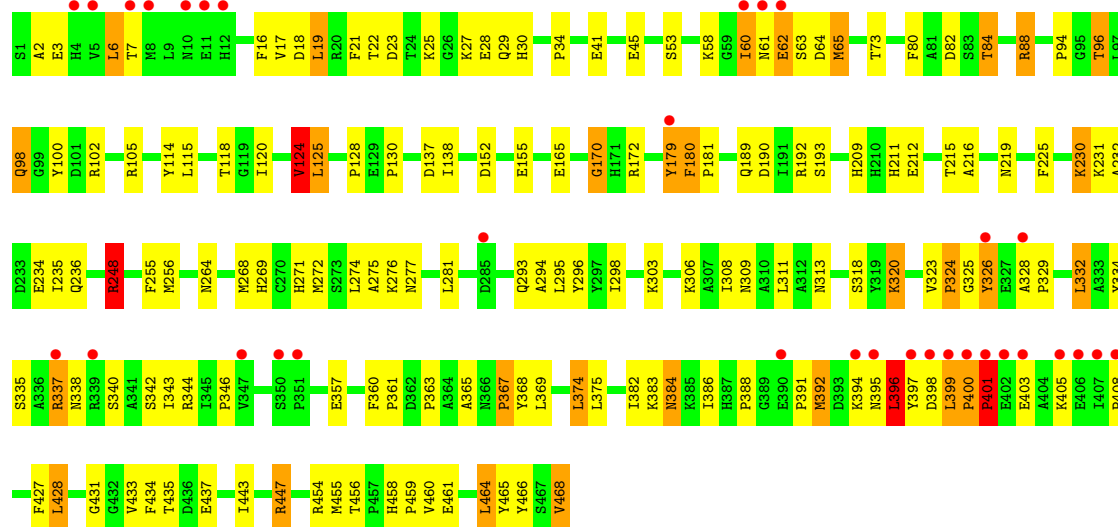
Chain G:





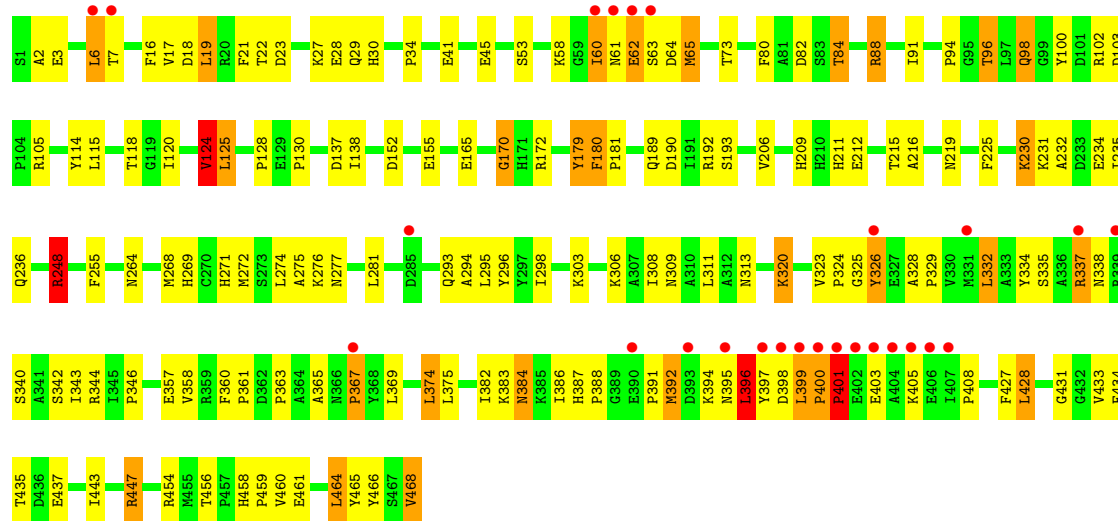
• Molecule 1: GLUTAMINE SYNTHETASE

Chain H:



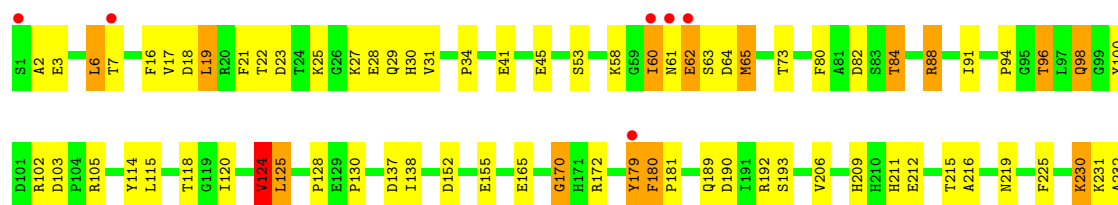
• Molecule 1: GLUTAMINE SYNTHETASE

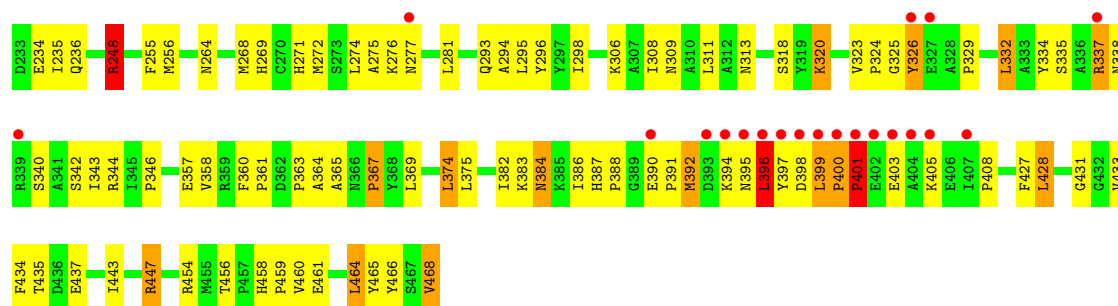
Chain I:



• Molecule 1: GLUTAMINE SYNTHETASE

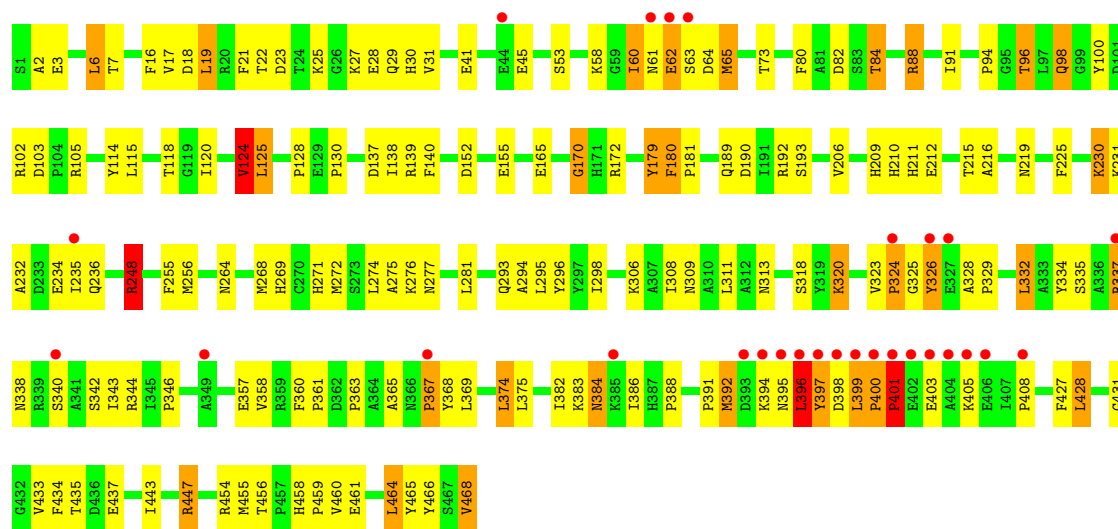
Chain J:





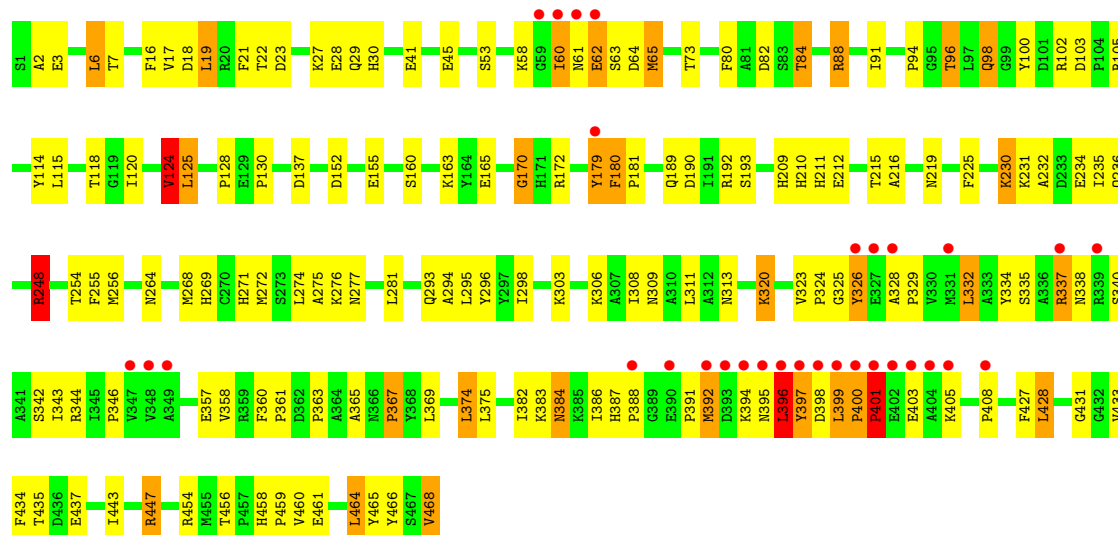
• Molecule 1: GLUTAMINE SYNTHETASE

Chain K: 



• Molecule 1: GLUTAMINE SYNTHETASE

Chain L: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	230.60Å 132.50Å 195.90Å 90.00° 102.40° 90.00°	Depositor
Resolution (Å)	34.90 – 2.49 34.90 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.90-2.49) 97.9 (34.90-2.49)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.67 (at 2.48Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.243 , 0.257 0.261 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 196561 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	47688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, MN, ADP

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	0.53	0/3724	0.85	4/5043 (0.1%)
1	B	0.53	0/3724	0.85	4/5043 (0.1%)
1	C	0.53	0/3724	0.85	4/5043 (0.1%)
1	D	0.53	0/3724	0.85	4/5043 (0.1%)
1	E	0.53	0/3724	0.85	4/5043 (0.1%)
1	F	0.53	0/3724	0.85	4/5043 (0.1%)
1	G	0.53	0/3724	0.85	4/5043 (0.1%)
1	H	0.53	0/3724	0.85	4/5043 (0.1%)
1	I	0.53	0/3724	0.85	4/5043 (0.1%)
1	J	0.53	0/3724	0.85	4/5043 (0.1%)
1	K	0.53	0/3724	0.85	4/5043 (0.1%)
1	L	0.53	0/3724	0.85	4/5043 (0.1%)
All	All	0.53	0/44688	0.85	48/60516 (0.1%)

There are no bond length outliers.

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	401	PRO	CA-N-CD	-6.91	101.83	111.50
1	J	401	PRO	CA-N-CD	-6.90	101.84	111.50
1	I	401	PRO	CA-N-CD	-6.89	101.86	111.50
1	L	401	PRO	CA-N-CD	-6.89	101.86	111.50
1	F	401	PRO	CA-N-CD	-6.88	101.86	111.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3637	0	3544	210	0
1	B	3637	0	3544	204	0
1	C	3637	0	3544	207	0
1	D	3637	0	3544	205	0
1	E	3637	0	3544	199	0
1	F	3637	0	3544	218	0
1	G	3637	0	3544	205	0
1	H	3637	0	3544	213	0
1	I	3637	0	3544	211	0
1	J	3637	0	3544	221	0
1	K	3637	0	3544	220	0
1	L	3637	0	3544	216	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	27	0	10	1	0
3	B	27	0	10	1	0
3	C	27	0	10	1	0
3	D	27	0	10	1	0
3	E	27	0	10	1	0
3	F	27	0	10	1	0
3	G	27	0	10	1	0
3	H	27	0	10	1	0
3	I	27	0	10	1	0
3	J	27	0	10	1	0
3	K	27	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	27	0	10	1	0
4	A	16	0	27	56	0
4	B	16	0	27	60	0
4	C	16	0	27	62	0
4	D	16	0	27	61	0
4	E	16	0	27	54	0
4	F	16	0	27	62	0
4	G	16	0	27	60	0
4	H	16	0	27	65	0
4	I	16	0	27	62	0
4	J	16	0	27	68	0
4	K	16	0	27	66	0
4	L	16	0	27	65	0
5	A	294	0	0	6	0
5	B	297	0	0	7	0
5	C	293	0	0	8	0
5	D	295	0	0	7	0
5	E	294	0	0	8	0
5	F	293	0	0	8	0
5	G	288	0	0	8	0
5	H	288	0	0	7	0
5	I	295	0	0	7	0
5	J	287	0	0	8	0
5	K	288	0	0	7	0
5	L	292	0	0	7	0
All	All	47688	0	42972	2421	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

The worst 5 of 2421 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:84:THR:HG21	4:J:5491:MPD:C5	1.53	1.36
1:J:84:THR:CG2	4:J:5491:MPD:H52	1.60	1.32
1:F:84:THR:HG21	4:F:5479:MPD:C5	1.57	1.32
1:L:84:THR:HG21	4:L:5483:MPD:C5	1.60	1.31
1:I:61:ASN:O	1:J:337:ARG:HB2	1.29	1.29

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	A	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	14	22
1	B	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	14	22
1	C	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	14	22
1	D	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	14	22
1	E	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	14	22
1	F	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	14	22
1	G	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	14	22
1	H	466/468 (100%)	427 (92%)	31 (7%)	8 (2%)	14	22
1	I	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	14	22
1	J	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	14	22
1	K	466/468 (100%)	427 (92%)	31 (7%)	8 (2%)	14	22
1	L	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	14	22
All	All	5592/5616 (100%)	5114 (92%)	382 (7%)	96 (2%)	14	22

5 of 96 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	PHE
1	A	400	PRO
1	A	401	PRO
1	B	180	PHE
1	B	400	PRO

### 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	A	384/384 (100%)	348 (91%)	36 (9%)	13	23
1	B	384/384 (100%)	349 (91%)	35 (9%)	14	24
1	C	384/384 (100%)	348 (91%)	36 (9%)	13	23
1	D	384/384 (100%)	348 (91%)	36 (9%)	13	23
1	E	384/384 (100%)	348 (91%)	36 (9%)	13	23
1	F	384/384 (100%)	349 (91%)	35 (9%)	14	24
1	G	384/384 (100%)	348 (91%)	36 (9%)	13	23
1	H	384/384 (100%)	348 (91%)	36 (9%)	13	23
1	I	384/384 (100%)	349 (91%)	35 (9%)	14	24
1	J	384/384 (100%)	349 (91%)	35 (9%)	14	24
1	K	384/384 (100%)	348 (91%)	36 (9%)	13	23
1	L	384/384 (100%)	349 (91%)	35 (9%)	14	24
All	All	4608/4608 (100%)	4181 (91%)	427 (9%)	13	23

5 of 427 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	165	GLU
1	G	374	LEU
1	L	60	ILE
1	F	264	ASN
1	G	60	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	244	ASN
1	G	313	ASN
1	L	30	HIS
1	F	264	ASN
1	G	30	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 60 ligands modelled in this entry, 24 are monoatomic - leaving 36 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	ADP	A	4471	2	29,29,29	3.24	14 (48%)	45,45,45	3.96	17 (37%)
4	MPD	A	5472	-	7,7,7	2.89	3 (42%)	10,10,10	1.36	1 (10%)
4	MPD	A	5481	-	7,7,7	1.35	1 (14%)	10,10,10	0.81	0
3	ADP	B	4472	2	29,29,29	3.23	14 (48%)	45,45,45	3.97	17 (37%)
4	MPD	B	5471	-	7,7,7	1.35	1 (14%)	10,10,10	0.81	0
4	MPD	B	5474	-	7,7,7	2.89	3 (42%)	10,10,10	1.36	1 (10%)
3	ADP	C	4473	2	29,29,29	3.24	14 (48%)	45,45,45	3.97	16 (35%)
4	MPD	C	5473	-	7,7,7	1.34	1 (14%)	10,10,10	0.81	0
4	MPD	C	5476	-	7,7,7	2.88	3 (42%)	10,10,10	1.36	1 (10%)
3	ADP	D	4474	2	29,29,29	3.24	14 (48%)	45,45,45	3.96	16 (35%)
4	MPD	D	5475	-	7,7,7	1.35	1 (14%)	10,10,10	0.80	0
4	MPD	D	5478	-	7,7,7	2.88	3 (42%)	10,10,10	1.36	1 (10%)
3	ADP	E	4475	2	29,29,29	3.24	14 (48%)	45,45,45	3.96	16 (35%)
4	MPD	E	5477	-	7,7,7	1.35	1 (14%)	10,10,10	0.81	0
4	MPD	E	5480	-	7,7,7	2.89	3 (42%)	10,10,10	1.37	1 (10%)
3	ADP	F	4476	2	29,29,29	3.24	14 (48%)	45,45,45	3.96	16 (35%)
4	MPD	F	5479	-	7,7,7	1.35	1 (14%)	10,10,10	0.81	0
4	MPD	F	5482	-	7,7,7	2.88	3 (42%)	10,10,10	1.37	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ADP	G	4477	2	29,29,29	3.23	14 (48%)	45,45,45	3.96	16 (35%)
4	MPD	G	5484	-	7,7,7	2.88	3 (42%)	10,10,10	1.36	1 (10%)
4	MPD	G	5485	-	7,7,7	1.35	1 (14%)	10,10,10	0.81	0
3	ADP	H	4478	2	29,29,29	3.24	14 (48%)	45,45,45	3.97	17 (37%)
4	MPD	H	5486	-	7,7,7	2.89	3 (42%)	10,10,10	1.36	1 (10%)
4	MPD	H	5487	-	7,7,7	1.35	1 (14%)	10,10,10	0.81	0
3	ADP	I	4479	2	29,29,29	3.24	14 (48%)	45,45,45	3.96	16 (35%)
4	MPD	I	5488	-	7,7,7	2.88	3 (42%)	10,10,10	1.37	1 (10%)
4	MPD	I	5489	-	7,7,7	1.35	1 (14%)	10,10,10	0.81	0
3	ADP	J	4480	2	29,29,29	3.24	14 (48%)	45,45,45	3.96	16 (35%)
4	MPD	J	5490	-	7,7,7	2.88	3 (42%)	10,10,10	1.37	1 (10%)
4	MPD	J	5491	-	7,7,7	1.35	1 (14%)	10,10,10	0.81	0
3	ADP	K	4481	2	29,29,29	3.24	14 (48%)	45,45,45	3.96	17 (37%)
4	MPD	K	5492	-	7,7,7	2.88	3 (42%)	10,10,10	1.36	1 (10%)
4	MPD	K	5493	-	7,7,7	1.35	1 (14%)	10,10,10	0.81	0
3	ADP	L	4482	2	29,29,29	3.24	14 (48%)	45,45,45	3.97	17 (37%)
4	MPD	L	5483	-	7,7,7	1.35	1 (14%)	10,10,10	0.81	0
4	MPD	L	5494	-	7,7,7	2.89	3 (42%)	10,10,10	1.36	1 (10%)

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	ADP	A	4471	2	-	0/16/32/32	0/1/3/3
4	MPD	A	5472	-	-	0/5/5/5	0/0/0/0
4	MPD	A	5481	-	-	0/5/5/5	0/0/0/0
3	ADP	B	4472	2	-	0/16/32/32	0/1/3/3
4	MPD	B	5471	-	-	0/5/5/5	0/0/0/0
4	MPD	B	5474	-	-	0/5/5/5	0/0/0/0
3	ADP	C	4473	2	-	0/16/32/32	0/1/3/3
4	MPD	C	5473	-	-	0/5/5/5	0/0/0/0
4	MPD	C	5476	-	-	0/5/5/5	0/0/0/0
3	ADP	D	4474	2	-	0/16/32/32	0/1/3/3
4	MPD	D	5475	-	-	0/5/5/5	0/0/0/0
4	MPD	D	5478	-	-	0/5/5/5	0/0/0/0
3	ADP	E	4475	2	-	0/16/32/32	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	E	5477	-	-	0/5/5/5	0/0/0/0
4	MPD	E	5480	-	-	0/5/5/5	0/0/0/0
3	ADP	F	4476	2	-	0/16/32/32	0/1/3/3
4	MPD	F	5479	-	-	0/5/5/5	0/0/0/0
4	MPD	F	5482	-	-	0/5/5/5	0/0/0/0
3	ADP	G	4477	2	-	0/16/32/32	0/1/3/3
4	MPD	G	5484	-	-	0/5/5/5	0/0/0/0
4	MPD	G	5485	-	-	0/5/5/5	0/0/0/0
3	ADP	H	4478	2	-	0/16/32/32	0/1/3/3
4	MPD	H	5486	-	-	0/5/5/5	0/0/0/0
4	MPD	H	5487	-	-	0/5/5/5	0/0/0/0
3	ADP	I	4479	2	-	0/16/32/32	0/1/3/3
4	MPD	I	5488	-	-	0/5/5/5	0/0/0/0
4	MPD	I	5489	-	-	0/5/5/5	0/0/0/0
3	ADP	J	4480	2	-	0/16/32/32	0/1/3/3
4	MPD	J	5490	-	-	0/5/5/5	0/0/0/0
4	MPD	J	5491	-	-	0/5/5/5	0/0/0/0
3	ADP	K	4481	2	-	0/16/32/32	0/1/3/3
4	MPD	K	5492	-	-	0/5/5/5	0/0/0/0
4	MPD	K	5493	-	-	0/5/5/5	0/0/0/0
3	ADP	L	4482	2	-	0/16/32/32	0/1/3/3
4	MPD	L	5483	-	-	0/5/5/5	0/0/0/0
4	MPD	L	5494	-	-	0/5/5/5	0/0/0/0

The worst 5 of 216 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	4481	ADP	O4'-C1'	7.85	1.53	1.41
3	L	4482	ADP	O4'-C1'	7.84	1.53	1.41
3	F	4476	ADP	O4'-C1'	7.83	1.53	1.41
3	C	4473	ADP	O4'-C1'	7.82	1.53	1.41
3	D	4474	ADP	O4'-C1'	7.81	1.53	1.41

The worst 5 of 209 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4472	ADP	O4'-C1'-N9	13.82	121.30	108.44
3	L	4482	ADP	O4'-C1'-N9	13.81	121.29	108.44
3	C	4473	ADP	O4'-C1'-N9	13.81	121.29	108.44
3	F	4476	ADP	O4'-C1'-N9	13.78	121.26	108.44
3	H	4478	ADP	O4'-C1'-N9	13.78	121.26	108.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	468/468 (100%)	1.40	134 (28%) 1 1	28, 48, 96, 100	19 (4%)
1	B	468/468 (100%)	0.80	60 (12%) 4 4	28, 48, 96, 100	19 (4%)
1	C	468/468 (100%)	0.68	52 (11%) 6 6	28, 48, 96, 100	19 (4%)
1	D	468/468 (100%)	0.35	36 (7%) 13 13	28, 48, 96, 100	19 (4%)
1	E	468/468 (100%)	0.71	59 (12%) 4 4	28, 48, 96, 100	19 (4%)
1	F	468/468 (100%)	0.72	41 (8%) 10 9	28, 48, 96, 100	19 (4%)
1	G	468/468 (100%)	0.40	35 (7%) 14 14	28, 48, 96, 100	19 (4%)
1	H	468/468 (100%)	0.43	33 (7%) 16 15	28, 48, 96, 100	19 (4%)
1	I	468/468 (100%)	0.38	26 (5%) 24 24	28, 48, 96, 100	19 (4%)
1	J	468/468 (100%)	0.39	26 (5%) 24 24	28, 48, 96, 100	19 (4%)
1	K	468/468 (100%)	0.33	28 (5%) 21 21	28, 48, 96, 100	19 (4%)
1	L	468/468 (100%)	0.50	31 (6%) 18 17	28, 48, 96, 100	19 (4%)
All	All	5616/5616 (100%)	0.59	561 (9%) 8 7	28, 48, 96, 100	228 (4%)

The worst 5 of 561 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	397	TYR	14.3
1	F	397	TYR	14.0
1	A	397	TYR	13.3
1	C	397	TYR	13.2
1	E	397	TYR	12.7

### 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. 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MPD	J	5491	8/8	0.39	20.15	37,50,65,66	8
4	MPD	I	5489	8/8	0.38	14.49	37,50,65,66	8
4	MPD	F	5479	8/8	0.42	14.45	37,50,65,66	8
4	MPD	L	5483	8/8	0.41	13.00	37,50,65,66	8
4	MPD	B	5474	8/8	0.45	12.54	63,68,75,98	8
4	MPD	H	5487	8/8	0.40	12.53	37,50,65,66	8
4	MPD	D	5478	8/8	0.46	11.19	63,68,75,98	8
4	MPD	C	5473	8/8	0.38	11.16	37,50,65,66	8
4	MPD	H	5486	8/8	0.50	11.03	63,68,75,98	8
4	MPD	I	5488	8/8	0.51	10.78	63,68,75,98	8
4	MPD	J	5490	8/8	0.49	10.57	63,68,75,98	8
4	MPD	G	5485	8/8	0.40	10.54	37,50,65,66	8
4	MPD	G	5484	8/8	0.49	10.52	63,68,75,98	8
4	MPD	B	5471	8/8	0.44	10.46	37,50,65,66	8
4	MPD	L	5494	8/8	0.50	10.38	63,68,75,98	8
4	MPD	E	5477	8/8	0.36	9.93	37,50,65,66	8
4	MPD	K	5492	8/8	0.48	9.40	63,68,75,98	8
4	MPD	D	5475	8/8	0.36	9.38	37,50,65,66	8
4	MPD	C	5476	8/8	0.44	9.27	63,68,75,98	8
4	MPD	E	5480	8/8	0.41	9.07	63,68,75,98	8
4	MPD	K	5493	8/8	0.40	8.94	37,50,65,66	8
4	MPD	A	5481	8/8	0.39	7.65	37,50,65,66	8
4	MPD	F	5482	8/8	0.34	7.39	63,68,75,98	8
3	ADP	I	4479	27/27	0.37	3.76	38,77,100,100	27
4	MPD	A	5472	8/8	0.51	3.44	63,68,75,98	8
3	ADP	L	4482	27/27	0.43	3.37	38,77,100,100	27
3	ADP	B	4472	27/27	0.42	3.11	38,77,100,100	27
3	ADP	J	4480	27/27	0.38	3.06	38,77,100,100	27
3	ADP	K	4481	27/27	0.38	3.03	38,77,100,100	27

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ADP	F	4476	27/27	0.42	2.78	38,77,100,100	27
3	ADP	G	4477	27/27	0.37	2.14	38,77,100,100	27
3	ADP	C	4473	27/27	0.33	1.98	38,77,100,100	27
3	ADP	H	4478	27/27	0.31	1.63	38,77,100,100	27
3	ADP	A	4471	27/27	0.52	1.59	38,77,100,100	27
3	ADP	E	4475	27/27	0.36	1.56	38,77,100,100	27
3	ADP	D	4474	27/27	0.33	1.53	38,77,100,100	27
2	MN	H	469	1/1	0.15	-0.97	47,47,47,47	0
2	MN	D	469	1/1	0.09	-1.10	47,47,47,47	0
2	MN	J	469	1/1	0.16	-1.13	47,47,47,47	0
2	MN	K	469	1/1	0.14	-1.48	47,47,47,47	0
2	MN	D	470	1/1	0.06	-1.68	46,46,46,46	0
2	MN	L	469	1/1	0.16	-1.69	47,47,47,47	0
2	MN	A	470	1/1	0.06	-2.05	46,46,46,46	0
2	MN	A	469	1/1	0.06	-2.11	47,47,47,47	0
2	MN	J	470	1/1	0.10	-2.11	46,46,46,46	0
2	MN	B	469	1/1	0.05	-2.16	47,47,47,47	0
2	MN	K	470	1/1	0.12	-2.16	46,46,46,46	0
2	MN	C	469	1/1	0.07	-2.23	47,47,47,47	0
2	MN	I	469	1/1	0.11	-2.38	47,47,47,47	0
2	MN	G	469	1/1	0.10	-2.49	47,47,47,47	0
2	MN	F	469	1/1	0.06	-2.51	47,47,47,47	0
2	MN	F	470	1/1	0.03	-3.06	46,46,46,46	0
2	MN	E	469	1/1	0.03	-3.11	47,47,47,47	0
2	MN	L	470	1/1	0.12	-3.14	46,46,46,46	0
2	MN	C	470	1/1	0.04	-3.22	46,46,46,46	0
2	MN	H	470	1/1	0.07	-3.32	46,46,46,46	0
2	MN	G	470	1/1	0.09	-3.43	46,46,46,46	0
2	MN	B	470	1/1	0.07	-3.68	46,46,46,46	0
2	MN	E	470	1/1	0.06	-3.98	46,46,46,46	0
2	MN	I	470	1/1	0.07	-5.01	46,46,46,46	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.