



# wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 12:11 AM GMT

PDB ID : 1F1H  
Title : CRYSTAL STRUCTURE OF GLUTAMINE SYNTHETASE FROM  
SALMONELLA TYPHIMURIUM WITH THALLIUM IONS  
Authors : Gill, H.S.; Eisenberg, D.  
Deposited on : 2000-05-19  
Resolution : 2.67 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>

---

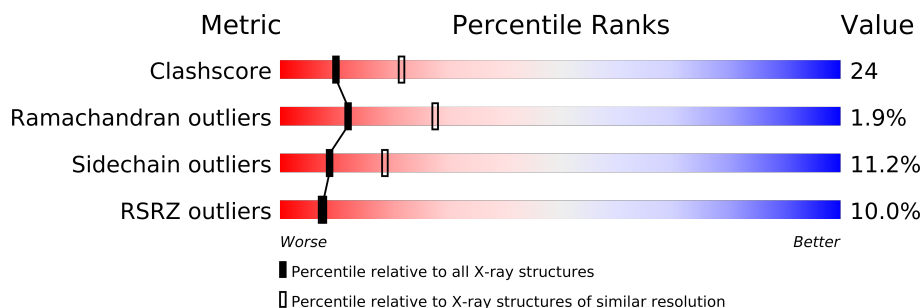
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.67 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	2450 (2.70-2.66)
Ramachandran outliers	78287	2410 (2.70-2.66)
Sidechain outliers	78261	2410 (2.70-2.66)
RSRZ outliers	66119	2013 (2.70-2.66)

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	B	1472	-	X
3	ADP	D	1474	-	X
3	ADP	F	1476	-	X
3	ADP	I	1479	-	X
3	ADP	L	1482	-	X
5	MPD	A	1483	-	X
5	MPD	B	1484	-	X
5	MPD	C	1485	-	X
5	MPD	D	1486	-	X
5	MPD	E	1487	-	X
5	MPD	F	1488	-	X
5	MPD	G	1489	-	X
5	MPD	H	1490	-	X
5	MPD	I	1491	-	X
5	MPD	J	1492	-	X
5	MPD	K	1493	-	X
5	MPD	L	1494	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 45564 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 PROTEIN (GLUTAMINE SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	B	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	C	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	D	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	E	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	F	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	G	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	H	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	I	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	J	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	K	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	L	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			

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

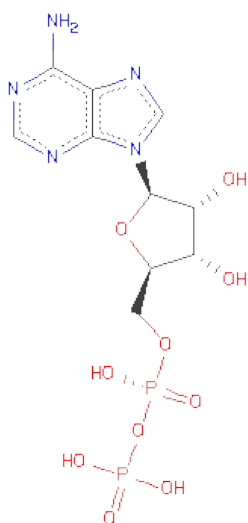
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

*Continued on next page...*

Continued from previous page...

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	
			27	10	5	10	2	

Continued on next page...

*Continued from previous page...*

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 THALLIUM (I) ION (three-letter code: Tl) (formula: Tl).

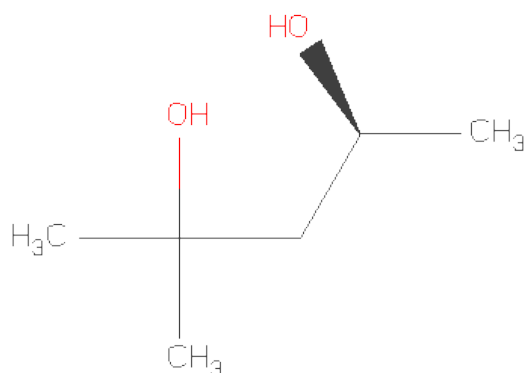
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Tl	0	0
			2	2		
4	J	2	Total	Tl	0	0
			2	2		
4	D	2	Total	Tl	0	0
			2	2		
4	K	2	Total	Tl	0	0
			2	2		
4	E	2	Total	Tl	0	0
			2	2		
4	H	2	Total	Tl	0	0
			2	2		
4	B	2	Total	Tl	0	0
			2	2		
4	I	2	Total	Tl	0	0
			2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	Tl 2	0	0
4	A	2	Total 2	Tl 2	0	0
4	L	2	Total 2	Tl 2	0	0
4	F	2	Total 2	Tl 2	0	0

- Molecule 5 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
5	A	1	Total 8	C 6	O 2	0	0
5	B	1	Total 8	C 6	O 2	0	0
5	C	1	Total 8	C 6	O 2	0	0
5	D	1	Total 8	C 6	O 2	0	0
5	E	1	Total 8	C 6	O 2	0	0
5	F	1	Total 8	C 6	O 2	0	0
5	G	1	Total 8	C 6	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			8	6	2		
5	I	1	Total	C	O	0	0
			8	6	2		
5	J	1	Total	C	O	0	0
			8	6	2		
5	K	1	Total	C	O	0	0
			8	6	2		
5	L	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

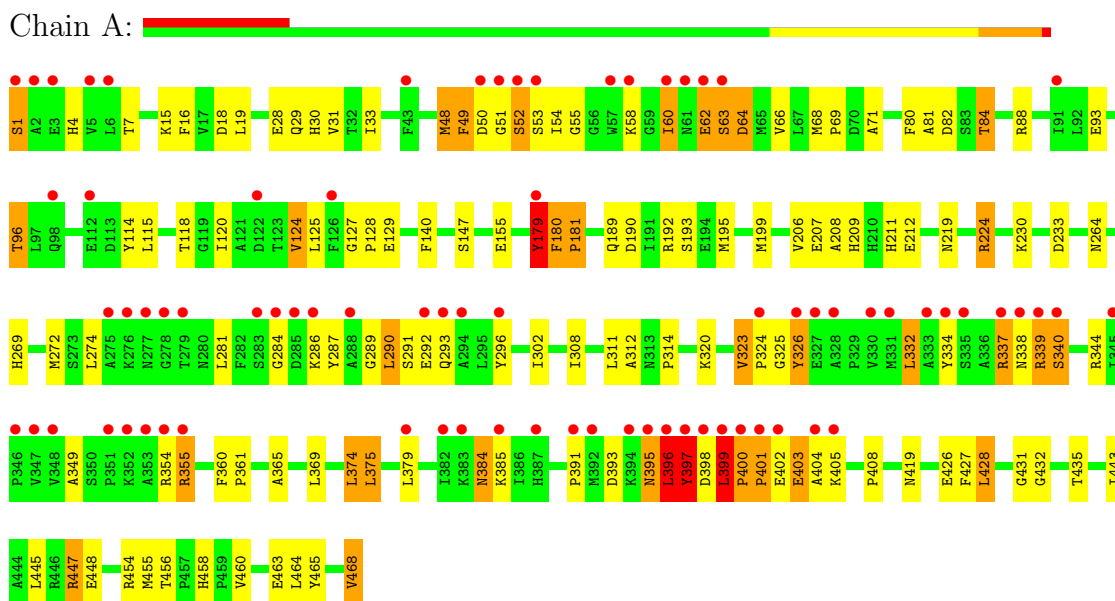
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	120	Total	O	0	0
			120	120		
6	B	121	Total	O	0	0
			121	121		
6	C	119	Total	O	0	0
			119	119		
6	D	122	Total	O	0	0
			122	122		
6	E	122	Total	O	0	0
			122	122		
6	F	121	Total	O	0	0
			121	121		
6	G	122	Total	O	0	0
			122	122		
6	H	121	Total	O	0	0
			121	121		
6	I	122	Total	O	0	0
			122	122		
6	J	120	Total	O	0	0
			120	120		
6	K	123	Total	O	0	0
			123	123		
6	L	119	Total	O	0	0
			119	119		



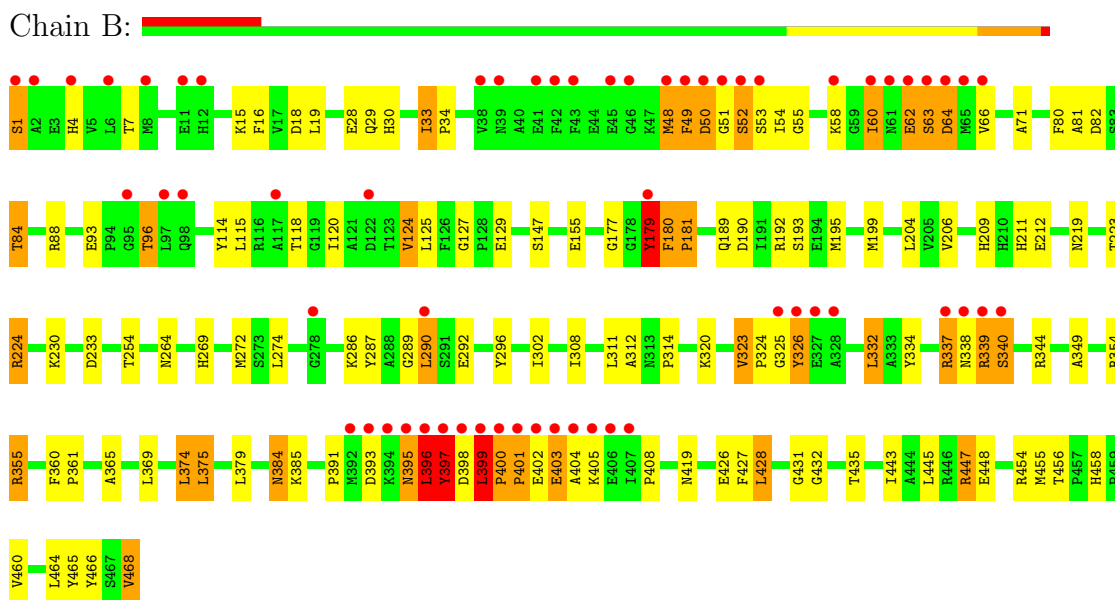
### 3 Residue-property plots

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: PROTEIN (GLUTAMINE SYNTHETASE)

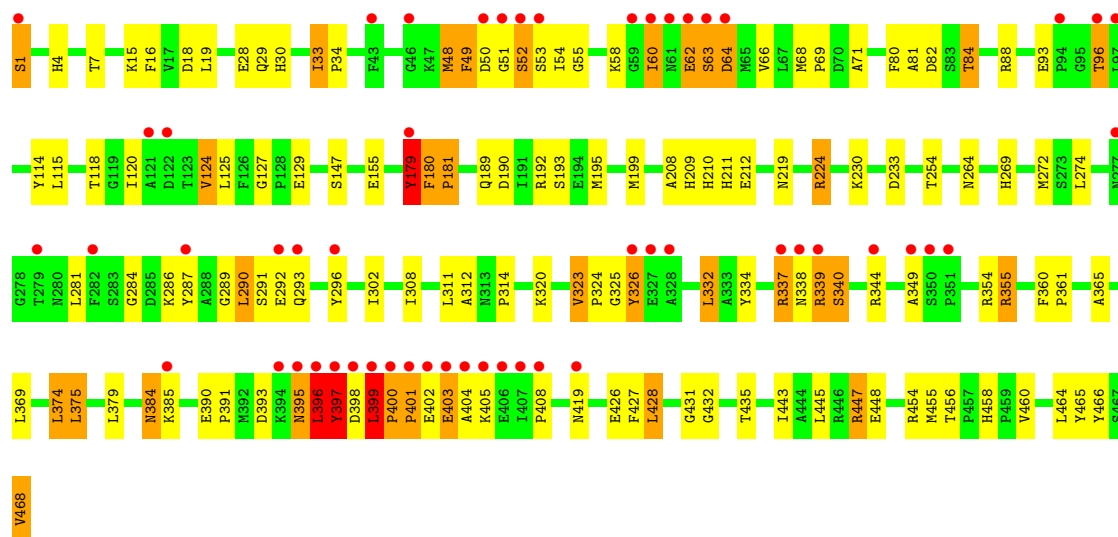


#### • Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)



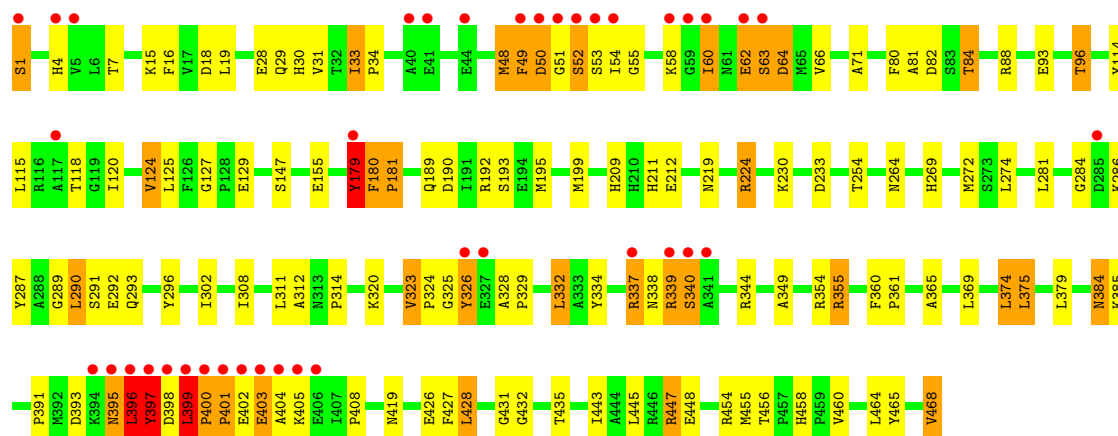
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

Chain C: 



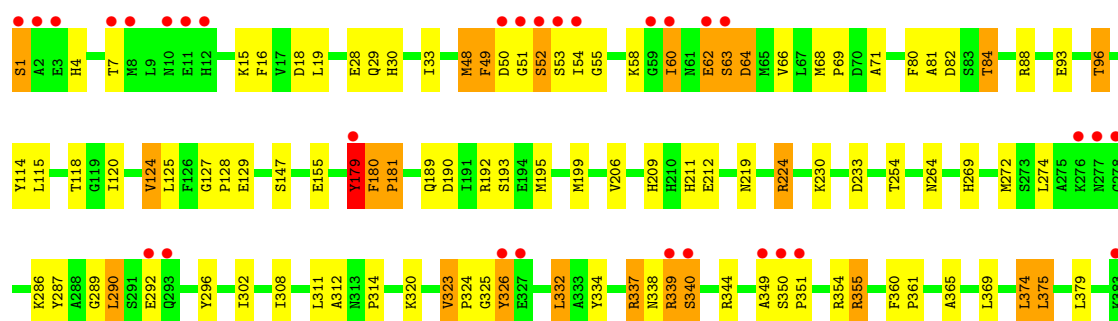
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

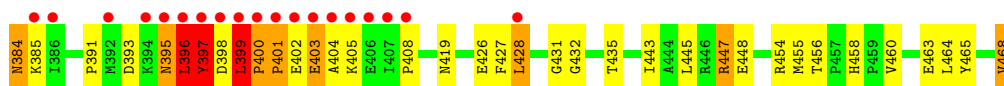
Chain D: 



• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

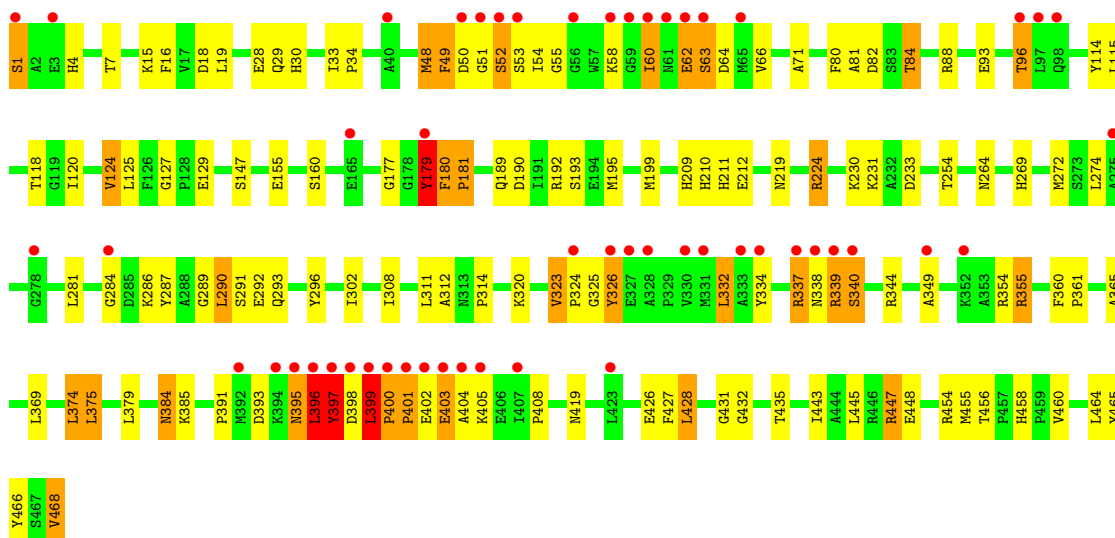
Chain E: 





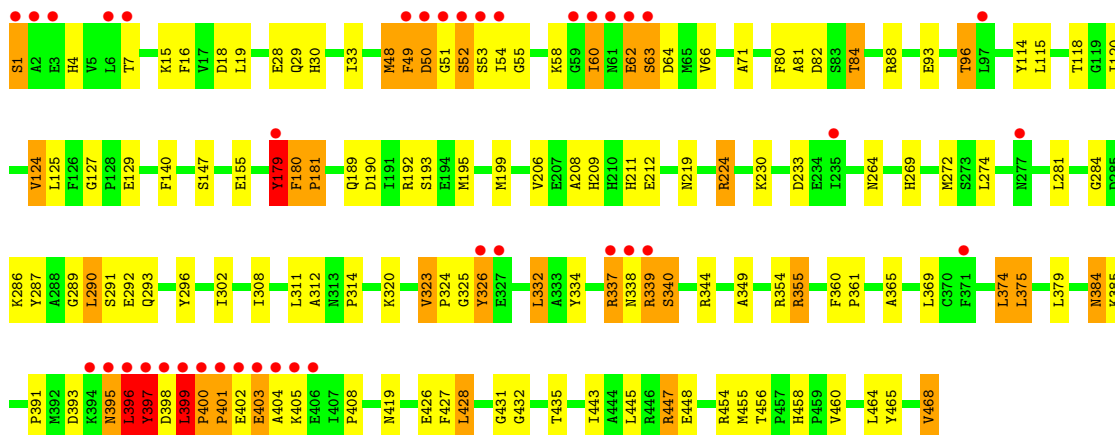
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

Chain F:



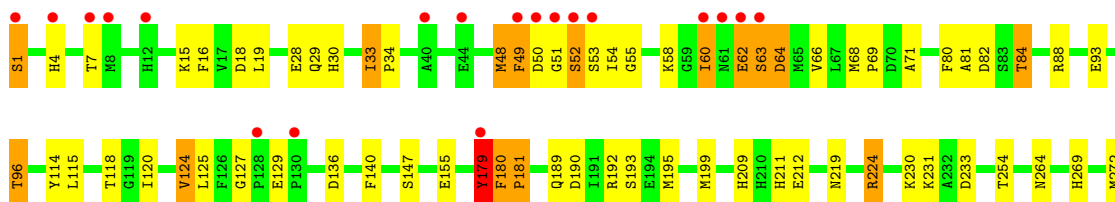
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

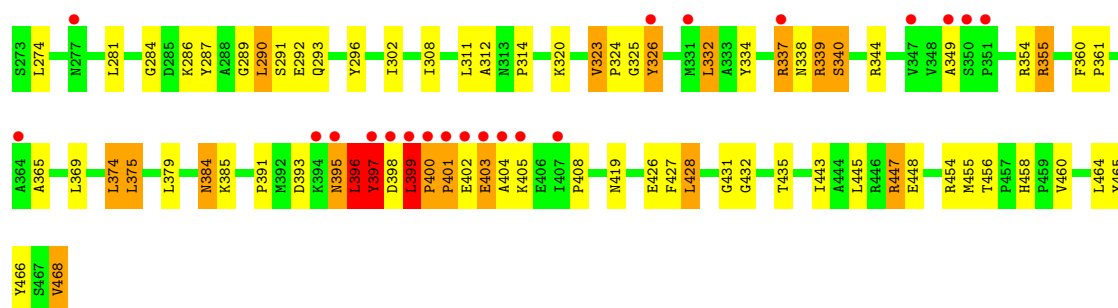
Chain G:



• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

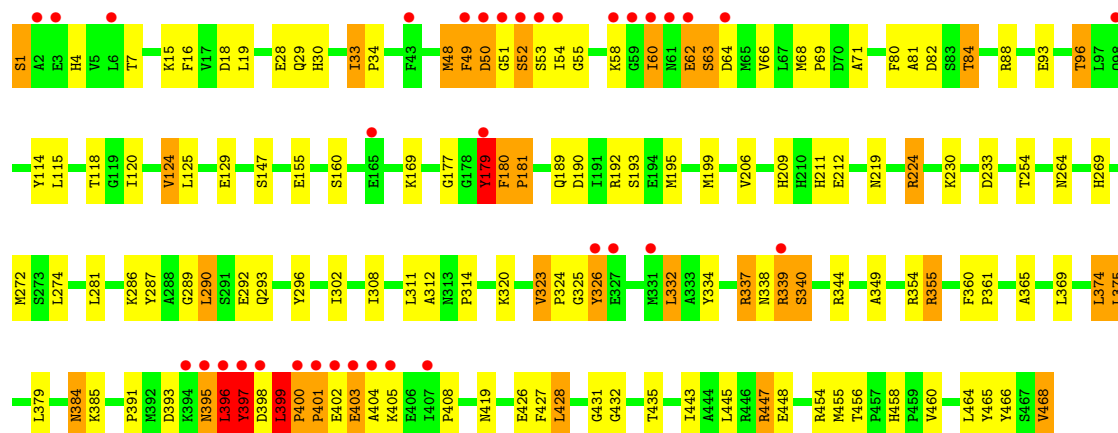
Chain H:





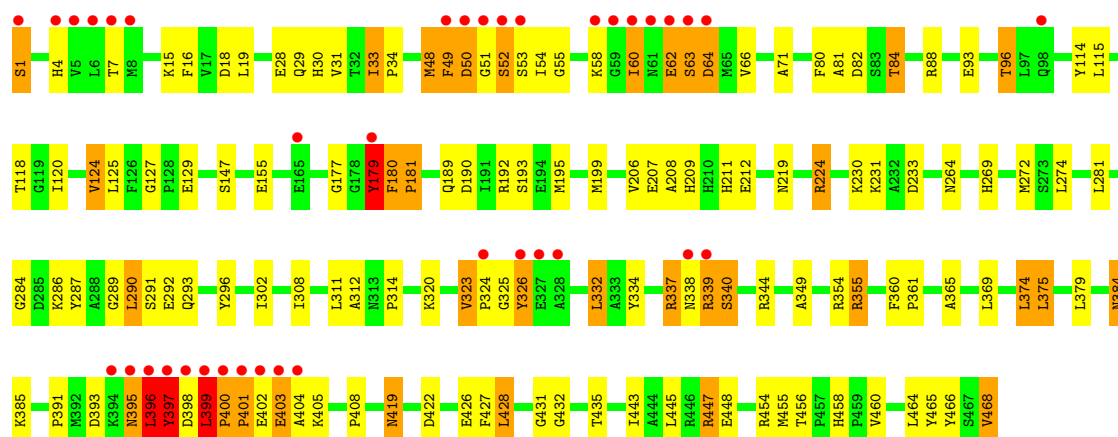
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

Chain I:



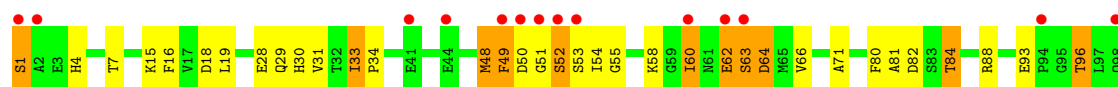
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

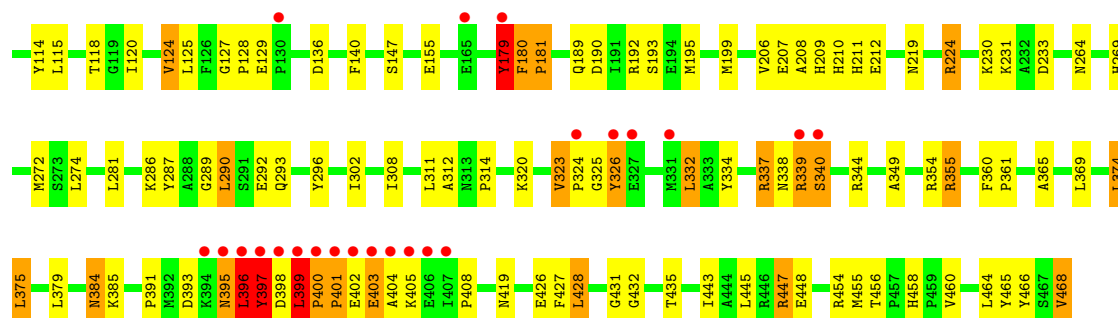
Chain J:



• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

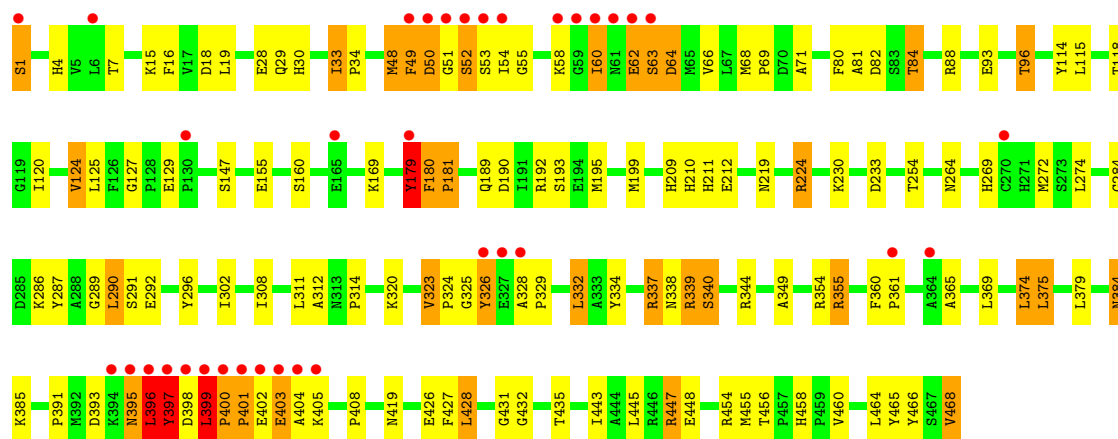
Chain K:





• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

Chain L:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.13Å 132.79Å 196.78Å 90.00° 102.44° 90.00°	Depositor
Resolution (Å)	32.00 – 2.67 36.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	82.0 (32.00-2.67) 82.0 (36.87-2.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.68Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.232 , 0.263 0.231 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.1	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 130547 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	45564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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, TL, 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	0.52	0/3724	0.85	4/5043 (0.1%)
1	B	0.52	0/3724	0.85	4/5043 (0.1%)
1	C	0.52	0/3724	0.85	4/5043 (0.1%)
1	D	0.52	0/3724	0.85	4/5043 (0.1%)
1	E	0.52	0/3724	0.85	4/5043 (0.1%)
1	F	0.52	0/3724	0.85	4/5043 (0.1%)
1	G	0.52	0/3724	0.85	4/5043 (0.1%)
1	H	0.52	0/3724	0.85	4/5043 (0.1%)
1	I	0.52	0/3724	0.85	4/5043 (0.1%)
1	J	0.52	0/3724	0.85	4/5043 (0.1%)
1	K	0.52	0/3724	0.85	4/5043 (0.1%)
1	L	0.52	0/3724	0.85	4/5043 (0.1%)
All	All	0.52	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	F	179	TYR	CB-CG-CD1	6.17	124.70	121.00
1	K	179	TYR	CB-CG-CD1	6.14	124.69	121.00
1	J	179	TYR	CB-CG-CD1	6.12	124.67	121.00
1	D	179	TYR	CB-CG-CD1	6.11	124.67	121.00
1	I	179	TYR	CB-CG-CD1	6.10	124.66	121.00

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	3542	186	0
1	B	3637	0	3543	185	0
1	C	3637	0	3543	188	0
1	D	3637	0	3542	180	0
1	E	3637	0	3543	175	0
1	F	3637	0	3543	176	0
1	G	3637	0	3542	176	0
1	H	3637	0	3543	180	0
1	I	3637	0	3542	189	0
1	J	3637	0	3543	193	0
1	K	3637	0	3543	189	0
1	L	3637	0	3543	179	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	4	0
3	B	27	0	10	4	0
3	C	27	0	10	4	0
3	D	27	0	10	4	0
3	E	27	0	10	4	0
3	F	27	0	10	4	0
3	G	27	0	10	4	0
3	H	27	0	10	4	0
3	I	27	0	10	3	0
3	J	27	0	10	4	0
3	K	27	0	10	4	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	27	0	10	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	8	0	14	29	0
5	B	8	0	14	34	0
5	C	8	0	14	33	0
5	D	8	0	14	34	0
5	E	8	0	14	29	0
5	F	8	0	14	34	0
5	G	8	0	14	31	0
5	H	8	0	14	33	0
5	I	8	0	14	35	0
5	J	8	0	14	34	0
5	K	8	0	14	33	0
5	L	8	0	14	32	0
6	A	120	0	0	6	0
6	B	121	0	0	6	0
6	C	119	0	0	5	0
6	D	122	0	0	6	0
6	E	122	0	0	6	0
6	F	121	0	0	5	0
6	G	122	0	0	6	0
6	H	121	0	0	5	0
6	I	122	0	0	6	0
6	J	120	0	0	6	0
6	K	123	0	0	6	0
6	L	119	0	0	6	0
All	All	45564	0	42800	2077	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 24.

The worst 5 of 2077 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:K:1481:ADP:C1'	3:K:1481:ADP:N9	1.71	1.54
3:I:1479:ADP:C1'	3:I:1479:ADP:N9	1.71	1.54
3:B:1472:ADP:C1'	3:B:1472:ADP:N9	1.71	1.52
3:F:1476:ADP:N9	3:F:1476:ADP:C1'	1.71	1.52
3:E:1475:ADP:N9	3:E:1475:ADP:C1'	1.71	1.51

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%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	B	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	C	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	D	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	E	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	F	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	G	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	H	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	I	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	J	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	K	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
1	L	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	12	28
All	All	5592/5616 (100%)	5148 (92%)	336 (6%)	108 (2%)	12	28

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	62	GLU
1	A	180	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	399	LEU
1	A	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%)	341 (89%)	43 (11%)	9	19
1	B	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	C	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	D	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	E	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	F	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	G	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	H	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	I	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	J	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	K	384/384 (100%)	341 (89%)	43 (11%)	9	19
1	L	384/384 (100%)	341 (89%)	43 (11%)	9	19
All	All	4608/4608 (100%)	4092 (89%)	516 (11%)	9	19

5 of 516 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	181	PRO
1	G	355	ARG
1	L	33	ILE
1	F	332	LEU
1	G	48	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	244	ASN
1	G	395	ASN
1	L	211	HIS
1	F	338	ASN
1	G	211	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 72 ligands modelled in this entry, 48 are monoatomic - leaving 24 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	1471	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	A	1483	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	B	1472	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	B	1484	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	C	1473	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	C	1485	-	7,7,7	1.02	0	10,10,10	0.63	0
3	ADP	D	1474	-	29,29,29	3.33	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	D	1486	-	7,7,7	1.00	0	10,10,10	0.63	0
3	ADP	E	1475	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MPD	E	1487	-	7,7,7	1.00	0	10,10,10	0.63	0
3	ADP	F	1476	-	29,29,29	3.33	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	F	1488	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	G	1477	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	G	1489	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	H	1478	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	H	1490	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	I	1479	-	29,29,29	3.34	13 (44%)	45,45,45	3.91	15 (33%)
5	MPD	I	1491	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	J	1480	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	J	1492	-	7,7,7	1.00	0	10,10,10	0.63	0
3	ADP	K	1481	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	K	1493	-	7,7,7	1.01	0	10,10,10	0.63	0
3	ADP	L	1482	-	29,29,29	3.34	13 (44%)	45,45,45	3.92	15 (33%)
5	MPD	L	1494	-	7,7,7	1.01	0	10,10,10	0.63	0

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	1471	-	-	0/16/32/32	0/1/3/3
5	MPD	A	1483	-	-	0/5/5/5	0/0/0/0
3	ADP	B	1472	-	-	0/16/32/32	0/1/3/3
5	MPD	B	1484	-	-	0/5/5/5	0/0/0/0
3	ADP	C	1473	-	-	0/16/32/32	0/1/3/3
5	MPD	C	1485	-	-	0/5/5/5	0/0/0/0
3	ADP	D	1474	-	-	0/16/32/32	0/1/3/3
5	MPD	D	1486	-	-	0/5/5/5	0/0/0/0
3	ADP	E	1475	-	-	0/16/32/32	0/1/3/3
5	MPD	E	1487	-	-	0/5/5/5	0/0/0/0
3	ADP	F	1476	-	-	0/16/32/32	0/1/3/3
5	MPD	F	1488	-	-	0/5/5/5	0/0/0/0
3	ADP	G	1477	-	-	0/16/32/32	0/1/3/3
5	MPD	G	1489	-	-	0/5/5/5	0/0/0/0
3	ADP	H	1478	-	-	0/16/32/32	0/1/3/3
5	MPD	H	1490	-	-	0/5/5/5	0/0/0/0
3	ADP	I	1479	-	-	0/16/32/32	0/1/3/3
5	MPD	I	1491	-	-	0/5/5/5	0/0/0/0
3	ADP	J	1480	-	-	0/16/32/32	0/1/3/3

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	J	1492	-	-	0/5/5/5	0/0/0/0
3	ADP	K	1481	-	-	0/16/32/32	0/1/3/3
5	MPD	K	1493	-	-	0/5/5/5	0/0/0/0
3	ADP	L	1482	-	-	0/16/32/32	0/1/3/3
5	MPD	L	1494	-	-	0/5/5/5	0/0/0/0

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1479	ADP	C1'-N9	7.21	1.71	1.48
3	L	1482	ADP	C1'-N9	7.20	1.71	1.48
3	D	1474	ADP	C1'-N9	7.19	1.71	1.48
3	C	1473	ADP	C1'-N9	7.19	1.71	1.48
3	H	1478	ADP	C1'-N9	7.19	1.71	1.48

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1475	ADP	O4'-C1'-N9	12.75	120.30	108.44
3	D	1474	ADP	O4'-C1'-N9	12.74	120.29	108.44
3	K	1481	ADP	O4'-C1'-N9	12.73	120.28	108.44
3	G	1477	ADP	O4'-C1'-N9	12.73	120.28	108.44
3	B	1472	ADP	O4'-C1'-N9	12.72	120.27	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%)	0.75	76 (16%) 2 2	18, 39, 91, 100	29 (6%)
1	B	468/468 (100%)	0.50	60 (12%) 4 4	18, 39, 91, 100	29 (6%)
1	C	468/468 (100%)	0.35	53 (11%) 6 5	18, 39, 91, 100	29 (6%)
1	D	468/468 (100%)	0.20	39 (8%) 11 11	18, 39, 91, 100	29 (6%)
1	E	468/468 (100%)	0.39	50 (10%) 6 6	18, 39, 91, 100	29 (6%)
1	F	468/468 (100%)	0.37	52 (11%) 6 6	18, 39, 91, 100	29 (6%)
1	G	468/468 (100%)	0.29	39 (8%) 11 11	18, 39, 91, 100	29 (6%)
1	H	468/468 (100%)	0.36	40 (8%) 11 10	18, 39, 91, 100	29 (6%)
1	I	468/468 (100%)	0.23	35 (7%) 14 14	18, 39, 91, 100	29 (6%)
1	J	468/468 (100%)	0.29	38 (8%) 12 12	18, 39, 91, 100	29 (6%)
1	K	468/468 (100%)	0.25	37 (7%) 13 13	18, 39, 91, 100	29 (6%)
1	L	468/468 (100%)	0.37	35 (7%) 14 14	18, 39, 91, 100	29 (6%)
All	All	5616/5616 (100%)	0.36	554 (9%) 8 7	18, 39, 92, 100	348 (6%)

The worst 5 of 554 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	TYR	15.5
1	L	397	TYR	14.9
1	A	397	TYR	14.0
1	A	395	ASN	14.0
1	K	397	TYR	12.3

### 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
5	MPD	L	1494	8/8	0.44	15.98	16,43,64,74	8
5	MPD	K	1493	8/8	0.39	13.14	16,43,64,74	8
5	MPD	G	1489	8/8	0.33	12.24	16,43,64,74	8
5	MPD	F	1488	8/8	0.42	11.79	16,43,64,74	8
5	MPD	C	1485	8/8	0.45	11.24	16,43,64,74	8
5	MPD	H	1490	8/8	0.38	9.98	16,43,64,74	8
5	MPD	I	1491	8/8	0.33	7.96	16,43,64,74	8
5	MPD	J	1492	8/8	0.35	7.76	16,43,64,74	8
5	MPD	B	1484	8/8	0.40	7.69	16,43,64,74	8
5	MPD	D	1486	8/8	0.36	7.17	16,43,64,74	8
5	MPD	E	1487	8/8	0.39	4.73	16,43,64,74	8
5	MPD	A	1483	8/8	0.32	4.25	16,43,64,74	8
3	ADP	L	1482	27/27	0.48	3.43	20,78,100,100	27
3	ADP	D	1474	27/27	0.47	2.97	20,78,100,100	27
3	ADP	I	1479	27/27	0.49	2.91	20,78,100,100	27
3	ADP	F	1476	27/27	0.49	2.86	20,78,100,100	27
3	ADP	B	1472	27/27	0.41	2.57	20,78,100,100	27
3	ADP	K	1481	27/27	0.41	1.78	20,78,100,100	27
3	ADP	C	1473	27/27	0.34	1.67	20,78,100,100	27
3	ADP	J	1480	27/27	0.35	1.65	20,78,100,100	27
3	ADP	H	1478	27/27	0.35	1.41	20,78,100,100	27
3	ADP	A	1471	27/27	0.38	1.15	20,78,100,100	27
3	ADP	E	1475	27/27	0.34	1.13	20,78,100,100	27
3	ADP	G	1477	27/27	0.33	1.06	20,78,100,100	27
4	TL	I	474	1/1	0.14	-0.44	75,75,75,75	1
4	TL	J	473	1/1	0.24	-0.51	67,67,67,67	1
4	TL	L	473	1/1	0.24	-0.65	67,67,67,67	1
4	TL	I	473	1/1	0.19	-0.73	67,67,67,67	1
2	MN	D	469	1/1	0.11	-0.75	34,34,34,34	0
4	TL	A	473	1/1	0.18	-0.77	67,67,67,67	1

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	TL	D	474	1/1	0.11	-0.79	75,75,75,75	1
4	TL	G	473	1/1	0.16	-0.80	67,67,67,67	1
4	TL	H	473	1/1	0.18	-0.82	67,67,67,67	1
2	MN	I	469	1/1	0.09	-0.97	34,34,34,34	0
2	MN	G	469	1/1	0.08	-0.98	34,34,34,34	0
4	TL	G	474	1/1	0.12	-1.00	75,75,75,75	1
2	MN	K	469	1/1	0.14	-1.00	34,34,34,34	0
2	MN	J	469	1/1	0.13	-1.01	34,34,34,34	0
2	MN	H	469	1/1	0.09	-1.04	34,34,34,34	0
2	MN	E	469	1/1	0.05	-1.06	34,34,34,34	0
2	MN	C	469	1/1	0.12	-1.07	34,34,34,34	0
2	MN	L	469	1/1	0.13	-1.08	34,34,34,34	0
4	TL	C	473	1/1	0.16	-1.08	67,67,67,67	1
2	MN	J	470	1/1	0.10	-1.10	41,41,41,41	0
2	MN	H	470	1/1	0.09	-1.20	41,41,41,41	0
4	TL	E	473	1/1	0.07	-1.20	67,67,67,67	1
4	TL	L	474	1/1	0.12	-1.20	75,75,75,75	1
4	TL	E	474	1/1	0.10	-1.21	75,75,75,75	1
2	MN	F	469	1/1	0.06	-1.23	34,34,34,34	0
4	TL	K	473	1/1	0.12	-1.34	67,67,67,67	1
2	MN	B	469	1/1	0.07	-1.34	34,34,34,34	0
2	MN	A	469	1/1	0.05	-1.35	34,34,34,34	0
4	TL	F	473	1/1	0.10	-1.40	67,67,67,67	1
4	TL	J	474	1/1	0.11	-1.53	75,75,75,75	1
4	TL	D	473	1/1	0.04	-1.57	67,67,67,67	1
2	MN	A	470	1/1	0.06	-1.57	41,41,41,41	0
4	TL	B	473	1/1	0.05	-1.60	67,67,67,67	1
2	MN	I	470	1/1	0.14	-1.74	41,41,41,41	0
2	MN	D	470	1/1	0.11	-1.77	41,41,41,41	0
4	TL	K	474	1/1	0.13	-1.78	75,75,75,75	1
2	MN	C	470	1/1	0.04	-1.98	41,41,41,41	0
4	TL	A	474	1/1	0.07	-2.77	75,75,75,75	1
4	TL	H	474	1/1	0.04	-2.83	75,75,75,75	1
2	MN	L	470	1/1	0.18	-2.88	41,41,41,41	0
2	MN	F	470	1/1	0.05	-3.60	41,41,41,41	0
2	MN	K	470	1/1	0.16	-3.91	41,41,41,41	0
4	TL	F	474	1/1	0.03	-3.93	75,75,75,75	1
2	MN	E	470	1/1	0.09	-4.10	41,41,41,41	0
2	MN	B	470	1/1	0.04	-4.14	41,41,41,41	0
2	MN	G	470	1/1	0.13	-4.49	41,41,41,41	0
4	TL	B	474	1/1	0.09	-4.71	75,75,75,75	1
4	TL	C	474	1/1	0.04	-4.89	75,75,75,75	1

## 6.5 Other polymers ⓘ

There are no such residues in this entry.