



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 05:39 am GMT

PDB ID : 1FPY
Title : CRYSTAL STRUCTURE OF GLUTAMINE SYNTHETASE FROM
SALMONELLA TYPHIMURIUM WITH INHIBITOR PHOS-
PHINOTHRICIN
Authors : Gill, H.S.; Eisenberg, D.
Deposited on : 2000-08-31
Resolution : 2.89 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

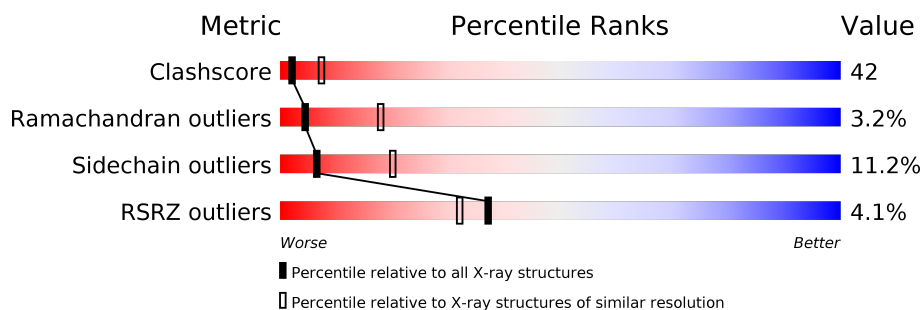
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	468	<div> <div>6%</div> <div>50% 41% 8%</div> </div>
1	B	468	<div> <div>4%</div> <div>52% 40% 8%</div> </div>
1	C	468	<div> <div>4%</div> <div>50% 41% 8%</div> </div>
1	D	468	<div> <div>4%</div> <div>51% 40% 8%</div> </div>
1	E	468	<div> <div>3%</div> <div>50% 41% 8%</div> </div>
1	F	468	<div> <div>5%</div> <div>52% 40% 8%</div> </div>
1	G	468	<div> <div>4%</div> <div>51% 41% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	468	
1	I	468	
1	J	468	
1	K	468	
1	L	468	

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
3	ADP	L	4482	-	-	-	X
4	PPQ	A	5900	-	-	X	-
4	PPQ	B	5901	-	-	X	-
4	PPQ	C	5902	-	-	X	-
4	PPQ	D	5903	-	-	X	-
4	PPQ	E	5904	-	-	X	-
4	PPQ	F	5905	-	-	X	-
4	PPQ	G	5906	-	-	X	-
4	PPQ	H	5907	-	-	X	-
4	PPQ	I	5908	-	-	X	-
4	PPQ	J	5909	-	-	X	-
4	PPQ	L	5911	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 47280 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	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	B	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	C	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	D	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	E	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	F	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	G	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	H	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	I	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	J	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	K	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			
1	L	468	Total	C	N	O	S	0	26	0
			3747	2371	643	713	20			

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

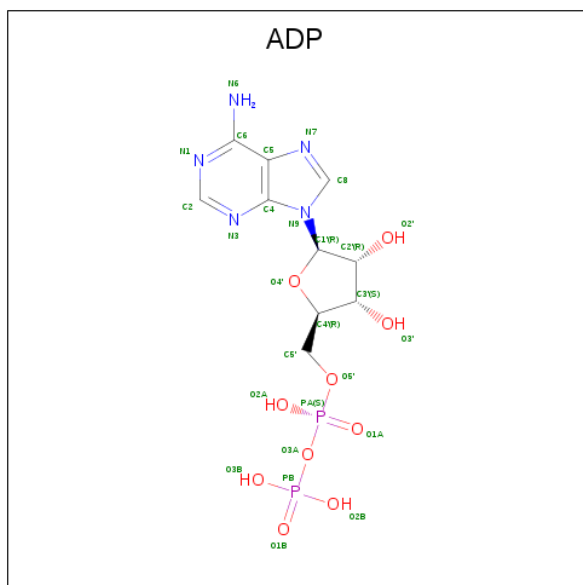
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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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: $C_{10}H_{15}N_5O_{10}P_2$).



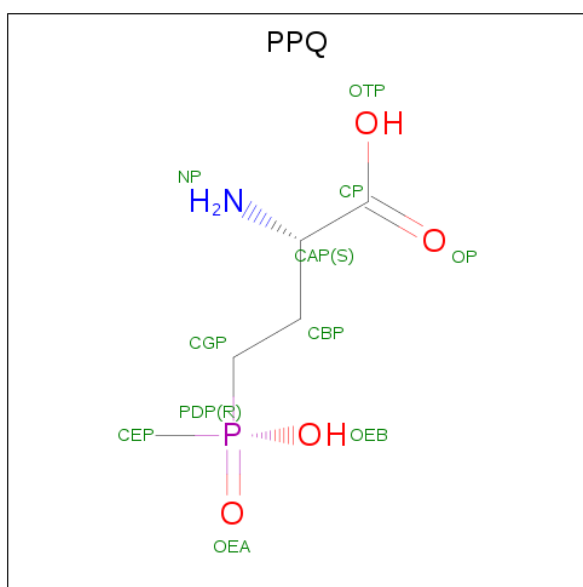
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	
			27	10	5	10	2	

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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 PHOSPHINOTHRICIN (three-letter code: PPQ) (formula: $C_5H_{12}NO_4P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	B	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	C	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	D	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	E	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	F	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	G	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	H	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	I	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	J	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	K	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
4	L	1	Total	C	N	O	P	0	0
			11	5	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total	O	0	0
			152	152		
5	B	155	Total	O	0	0
			155	155		
5	C	152	Total	O	0	0
			152	152		
5	D	153	Total	O	0	0
			153	153		
5	E	154	Total	O	0	0
			154	154		
5	F	152	Total	O	0	0
			152	152		
5	G	155	Total	O	0	0
			155	155		
5	H	150	Total	O	0	0
			150	150		

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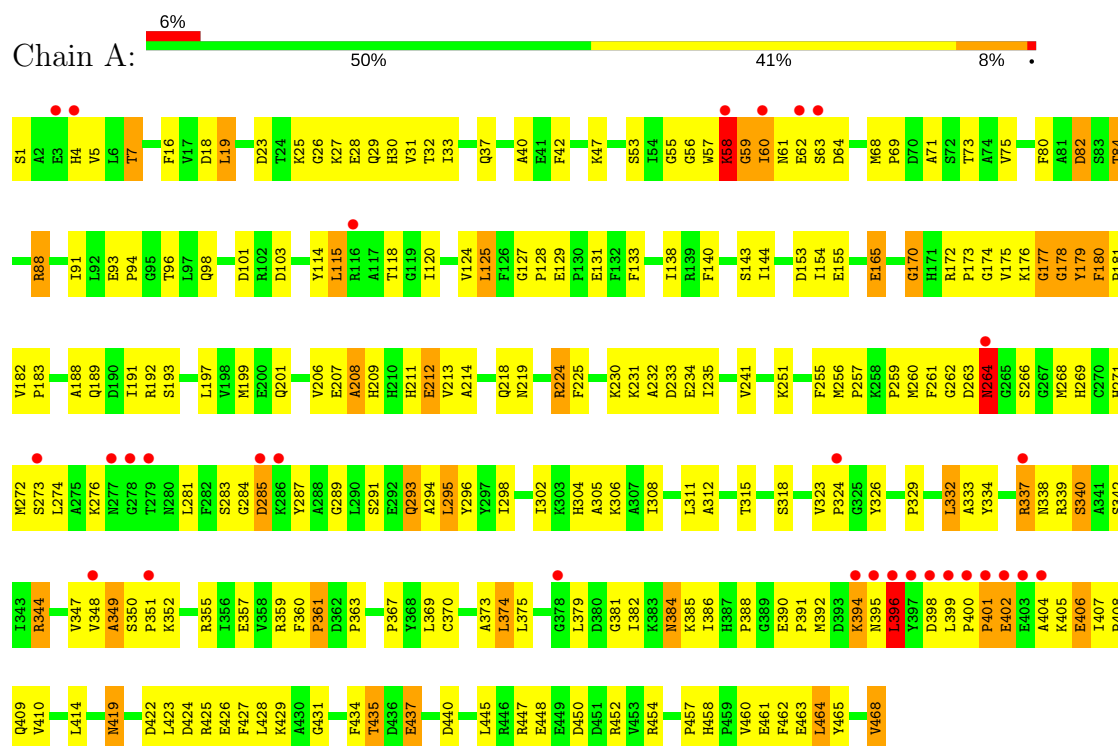
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	156	Total 156	O 156	0	0
5	J	151	Total 151	O 151	0	0
5	K	153	Total 153	O 153	0	0
5	L	153	Total 153	O 153	0	0

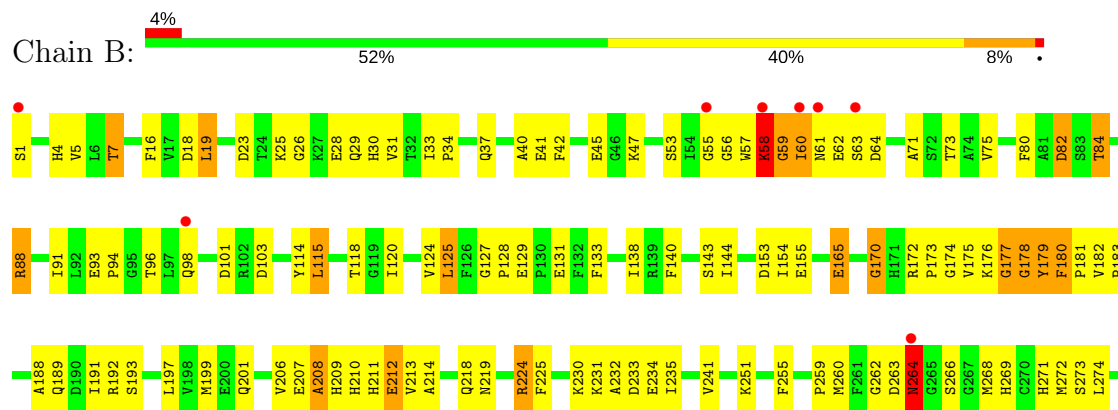
3 Residue-property plots

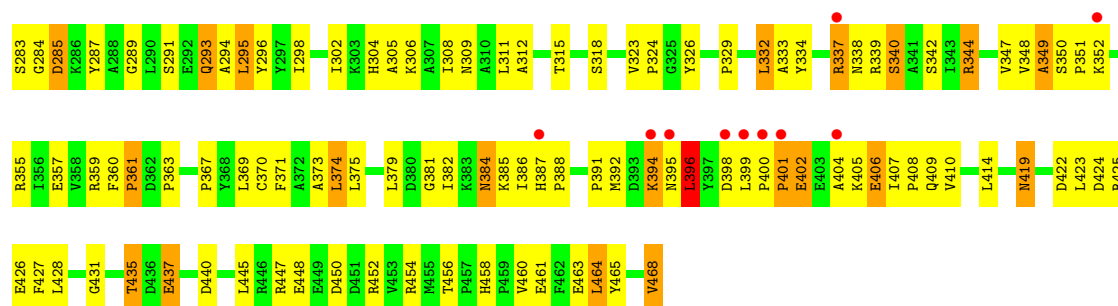
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: GLUTAMINE SYNTHETASE

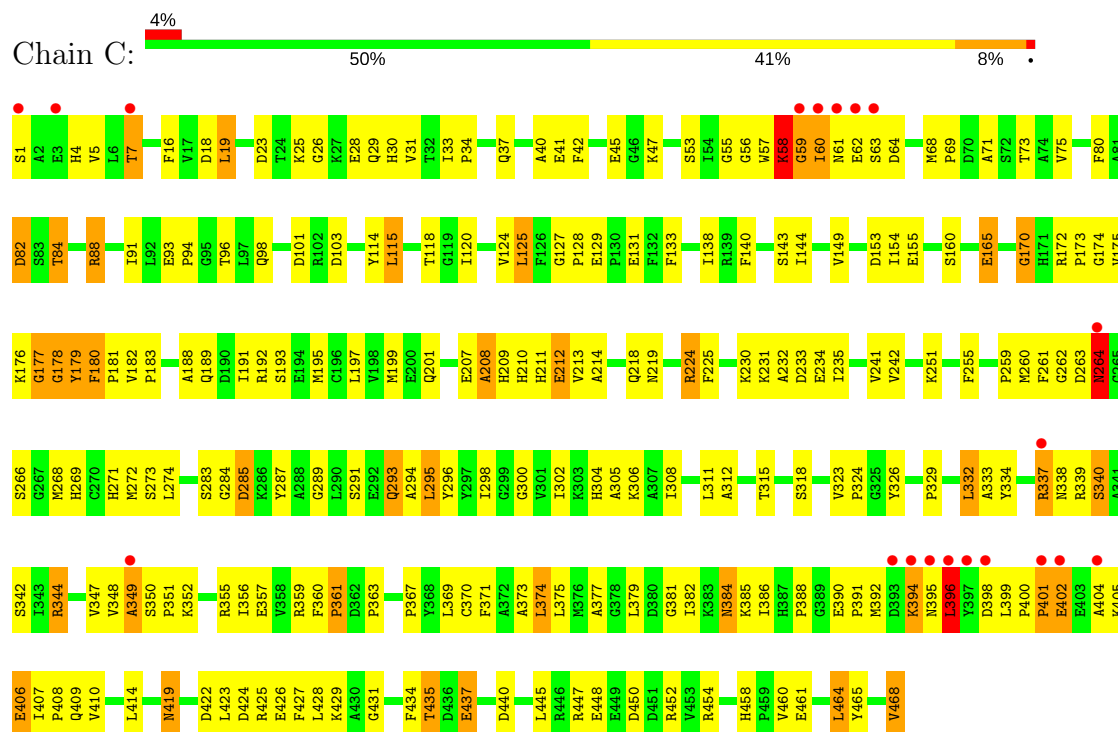


• Molecule 1: GLUTAMINE SYNTHETASE

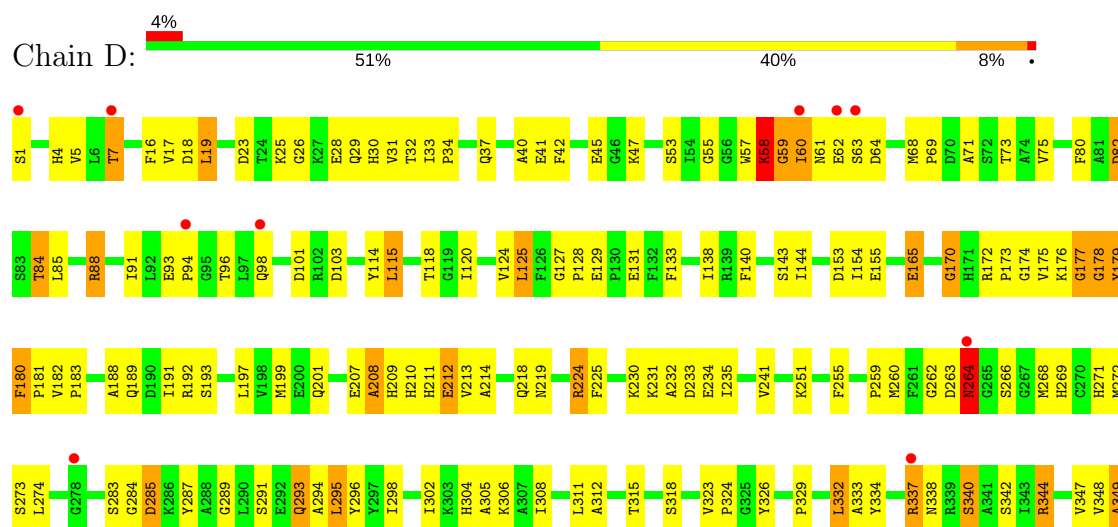


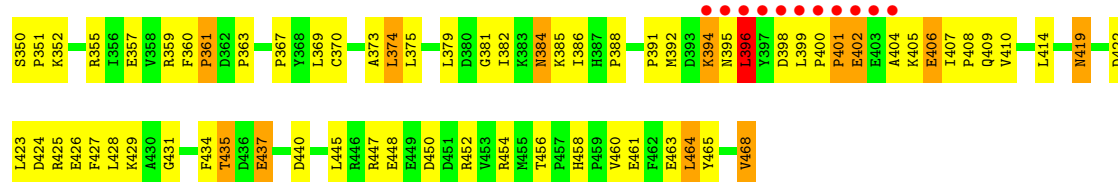


• Molecule 1: GLUTAMINE SYNTHETASE

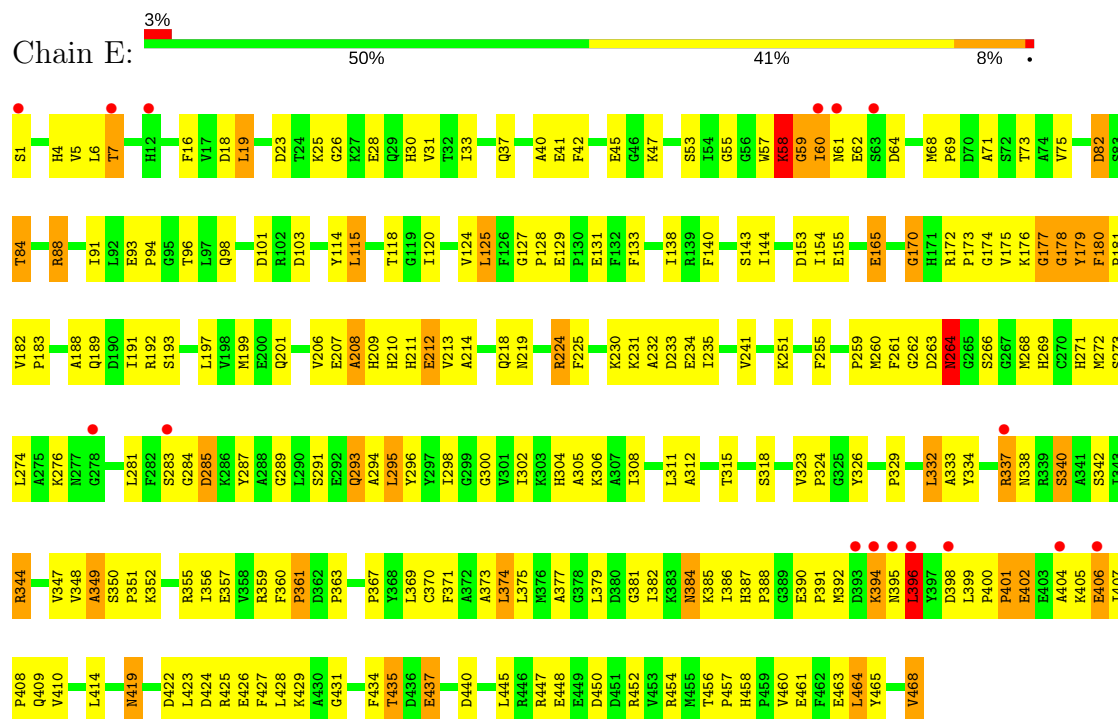


• Molecule 1: GLUTAMINE SYNTHETASE

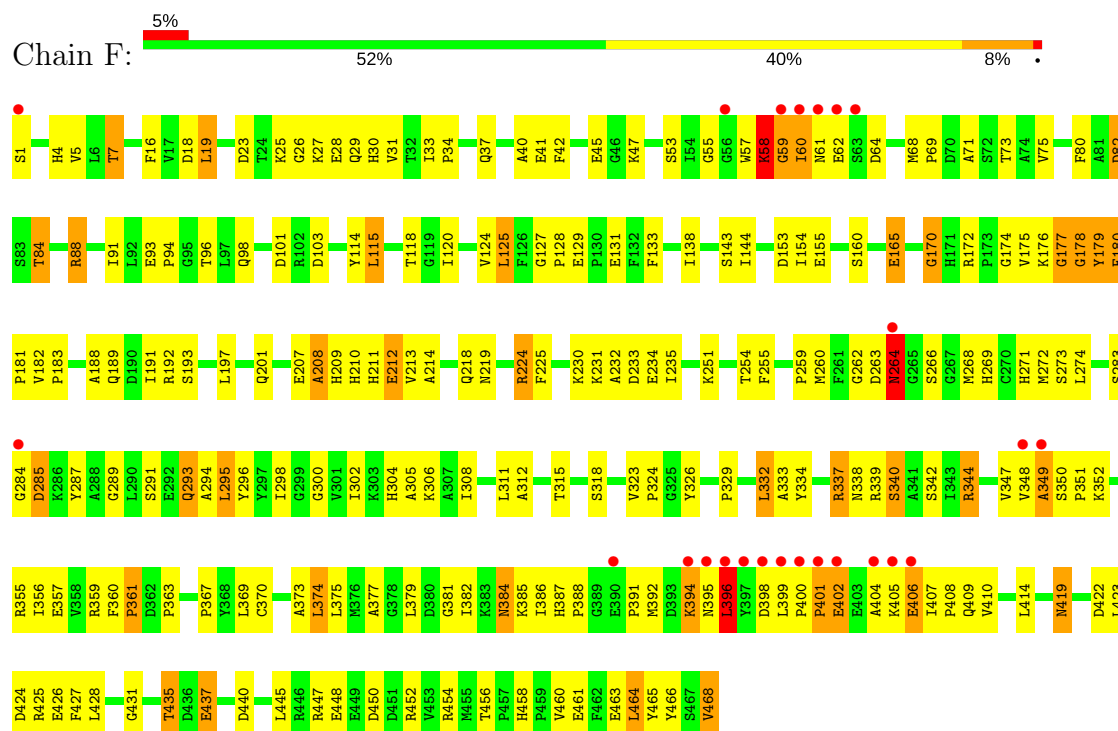




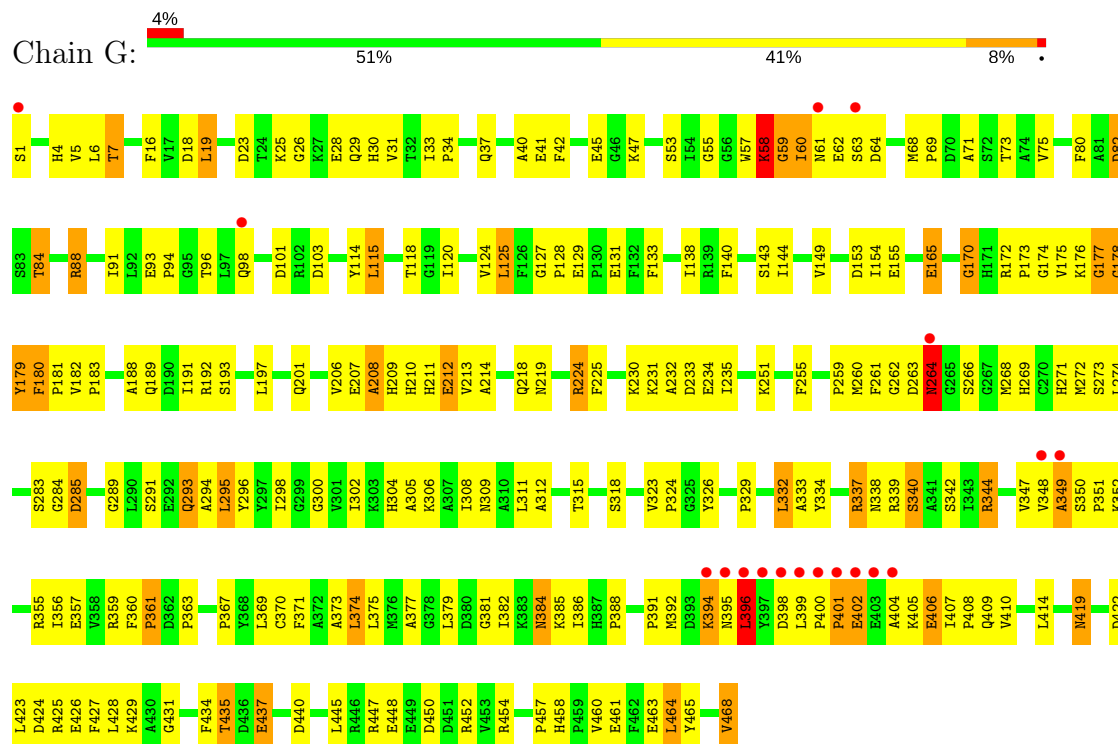
• Molecule 1: GLUTAMINE SYNTHETASE



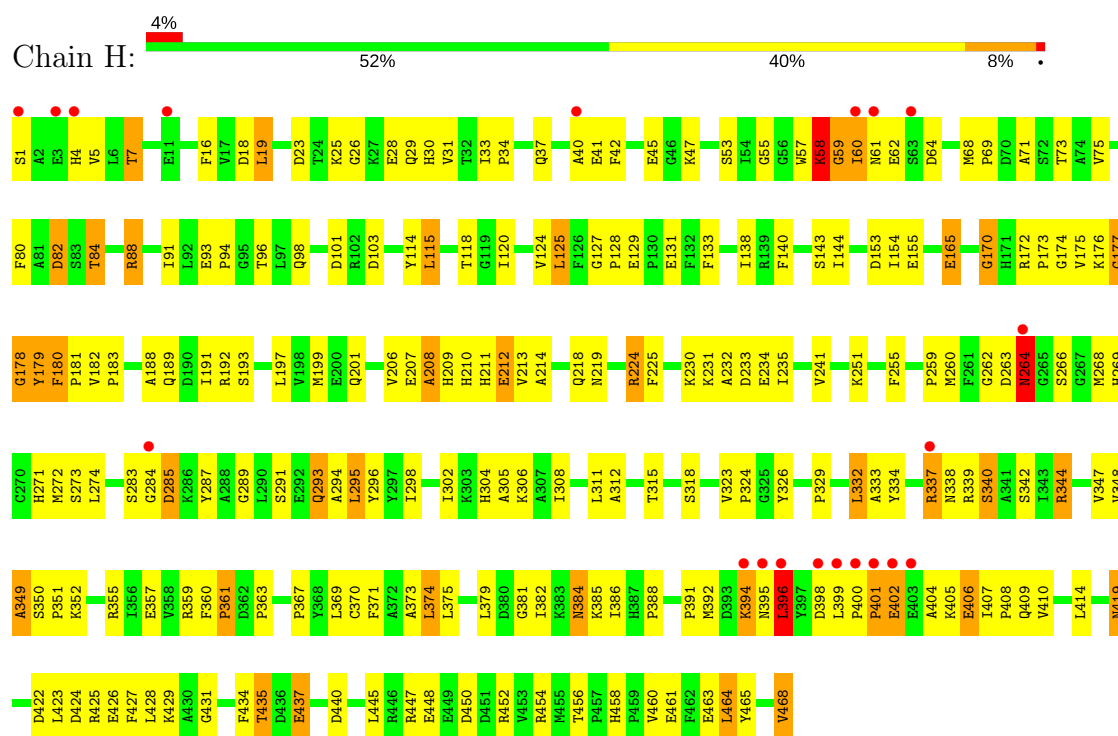
• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE

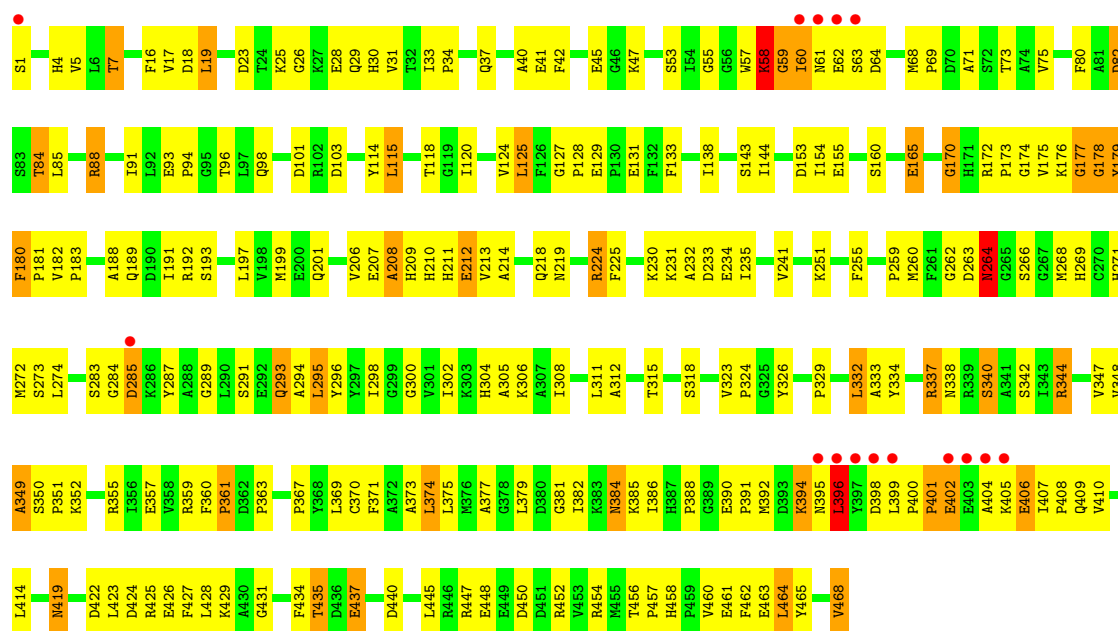


• Molecule 1: GLUTAMINE SYNTHETASE

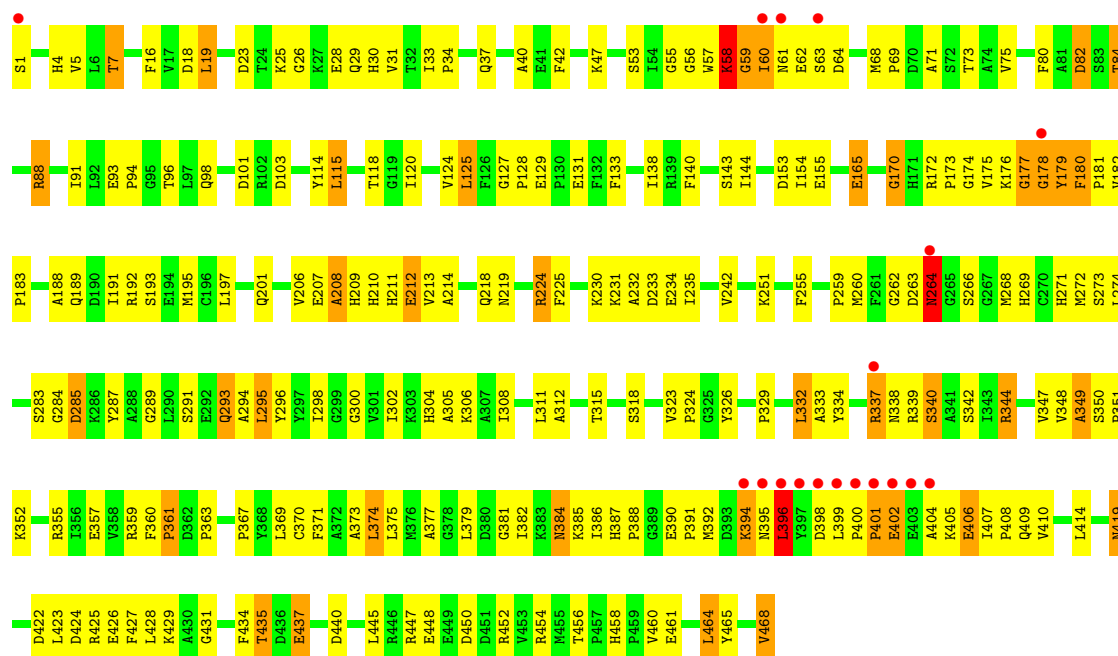


• Molecule 1: GLUTAMINE SYNTHETASE



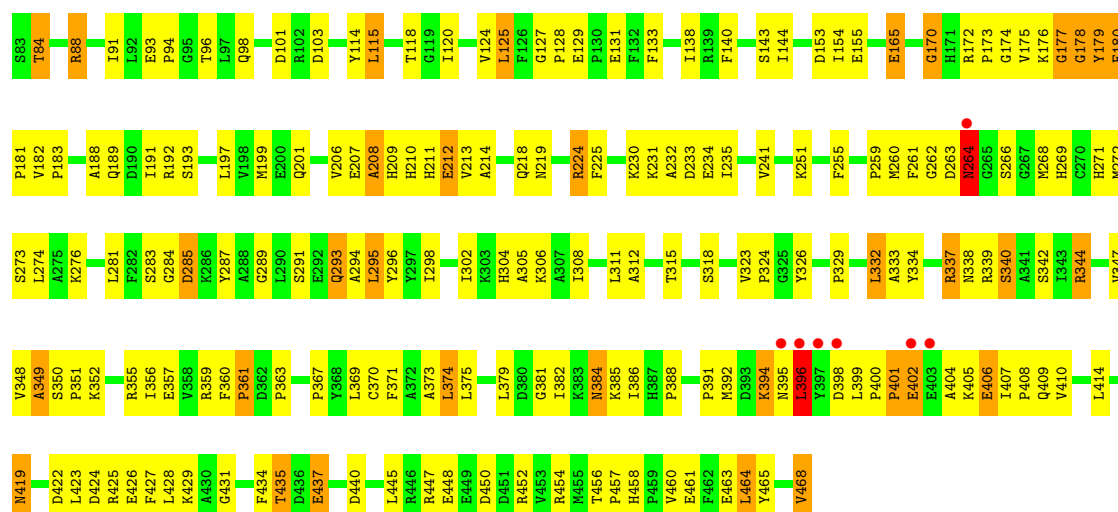


• Molecule 1: GLUTAMINE SYNTHETASE

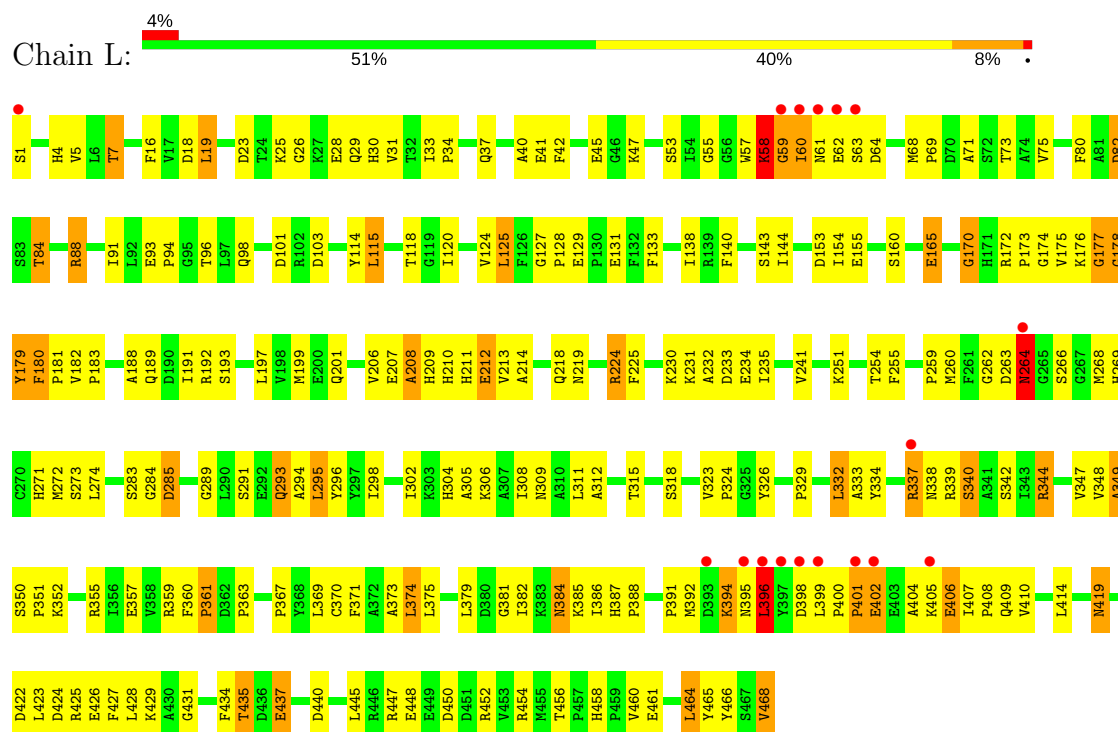


• Molecule 1: GLUTAMINE SYNTHETASE





• Molecule 1: GLUTAMINE SYNTHETASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	230.60Å 132.50Å 195.90Å 90.00° 102.40° 90.00°	Depositor
Resolution (Å)	15.00 – 2.89 15.00 – 2.89	Depositor EDS
% Data completeness (in resolution range)	70.0 (15.00-2.89) 68.7 (15.00-2.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.91Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.248 , 0.263 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47280	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PPQ, 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	0.63	0/3850	0.90	2/5212 (0.0%)
1	B	0.63	0/3850	0.90	2/5212 (0.0%)
1	C	0.63	0/3850	0.90	2/5212 (0.0%)
1	D	0.63	0/3850	0.90	2/5212 (0.0%)
1	E	0.63	0/3850	0.90	2/5212 (0.0%)
1	F	0.63	0/3850	0.90	2/5212 (0.0%)
1	G	0.63	0/3850	0.90	2/5212 (0.0%)
1	H	0.63	0/3850	0.90	2/5212 (0.0%)
1	I	0.63	0/3850	0.90	2/5212 (0.0%)
1	J	0.63	0/3850	0.90	2/5212 (0.0%)
1	K	0.63	0/3850	0.90	2/5212 (0.0%)
1	L	0.63	0/3850	0.90	2/5212 (0.0%)
All	All	0.63	0/46200	0.90	24/62544 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
All	All	0	12

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179[A]	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	B	179[B]	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	J	179[A]	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	J	179[B]	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	C	179[A]	TYR	CB-CG-CD2	-5.66	117.60	121.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ALA	Mainchain
1	B	208	ALA	Mainchain
1	C	208	ALA	Mainchain
1	D	208	ALA	Mainchain
1	E	208	ALA	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3747	0	3621	330	0
1	B	3747	0	3621	325	0
1	C	3747	0	3621	330	0
1	D	3747	0	3621	320	0
1	E	3747	0	3621	322	0
1	F	3747	0	3621	325	0
1	G	3747	0	3621	328	0
1	H	3747	0	3621	324	0
1	I	3747	0	3621	334	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3747	0	3621	333	0
1	K	3747	0	3621	328	0
1	L	3747	0	3621	323	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	8	0
3	B	27	0	10	8	0
3	C	27	0	10	8	0
3	D	27	0	10	8	0
3	E	27	0	10	8	0
3	F	27	0	10	8	0
3	G	27	0	10	8	0
3	H	27	0	10	8	0
3	I	27	0	10	8	0
3	J	27	0	10	8	0
3	K	27	0	10	8	0
3	L	27	0	10	8	0
4	A	11	0	10	7	0
4	B	11	0	10	7	0
4	C	11	0	10	6	0
4	D	11	0	10	6	0
4	E	11	0	10	6	0
4	F	11	0	10	7	0
4	G	11	0	10	6	0
4	H	11	0	10	7	0
4	I	11	0	10	6	0
4	J	11	0	10	6	0
4	K	11	0	10	5	0
4	L	11	0	10	7	0
5	A	152	0	0	89	0
5	B	155	0	0	91	0
5	C	152	0	0	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	153	0	0	85	0
5	E	154	0	0	91	0
5	F	152	0	0	91	0
5	G	155	0	0	91	0
5	H	150	0	0	88	0
5	I	156	0	0	92	0
5	J	151	0	0	90	0
5	K	153	0	0	85	0
5	L	153	0	0	90	0
All	All	47280	0	43692	3738	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 42.

The worst 5 of 3738 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:L:4482:ADP:C1'	3:L:4482:ADP:N9	1.70	1.54
3:C:4473:ADP:N9	3:C:4473:ADP:C1'	1.70	1.53
3:I:4479:ADP:N9	3:I:4479:ADP:C1'	1.70	1.53
3:H:4478:ADP:N9	3:H:4478:ADP:C1'	1.70	1.52
3:B:4472:ADP:C1'	3:B:4472:ADP:N9	1.70	1.52

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	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	B	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	D	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	E	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	F	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	G	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	H	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	I	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	J	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	K	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
1	L	482/468 (103%)	411 (85%)	50 (10%)	21 (4%)	3	11
All	All	5784/5616 (103%)	4932 (85%)	600 (10%)	252 (4%)	4	11

5 of 252 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	177[A]	GLY
1	A	177[B]	GLY
1	A	180[A]	PHE
1	A	180[B]	PHE

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	395/384 (103%)	350 (89%)	45 (11%)	6	19
1	B	395/384 (103%)	350 (89%)	45 (11%)	6	19
1	C	395/384 (103%)	350 (89%)	45 (11%)	6	19
1	D	395/384 (103%)	350 (89%)	45 (11%)	6	19
1	E	395/384 (103%)	350 (89%)	45 (11%)	6	19
1	F	395/384 (103%)	350 (89%)	45 (11%)	6	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	395/384 (103%)	350 (89%)	45 (11%)	6	19
1	H	395/384 (103%)	350 (89%)	45 (11%)	6	19
1	I	395/384 (103%)	350 (89%)	45 (11%)	6	19
1	J	395/384 (103%)	350 (89%)	45 (11%)	6	19
1	K	395/384 (103%)	350 (89%)	45 (11%)	6	19
1	L	395/384 (103%)	350 (89%)	45 (11%)	6	19
All	All	4740/4608 (103%)	4200 (89%)	540 (11%)	6	19

5 of 540 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	264[B]	ASN
1	G	384	ASN
1	L	58	LYS
1	F	337	ARG
1	G	58	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	218	GLN
1	G	277	ASN
1	L	29[A]	GLN
1	F	219	ASN
1	F	458	HIS

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 48 ligands modelled in this entry, 24 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	4471	2	25,29,29	3.40	10 (40%)	25,45,45	3.24	9 (36%)
4	PPQ	A	5900	2	2,10,10	1.68	0	2,14,14	8.52	2 (100%)
3	ADP	B	4472	2	25,29,29	3.39	10 (40%)	25,45,45	3.24	10 (40%)
4	PPQ	B	5901	2	2,10,10	1.67	0	2,14,14	8.53	2 (100%)
3	ADP	C	4473	2	25,29,29	3.40	10 (40%)	25,45,45	3.24	9 (36%)
4	PPQ	C	5902	2	2,10,10	1.69	0	2,14,14	8.52	2 (100%)
3	ADP	D	4474	2	25,29,29	3.40	10 (40%)	25,45,45	3.23	9 (36%)
4	PPQ	D	5903	2	2,10,10	1.68	0	2,14,14	8.52	2 (100%)
3	ADP	E	4475	2	25,29,29	3.40	10 (40%)	25,45,45	3.24	10 (40%)
4	PPQ	E	5904	2	2,10,10	1.69	0	2,14,14	8.53	2 (100%)
3	ADP	F	4476	2	25,29,29	3.39	10 (40%)	25,45,45	3.24	10 (40%)
4	PPQ	F	5905	2	2,10,10	1.66	0	2,14,14	8.52	2 (100%)
3	ADP	G	4477	2	25,29,29	3.40	10 (40%)	25,45,45	3.24	9 (36%)
4	PPQ	G	5906	2	2,10,10	1.67	0	2,14,14	8.53	2 (100%)
3	ADP	H	4478	2	25,29,29	3.39	10 (40%)	25,45,45	3.24	9 (36%)
4	PPQ	H	5907	2	2,10,10	1.70	0	2,14,14	8.54	2 (100%)
3	ADP	I	4479	2	25,29,29	3.40	10 (40%)	25,45,45	3.24	9 (36%)
4	PPQ	I	5908	2	2,10,10	1.72	0	2,14,14	8.53	2 (100%)
3	ADP	J	4480	2	25,29,29	3.39	10 (40%)	25,45,45	3.24	10 (40%)
4	PPQ	J	5909	2	2,10,10	1.69	0	2,14,14	8.53	2 (100%)
3	ADP	K	4481	2	25,29,29	3.40	10 (40%)	25,45,45	3.25	10 (40%)
4	PPQ	K	5910	2	2,10,10	1.62	0	2,14,14	8.51	2 (100%)
3	ADP	L	4482	2	25,29,29	3.41	10 (40%)	25,45,45	3.24	10 (40%)
4	PPQ	L	5911	2	2,10,10	1.66	0	2,14,14	8.53	2 (100%)

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	-	0/12/32/32	0/3/3/3
4	PPQ	A	5900	2	-	0/6/10/10	0/0/0/0
3	ADP	B	4472	2	-	0/12/32/32	0/3/3/3
4	PPQ	B	5901	2	-	0/6/10/10	0/0/0/0
3	ADP	C	4473	2	-	0/12/32/32	0/3/3/3
4	PPQ	C	5902	2	-	0/6/10/10	0/0/0/0
3	ADP	D	4474	2	-	0/12/32/32	0/3/3/3
4	PPQ	D	5903	2	-	0/6/10/10	0/0/0/0
3	ADP	E	4475	2	-	0/12/32/32	0/3/3/3
4	PPQ	E	5904	2	-	0/6/10/10	0/0/0/0
3	ADP	F	4476	2	-	0/12/32/32	0/3/3/3
4	PPQ	F	5905	2	-	0/6/10/10	0/0/0/0
3	ADP	G	4477	2	-	0/12/32/32	0/3/3/3
4	PPQ	G	5906	2	-	0/6/10/10	0/0/0/0
3	ADP	H	4478	2	-	0/12/32/32	0/3/3/3
4	PPQ	H	5907	2	-	0/6/10/10	0/0/0/0
3	ADP	I	4479	2	-	0/12/32/32	0/3/3/3
4	PPQ	I	5908	2	-	0/6/10/10	0/0/0/0
3	ADP	J	4480	2	-	0/12/32/32	0/3/3/3
4	PPQ	J	5909	2	-	0/6/10/10	0/0/0/0
3	ADP	K	4481	2	-	0/12/32/32	0/3/3/3
4	PPQ	K	5910	2	-	0/6/10/10	0/0/0/0
3	ADP	L	4482	2	-	0/12/32/32	0/3/3/3
4	PPQ	L	5911	2	-	0/6/10/10	0/0/0/0

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	4479	ADP	C6-N6	-2.88	1.22	1.34
3	E	4475	ADP	C6-N6	-2.88	1.22	1.34
3	D	4474	ADP	C6-N6	-2.88	1.22	1.34
3	J	4480	ADP	C6-N6	-2.87	1.22	1.34
3	B	4472	ADP	C6-N6	-2.87	1.22	1.34

The worst 5 of 138 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	4478	ADP	C4'-O4'-C1'	-8.59	100.87	109.83
3	I	4479	ADP	C4'-O4'-C1'	-8.59	100.88	109.83
3	E	4475	ADP	C4'-O4'-C1'	-8.59	100.88	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	4482	ADP	C4'-O4'-C1'	-8.57	100.89	109.83
3	K	4481	ADP	C4'-O4'-C1'	-8.57	100.90	109.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 172 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4471	ADP	8	0
4	A	5900	PPQ	7	0
3	B	4472	ADP	8	0
4	B	5901	PPQ	7	0
3	C	4473	ADP	8	0
4	C	5902	PPQ	6	0
3	D	4474	ADP	8	0
4	D	5903	PPQ	6	0
3	E	4475	ADP	8	0
4	E	5904	PPQ	6	0
3	F	4476	ADP	8	0
4	F	5905	PPQ	7	0
3	G	4477	ADP	8	0
4	G	5906	PPQ	6	0
3	H	4478	ADP	8	0
4	H	5907	PPQ	7	0
3	I	4479	ADP	8	0
4	I	5908	PPQ	6	0
3	J	4480	ADP	8	0
4	J	5909	PPQ	6	0
3	K	4481	ADP	8	0
4	K	5910	PPQ	5	0
3	L	4482	ADP	8	0
4	L	5911	PPQ	7	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	468/468 (100%)	0.10	30 (6%)	19	15	20, 47, 80, 100	94 (20%)
1	B	468/468 (100%)	-0.16	18 (3%)	40	35	20, 47, 80, 100	94 (20%)
1	C	468/468 (100%)	-0.19	20 (4%)	35	30	20, 47, 80, 100	94 (20%)
1	D	468/468 (100%)	-0.29	21 (4%)	33	29	20, 47, 80, 100	94 (20%)
1	E	468/468 (100%)	-0.22	16 (3%)	45	39	20, 47, 80, 100	94 (20%)
1	F	468/468 (100%)	-0.16	24 (5%)	28	23	20, 47, 80, 100	94 (20%)
1	G	468/468 (100%)	-0.30	18 (3%)	40	35	20, 47, 80, 100	94 (20%)
1	H	468/468 (100%)	-0.25	20 (4%)	35	30	20, 47, 80, 100	94 (20%)
1	I	468/468 (100%)	-0.36	15 (3%)	47	42	20, 47, 80, 100	94 (20%)
1	J	468/468 (100%)	-0.26	18 (3%)	40	35	20, 47, 80, 100	94 (20%)
1	K	468/468 (100%)	-0.35	11 (2%)	59	56	20, 47, 80, 100	94 (20%)
1	L	468/468 (100%)	-0.30	17 (3%)	42	37	20, 47, 80, 100	94 (20%)
All	All	5616/5616 (100%)	-0.23	228 (4%)	37	32	20, 47, 81, 100	1128 (20%)

The worst 5 of 228 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	396	LEU	10.3
1	F	396	LEU	8.7
1	L	396	LEU	7.7
1	D	395	ASN	7.4
1	J	60	ILE	7.3

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADP	L	4482	27/27	0.73	0.42	42,80,100,100	27
3	ADP	C	4473	27/27	0.76	0.36	42,80,100,100	27
3	ADP	I	4479	27/27	0.78	0.36	42,80,100,100	27
3	ADP	K	4481	27/27	0.78	0.35	42,80,100,100	27
3	ADP	E	4475	27/27	0.79	0.39	42,80,100,100	27
3	ADP	H	4478	27/27	0.81	0.32	42,80,100,100	27
3	ADP	B	4472	27/27	0.82	0.31	42,80,100,100	27
3	ADP	F	4476	27/27	0.82	0.41	42,80,100,100	27
3	ADP	J	4480	27/27	0.84	0.30	42,80,100,100	27
3	ADP	A	4471	27/27	0.84	0.35	42,80,100,100	27
3	ADP	G	4477	27/27	0.84	0.28	42,80,100,100	27
3	ADP	D	4474	27/27	0.88	0.34	42,80,100,100	27
2	MN	H	470	1/1	0.91	0.07	43,43,43,43	0
4	PPQ	B	5901	11/11	0.91	0.20	16,36,70,83	11
4	PPQ	F	5905	11/11	0.92	0.20	16,36,70,83	11
2	MN	C	469	1/1	0.92	0.07	41,41,41,41	0
2	MN	G	469	1/1	0.92	0.08	41,41,41,41	0
4	PPQ	H	5907	11/11	0.93	0.20	16,36,70,83	11
2	MN	D	469	1/1	0.93	0.07	41,41,41,41	0
4	PPQ	I	5908	11/11	0.93	0.22	16,36,70,83	11
4	PPQ	G	5906	11/11	0.93	0.17	16,36,70,83	11
4	PPQ	D	5903	11/11	0.93	0.19	16,36,70,83	11
4	PPQ	C	5902	11/11	0.94	0.16	16,36,70,83	11
4	PPQ	K	5910	11/11	0.94	0.17	16,36,70,83	11
4	PPQ	E	5904	11/11	0.94	0.15	16,36,70,83	11
4	PPQ	A	5900	11/11	0.95	0.16	16,36,70,83	11
4	PPQ	J	5909	11/11	0.95	0.19	16,36,70,83	11
2	MN	E	469	1/1	0.95	0.04	41,41,41,41	0
4	PPQ	L	5911	11/11	0.95	0.21	16,36,70,83	11
2	MN	H	469	1/1	0.96	0.10	41,41,41,41	0
2	MN	A	469	1/1	0.97	0.06	41,41,41,41	0
2	MN	F	469	1/1	0.97	0.06	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	A	470	1/1	0.97	0.03	43,43,43,43	0
2	MN	E	470	1/1	0.97	0.06	43,43,43,43	0
2	MN	K	469	1/1	0.97	0.11	41,41,41,41	0
2	MN	F	470	1/1	0.98	0.06	43,43,43,43	0
2	MN	D	470	1/1	0.98	0.08	43,43,43,43	0
2	MN	L	470	1/1	0.98	0.05	43,43,43,43	0
2	MN	L	469	1/1	0.98	0.11	41,41,41,41	0
2	MN	C	470	1/1	0.98	0.03	43,43,43,43	0
2	MN	B	470	1/1	0.98	0.05	43,43,43,43	0
2	MN	B	469	1/1	0.98	0.04	41,41,41,41	0
2	MN	K	470	1/1	0.98	0.04	43,43,43,43	0
2	MN	I	470	1/1	0.99	0.04	43,43,43,43	0
2	MN	J	470	1/1	0.99	0.02	43,43,43,43	0
2	MN	I	469	1/1	0.99	0.06	41,41,41,41	0
2	MN	J	469	1/1	0.99	0.07	41,41,41,41	0
2	MN	G	470	1/1	0.99	0.04	43,43,43,43	0

6.5 Other polymers

There are no such residues in this entry.