wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2023 – 07:26 PM EST

PDB ID	:	8TGE
Title	:	Crystal structure of the Methanosarcina mazei glutamine synthetase in complex with GlnK1
Authors	:	Schumacher, M.A.
Deposited on	:	2023-07-12
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

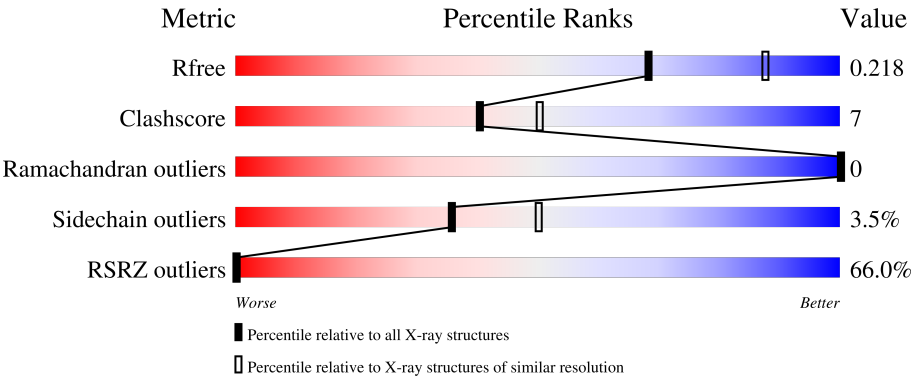
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	467	59% 79% 15% • 5%
1	B	467	53% 78% 16% 5%
1	D	467	68% 81% 13% • 5%
1	M	467	55% 81% 13% • 5%
1	P	467	64% 80% 14% 5%

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Mol	Chain	Length	Quality of chain
1	Y	467	57% 82% 12% 5%
2	G	137	69% 45% 23% 31%
2	J	137	69% 41% 27% 29%
2	Z	137	69% 42% 26% 29%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24784 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	442	Total	C	N	O	S	0	0	0
			3479	2225	588	649	17			
1	B	442	Total	C	N	O	S	0	0	0
			3490	2230	586	657	17			
1	D	442	Total	C	N	O	S	0	0	0
			3495	2233	588	657	17			
1	Y	443	Total	C	N	O	S	0	0	0
			3506	2242	589	658	17			
1	M	443	Total	C	N	O	S	0	0	0
			3518	2248	595	658	17			
1	P	443	Total	C	N	O	S	0	0	0
			3512	2245	592	658	17			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8PY99
A	-18	GLY	-	expression tag	UNP Q8PY99
A	-17	SER	-	expression tag	UNP Q8PY99
A	-16	SER	-	expression tag	UNP Q8PY99
A	-15	HIS	-	expression tag	UNP Q8PY99
A	-14	HIS	-	expression tag	UNP Q8PY99
A	-13	HIS	-	expression tag	UNP Q8PY99
A	-12	HIS	-	expression tag	UNP Q8PY99
A	-11	HIS	-	expression tag	UNP Q8PY99
A	-10	HIS	-	expression tag	UNP Q8PY99
A	-9	SER	-	expression tag	UNP Q8PY99
A	-8	SER	-	expression tag	UNP Q8PY99
A	-7	GLY	-	expression tag	UNP Q8PY99
A	-6	LEU	-	expression tag	UNP Q8PY99
A	-5	VAL	-	expression tag	UNP Q8PY99
A	-4	PRO	-	expression tag	UNP Q8PY99
A	-3	ARG	-	expression tag	UNP Q8PY99

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q8PY99
A	-1	SER	-	expression tag	UNP Q8PY99
A	0	HIS	-	expression tag	UNP Q8PY99
B	-19	MET	-	initiating methionine	UNP Q8PY99
B	-18	GLY	-	expression tag	UNP Q8PY99
B	-17	SER	-	expression tag	UNP Q8PY99
B	-16	SER	-	expression tag	UNP Q8PY99
B	-15	HIS	-	expression tag	UNP Q8PY99
B	-14	HIS	-	expression tag	UNP Q8PY99
B	-13	HIS	-	expression tag	UNP Q8PY99
B	-12	HIS	-	expression tag	UNP Q8PY99
B	-11	HIS	-	expression tag	UNP Q8PY99
B	-10	HIS	-	expression tag	UNP Q8PY99
B	-9	SER	-	expression tag	UNP Q8PY99
B	-8	SER	-	expression tag	UNP Q8PY99
B	-7	GLY	-	expression tag	UNP Q8PY99
B	-6	LEU	-	expression tag	UNP Q8PY99
B	-5	VAL	-	expression tag	UNP Q8PY99
B	-4	PRO	-	expression tag	UNP Q8PY99
B	-3	ARG	-	expression tag	UNP Q8PY99
B	-2	GLY	-	expression tag	UNP Q8PY99
B	-1	SER	-	expression tag	UNP Q8PY99
B	0	HIS	-	expression tag	UNP Q8PY99
D	-19	MET	-	initiating methionine	UNP Q8PY99
D	-18	GLY	-	expression tag	UNP Q8PY99
D	-17	SER	-	expression tag	UNP Q8PY99
D	-16	SER	-	expression tag	UNP Q8PY99
D	-15	HIS	-	expression tag	UNP Q8PY99
D	-14	HIS	-	expression tag	UNP Q8PY99
D	-13	HIS	-	expression tag	UNP Q8PY99
D	-12	HIS	-	expression tag	UNP Q8PY99
D	-11	HIS	-	expression tag	UNP Q8PY99
D	-10	HIS	-	expression tag	UNP Q8PY99
D	-9	SER	-	expression tag	UNP Q8PY99
D	-8	SER	-	expression tag	UNP Q8PY99
D	-7	GLY	-	expression tag	UNP Q8PY99
D	-6	LEU	-	expression tag	UNP Q8PY99
D	-5	VAL	-	expression tag	UNP Q8PY99
D	-4	PRO	-	expression tag	UNP Q8PY99
D	-3	ARG	-	expression tag	UNP Q8PY99
D	-2	GLY	-	expression tag	UNP Q8PY99
D	-1	SER	-	expression tag	UNP Q8PY99

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP Q8PY99
Y	-19	MET	-	initiating methionine	UNP Q8PY99
Y	-18	GLY	-	expression tag	UNP Q8PY99
Y	-17	SER	-	expression tag	UNP Q8PY99
Y	-16	SER	-	expression tag	UNP Q8PY99
Y	-15	HIS	-	expression tag	UNP Q8PY99
Y	-14	HIS	-	expression tag	UNP Q8PY99
Y	-13	HIS	-	expression tag	UNP Q8PY99
Y	-12	HIS	-	expression tag	UNP Q8PY99
Y	-11	HIS	-	expression tag	UNP Q8PY99
Y	-10	HIS	-	expression tag	UNP Q8PY99
Y	-9	SER	-	expression tag	UNP Q8PY99
Y	-8	SER	-	expression tag	UNP Q8PY99
Y	-7	GLY	-	expression tag	UNP Q8PY99
Y	-6	LEU	-	expression tag	UNP Q8PY99
Y	-5	VAL	-	expression tag	UNP Q8PY99
Y	-4	PRO	-	expression tag	UNP Q8PY99
Y	-3	ARG	-	expression tag	UNP Q8PY99
Y	-2	GLY	-	expression tag	UNP Q8PY99
Y	-1	SER	-	expression tag	UNP Q8PY99
Y	0	HIS	-	expression tag	UNP Q8PY99
M	-19	MET	-	initiating methionine	UNP Q8PY99
M	-18	GLY	-	expression tag	UNP Q8PY99
M	-17	SER	-	expression tag	UNP Q8PY99
M	-16	SER	-	expression tag	UNP Q8PY99
M	-15	HIS	-	expression tag	UNP Q8PY99
M	-14	HIS	-	expression tag	UNP Q8PY99
M	-13	HIS	-	expression tag	UNP Q8PY99
M	-12	HIS	-	expression tag	UNP Q8PY99
M	-11	HIS	-	expression tag	UNP Q8PY99
M	-10	HIS	-	expression tag	UNP Q8PY99
M	-9	SER	-	expression tag	UNP Q8PY99
M	-8	SER	-	expression tag	UNP Q8PY99
M	-7	GLY	-	expression tag	UNP Q8PY99
M	-6	LEU	-	expression tag	UNP Q8PY99
M	-5	VAL	-	expression tag	UNP Q8PY99
M	-4	PRO	-	expression tag	UNP Q8PY99
M	-3	ARG	-	expression tag	UNP Q8PY99
M	-2	GLY	-	expression tag	UNP Q8PY99
M	-1	SER	-	expression tag	UNP Q8PY99
M	0	HIS	-	expression tag	UNP Q8PY99
P	-19	MET	-	initiating methionine	UNP Q8PY99

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-18	GLY	-	expression tag	UNP Q8PY99
P	-17	SER	-	expression tag	UNP Q8PY99
P	-16	SER	-	expression tag	UNP Q8PY99
P	-15	HIS	-	expression tag	UNP Q8PY99
P	-14	HIS	-	expression tag	UNP Q8PY99
P	-13	HIS	-	expression tag	UNP Q8PY99
P	-12	HIS	-	expression tag	UNP Q8PY99
P	-11	HIS	-	expression tag	UNP Q8PY99
P	-10	HIS	-	expression tag	UNP Q8PY99
P	-9	SER	-	expression tag	UNP Q8PY99
P	-8	SER	-	expression tag	UNP Q8PY99
P	-7	GLY	-	expression tag	UNP Q8PY99
P	-6	LEU	-	expression tag	UNP Q8PY99
P	-5	VAL	-	expression tag	UNP Q8PY99
P	-4	PRO	-	expression tag	UNP Q8PY99
P	-3	ARG	-	expression tag	UNP Q8PY99
P	-2	GLY	-	expression tag	UNP Q8PY99
P	-1	SER	-	expression tag	UNP Q8PY99
P	0	HIS	-	expression tag	UNP Q8PY99

- Molecule 2 is a protein called Nitrogen regulatory protein GlnK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	97	Total	C	N	O	S	0	0	0
			733	470	122	137	4			
2	G	95	Total	C	N	O	S	0	0	0
			706	451	117	134	4			
2	Z	97	Total	C	N	O	S	0	0	0
			731	469	121	137	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-19	MET	-	initiating methionine	UNP Q8PYW7
J	-18	GLY	-	expression tag	UNP Q8PYW7
J	-17	SER	-	expression tag	UNP Q8PYW7
J	-16	SER	-	expression tag	UNP Q8PYW7
J	-15	HIS	-	expression tag	UNP Q8PYW7
J	-14	HIS	-	expression tag	UNP Q8PYW7
J	-13	HIS	-	expression tag	UNP Q8PYW7
J	-12	HIS	-	expression tag	UNP Q8PYW7
J	-11	HIS	-	expression tag	UNP Q8PYW7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-10	HIS	-	expression tag	UNP Q8PYW7
J	-9	SER	-	expression tag	UNP Q8PYW7
J	-8	SER	-	expression tag	UNP Q8PYW7
J	-7	GLY	-	expression tag	UNP Q8PYW7
J	-6	LEU	-	expression tag	UNP Q8PYW7
J	-5	VAL	-	expression tag	UNP Q8PYW7
J	-4	PRO	-	expression tag	UNP Q8PYW7
J	-3	ARG	-	expression tag	UNP Q8PYW7
J	-2	GLY	-	expression tag	UNP Q8PYW7
J	-1	SER	-	expression tag	UNP Q8PYW7
J	0	HIS	-	expression tag	UNP Q8PYW7
G	-19	MET	-	initiating methionine	UNP Q8PYW7
G	-18	GLY	-	expression tag	UNP Q8PYW7
G	-17	SER	-	expression tag	UNP Q8PYW7
G	-16	SER	-	expression tag	UNP Q8PYW7
G	-15	HIS	-	expression tag	UNP Q8PYW7
G	-14	HIS	-	expression tag	UNP Q8PYW7
G	-13	HIS	-	expression tag	UNP Q8PYW7
G	-12	HIS	-	expression tag	UNP Q8PYW7
G	-11	HIS	-	expression tag	UNP Q8PYW7
G	-10	HIS	-	expression tag	UNP Q8PYW7
G	-9	SER	-	expression tag	UNP Q8PYW7
G	-8	SER	-	expression tag	UNP Q8PYW7
G	-7	GLY	-	expression tag	UNP Q8PYW7
G	-6	LEU	-	expression tag	UNP Q8PYW7
G	-5	VAL	-	expression tag	UNP Q8PYW7
G	-4	PRO	-	expression tag	UNP Q8PYW7
G	-3	ARG	-	expression tag	UNP Q8PYW7
G	-2	GLY	-	expression tag	UNP Q8PYW7
G	-1	SER	-	expression tag	UNP Q8PYW7
G	0	HIS	-	expression tag	UNP Q8PYW7
Z	-19	MET	-	initiating methionine	UNP Q8PYW7
Z	-18	GLY	-	expression tag	UNP Q8PYW7
Z	-17	SER	-	expression tag	UNP Q8PYW7
Z	-16	SER	-	expression tag	UNP Q8PYW7
Z	-15	HIS	-	expression tag	UNP Q8PYW7
Z	-14	HIS	-	expression tag	UNP Q8PYW7
Z	-13	HIS	-	expression tag	UNP Q8PYW7
Z	-12	HIS	-	expression tag	UNP Q8PYW7
Z	-11	HIS	-	expression tag	UNP Q8PYW7
Z	-10	HIS	-	expression tag	UNP Q8PYW7
Z	-9	SER	-	expression tag	UNP Q8PYW7

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	-8	SER	-	expression tag	UNP Q8PYW7
Z	-7	GLY	-	expression tag	UNP Q8PYW7
Z	-6	LEU	-	expression tag	UNP Q8PYW7
Z	-5	VAL	-	expression tag	UNP Q8PYW7
Z	-4	PRO	-	expression tag	UNP Q8PYW7
Z	-3	ARG	-	expression tag	UNP Q8PYW7
Z	-2	GLY	-	expression tag	UNP Q8PYW7
Z	-1	SER	-	expression tag	UNP Q8PYW7
Z	0	HIS	-	expression tag	UNP Q8PYW7

- Molecule 3 is water.

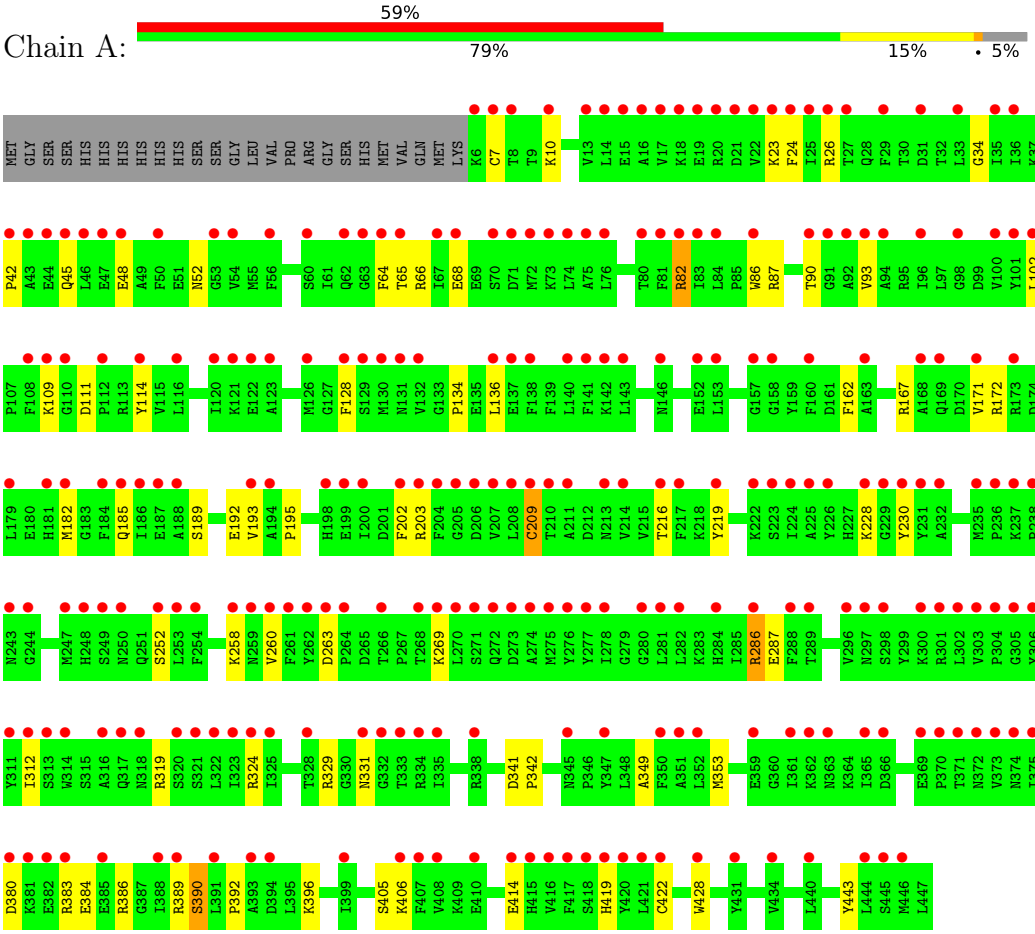
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	281	Total O 281 281	0	0
3	B	270	Total O 270 270	0	0
3	D	266	Total O 266 266	0	0
3	Y	261	Total O 261 261	0	0
3	M	253	Total O 253 253	0	0
3	P	268	Total O 268 268	0	0
3	J	6	Total O 6 6	0	0
3	G	5	Total O 5 5	0	0
3	Z	4	Total O 4 4	0	0

3 Residue-property plots (i)

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

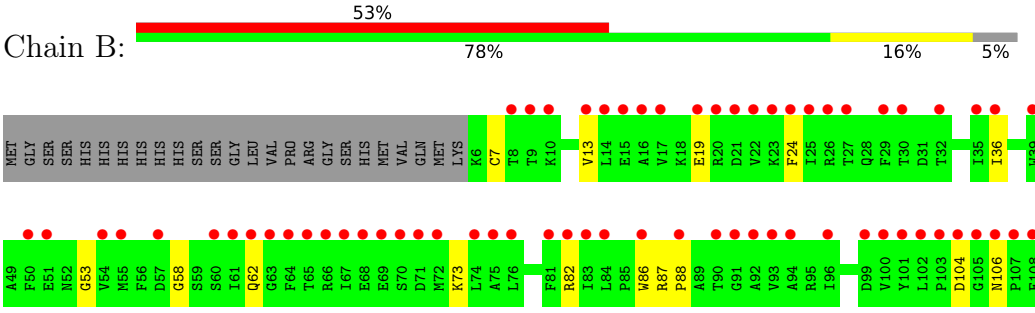
• Molecule 1: Glutamine synthetase

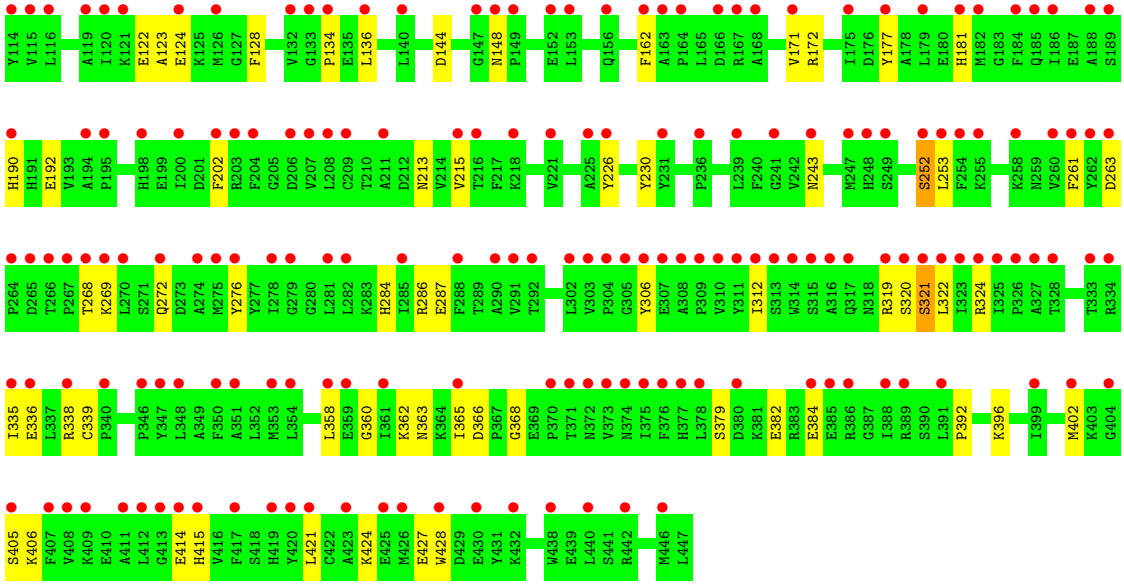
Chain A:



• Molecule 1: Glutamine synthetase

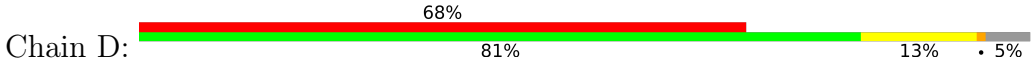
Chain B:

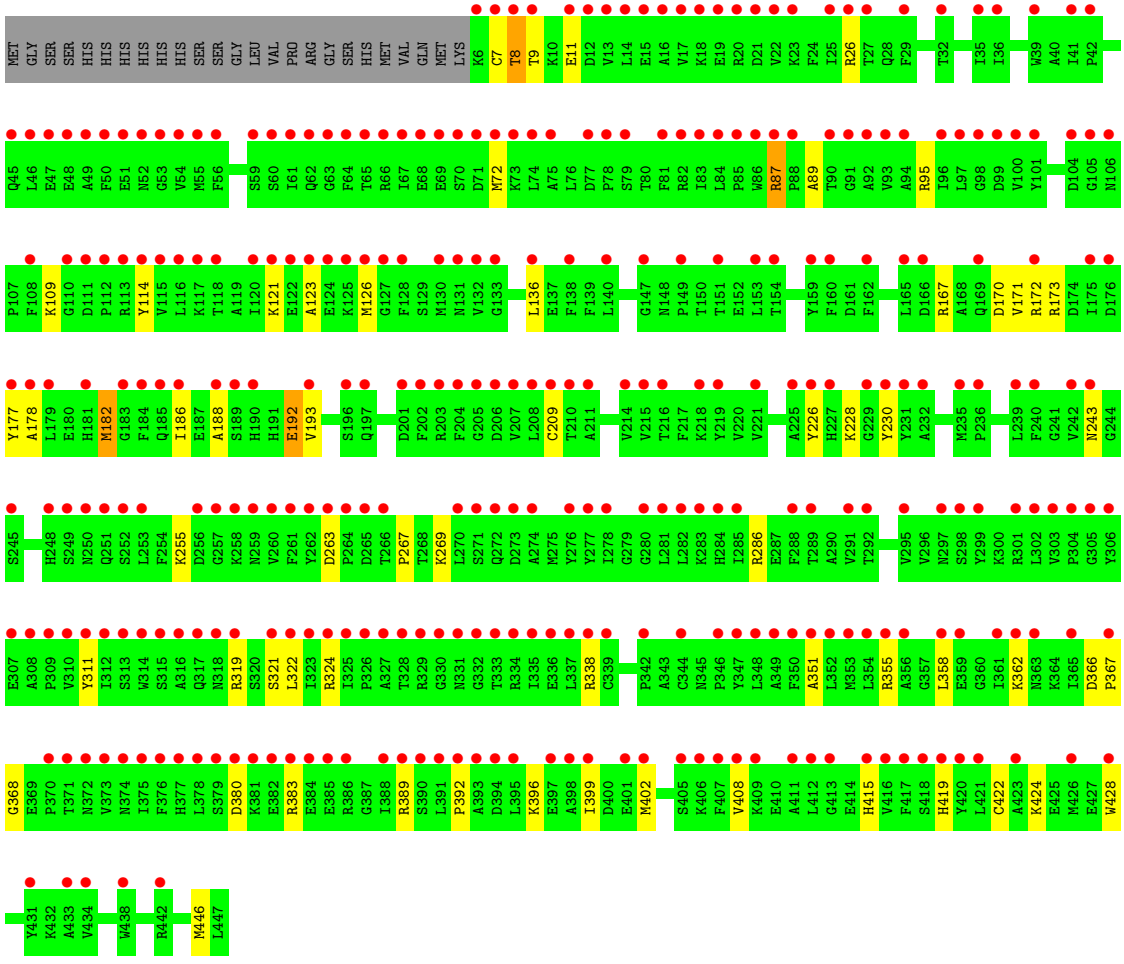




• Molecule 1: Glutamine synthetase

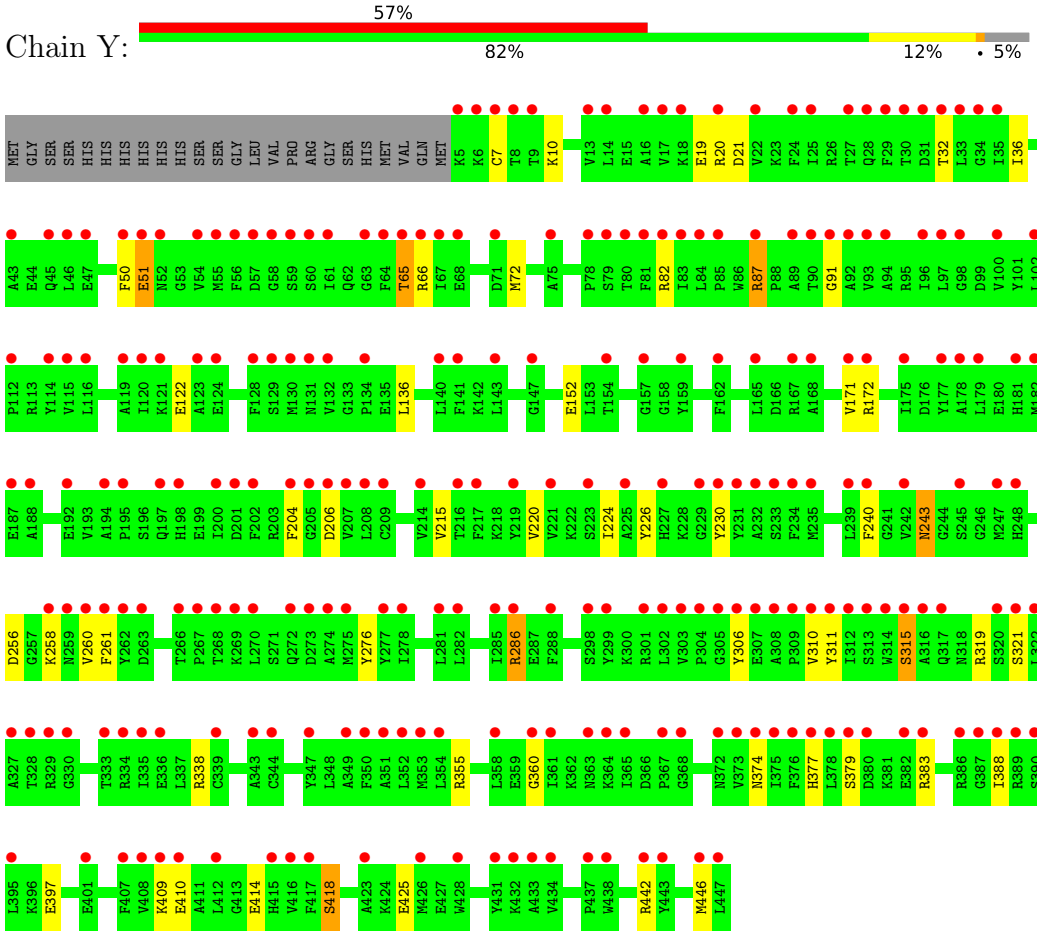
Chain D:





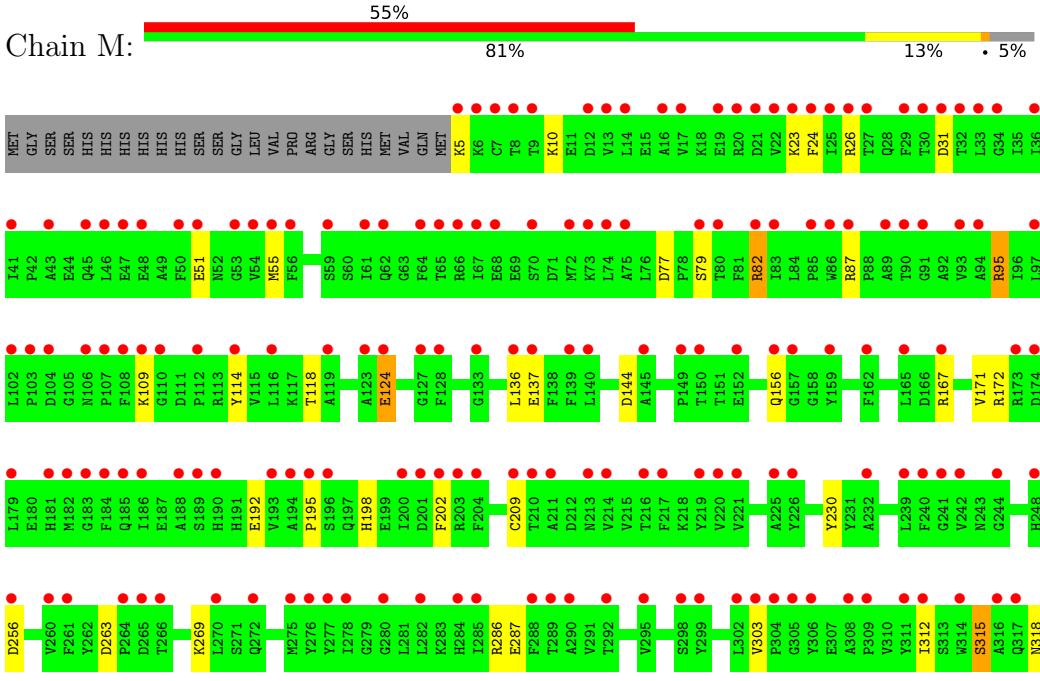
• Molecule 1: Glutamine synthetase

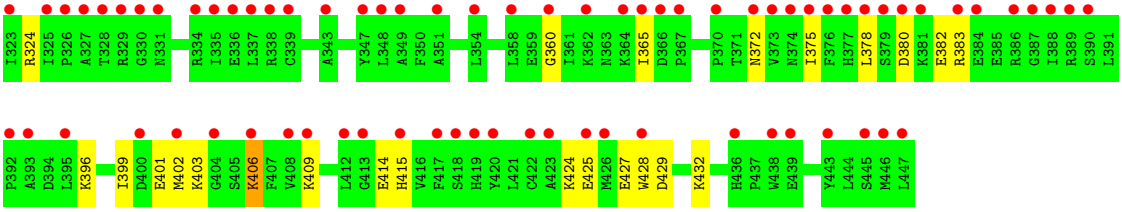
Chain Y:



• Molecule 1: Glutamine synthetase

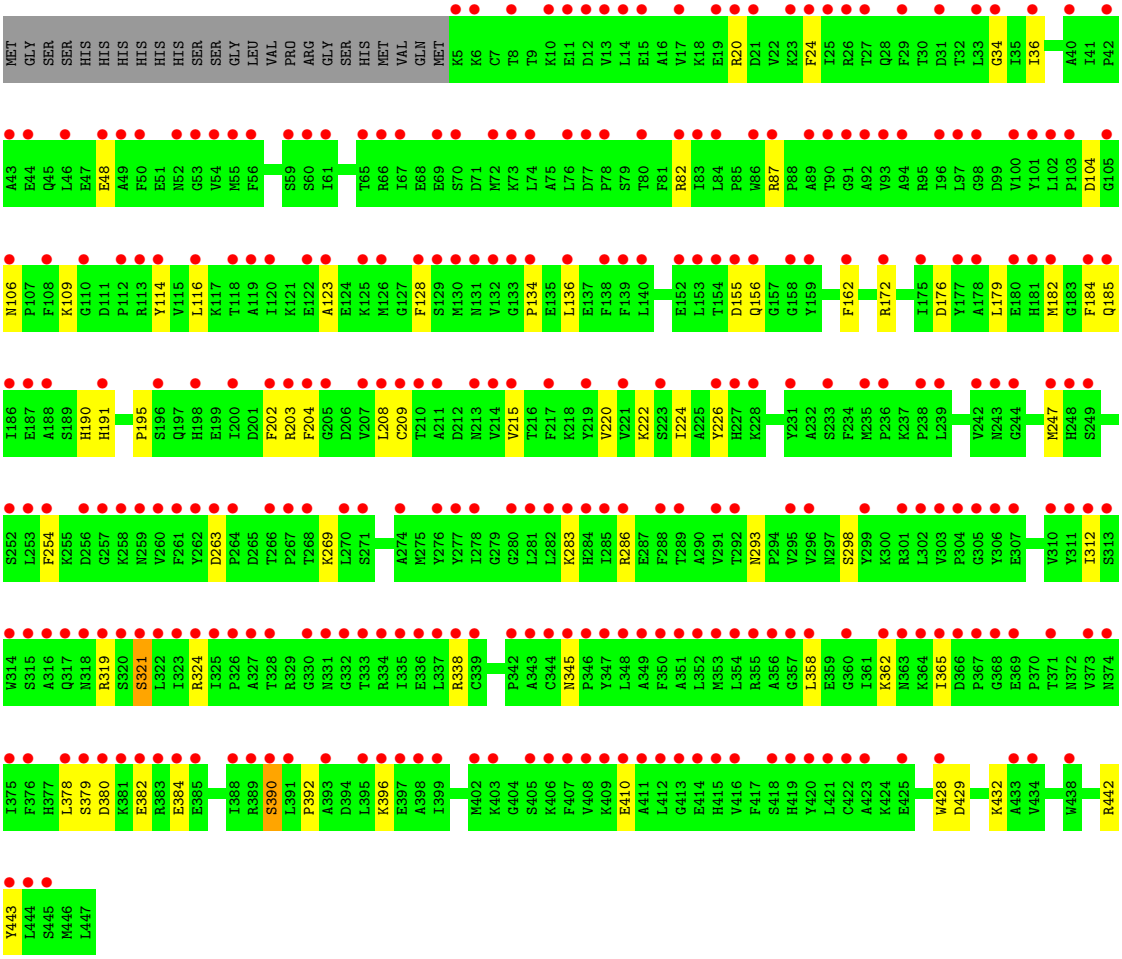
Chain M:





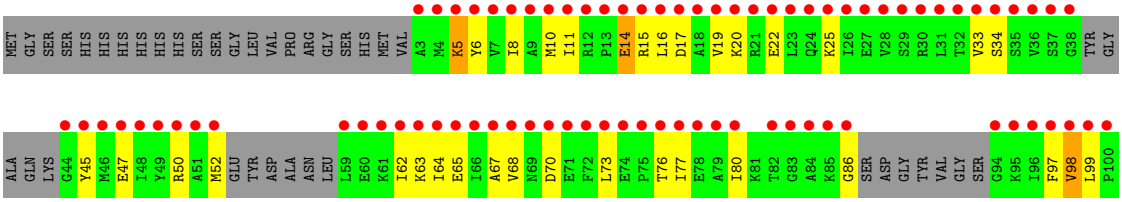
• Molecule 1: Glutamine synthetase

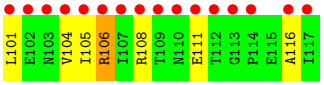
Chain P:



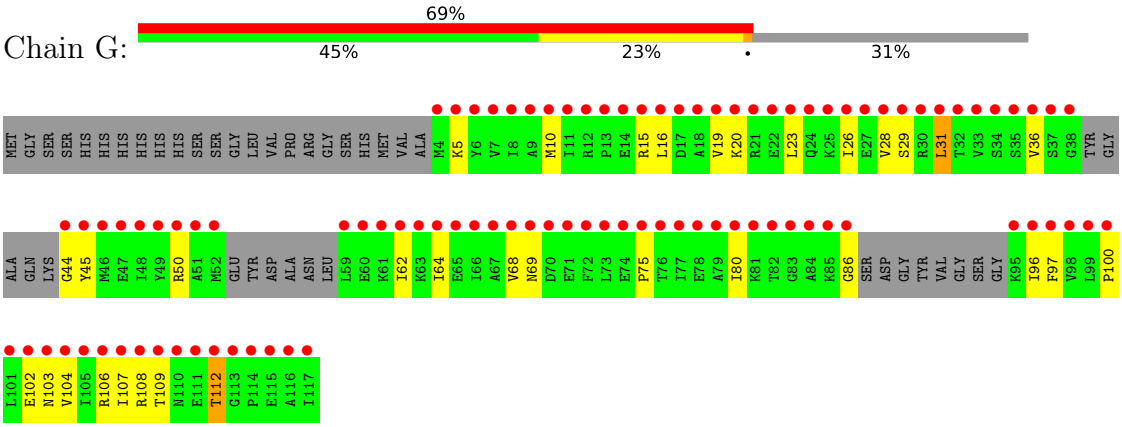
• Molecule 2: Nitrogen regulatory protein GlnK1

Chain J:

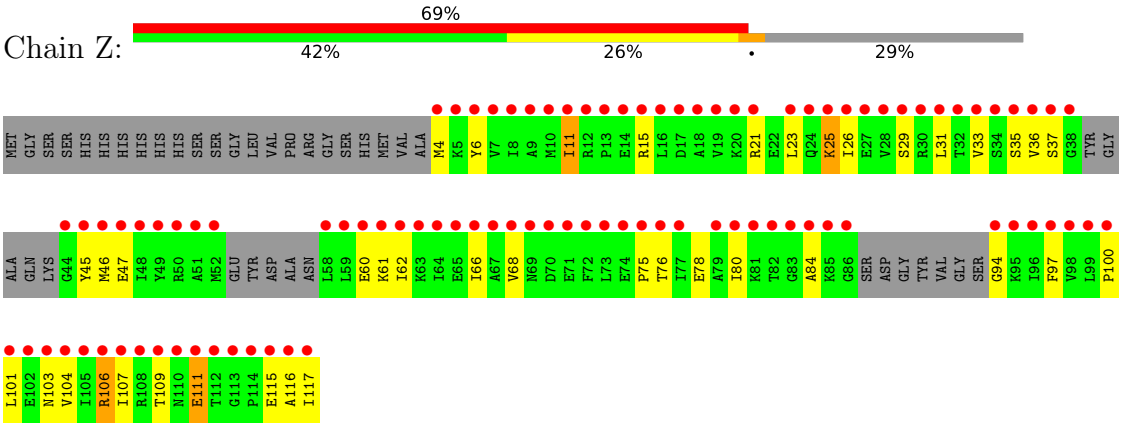




• Molecule 2: Nitrogen regulatory protein GlnK1



• Molecule 2: Nitrogen regulatory protein GlnK1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	137.99Å 178.03Å 169.05Å 90.00° 90.36° 90.00°	Depositor
Resolution (Å)	89.02 – 2.30 89.01 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (89.02-2.30) 98.1 (89.01-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	60.41 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.165 , 0.223 0.167 , 0.218	Depositor DCC
R_{free} test set	1759 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.437 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	24784	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.41	0/3568	0.62	0/4837
1	B	0.43	0/3578	0.63	0/4849
1	D	0.44	0/3584	0.63	0/4857
1	M	0.43	0/3607	0.63	0/4883
1	P	0.41	0/3601	0.61	0/4876
1	Y	0.42	0/3595	0.64	0/4869
2	G	0.39	0/710	0.59	0/956
2	J	0.35	0/738	0.60	0/992
2	Z	0.37	0/736	0.60	0/991
All	All	0.42	0/23717	0.62	0/32110

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

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	3479	0	3377	51	1
1	B	3490	0	3388	51	2
1	D	3495	0	3393	37	1
1	M	3518	0	3439	42	0
1	P	3512	0	3428	43	0
1	Y	3506	0	3417	34	1
2	G	706	0	710	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	733	0	752	41	0
2	Z	731	0	745	28	0
3	A	281	0	0	15	0
3	B	270	0	0	13	0
3	D	266	0	0	6	0
3	G	5	0	0	1	0
3	J	6	0	0	3	0
3	M	253	0	0	12	0
3	P	268	0	0	4	1
3	Y	261	0	0	6	0
3	Z	4	0	0	0	0
All	All	24784	0	22649	331	3

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 7.

The worst 5 of 331 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:THR:HG22	1:D:9:THR:HG23	1.57	0.86
1:P:319:ARG:HA	1:P:324:ARG:HD2	1.59	0.83
1:A:209:CYS:SG	3:A:728:HOH:O	2.37	0.81
2:J:11:ILE:HD13	2:J:19:VAL:HG21	1.65	0.79
1:P:209:CYS:SG	3:P:715:HOH:O	2.40	0.79

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:TYR:OH	1:B:427:GLU:OE2[2_555]	2.01	0.19
1:D:226:TYR:OH	3:P:699:HOH:O[2_555]	2.12	0.08
1:B:124:GLU:OE1	1:Y:258:LYS:NZ[4_445]	2.17	0.03

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	440/467 (94%)	426 (97%)	14 (3%)	0	100	100
1	B	440/467 (94%)	424 (96%)	16 (4%)	0	100	100
1	D	440/467 (94%)	429 (98%)	11 (2%)	0	100	100
1	M	441/467 (94%)	431 (98%)	10 (2%)	0	100	100
1	P	441/467 (94%)	429 (97%)	12 (3%)	0	100	100
1	Y	441/467 (94%)	433 (98%)	8 (2%)	0	100	100
2	G	87/137 (64%)	82 (94%)	5 (6%)	0	100	100
2	J	89/137 (65%)	86 (97%)	3 (3%)	0	100	100
2	Z	89/137 (65%)	87 (98%)	2 (2%)	0	100	100
All	All	2908/3213 (90%)	2827 (97%)	81 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	368/400 (92%)	356 (97%)	12 (3%)	38	53
1	B	371/400 (93%)	362 (98%)	9 (2%)	49	66
1	D	372/400 (93%)	361 (97%)	11 (3%)	41	57
1	M	376/400 (94%)	366 (97%)	10 (3%)	44	61
1	P	375/400 (94%)	366 (98%)	9 (2%)	49	66
1	Y	374/400 (94%)	356 (95%)	18 (5%)	25	36
2	G	72/115 (63%)	68 (94%)	4 (6%)	21	29
2	J	76/115 (66%)	72 (95%)	4 (5%)	22	31
2	Z	76/115 (66%)	67 (88%)	9 (12%)	5	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2460/2745 (90%)	2374 (96%)	86 (4%)	36 50

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	256	ASP
2	J	98	VAL
1	M	406	LYS
1	P	226	TYR
2	G	106	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	HIS
1	B	181	HIS
1	M	372	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	442/467 (94%)	2.62	275 (62%)	0	0	17, 26, 49, 81	0
1	B	442/467 (94%)	2.42	248 (56%)	0	0	17, 27, 49, 97	0
1	D	442/467 (94%)	2.84	316 (71%)	0	0	17, 27, 46, 76	0
1	M	443/467 (94%)	2.47	257 (58%)	0	0	17, 27, 54, 83	0
1	P	443/467 (94%)	2.80	298 (67%)	0	0	17, 27, 47, 90	0
1	Y	443/467 (94%)	2.45	264 (59%)	0	0	16, 26, 47, 97	0
2	G	95/137 (69%)	7.75	95 (100%)	0	0	38, 76, 105, 124	0
2	J	97/137 (70%)	7.24	95 (97%)	0	0	37, 75, 103, 125	0
2	Z	97/137 (70%)	7.76	95 (97%)	0	0	38, 84, 113, 133	0
All	All	2944/3213 (91%)	3.09	1943 (65%)	0	0	16, 28, 78, 133	0

The worst 5 of 1943 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	16	LEU	28.7
2	Z	29	SER	27.5
2	G	66	ILE	24.3
2	G	80	ILE	21.6
2	G	95	LYS	21.2

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.