



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:58 AM EDT

PDB ID : 8TGE / pdb_00008tge
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 Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

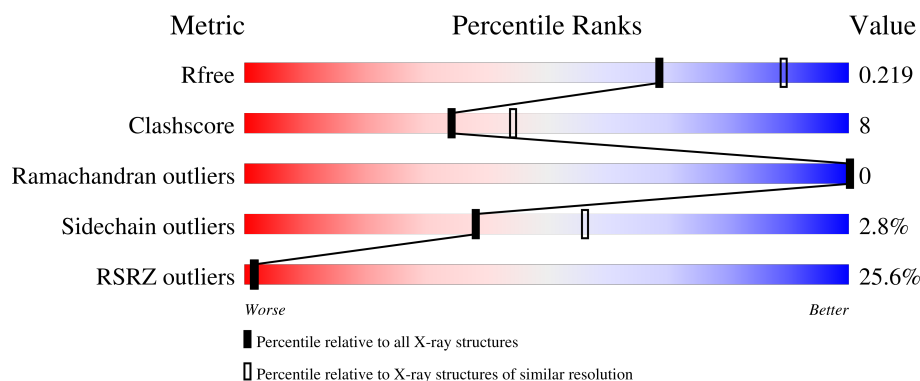
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	467	
1	B	467	
1	D	467	
1	M	467	
1	P	467	

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Mol	Chain	Length	Quality of chain
1	Y	467	16% 81% 13% 5%
2	G	137	61% 43% 24% 31%
2	J	137	64% 39% 29% 29%
2	Z	137	63% 40% 27% 29%

2 Entry composition

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

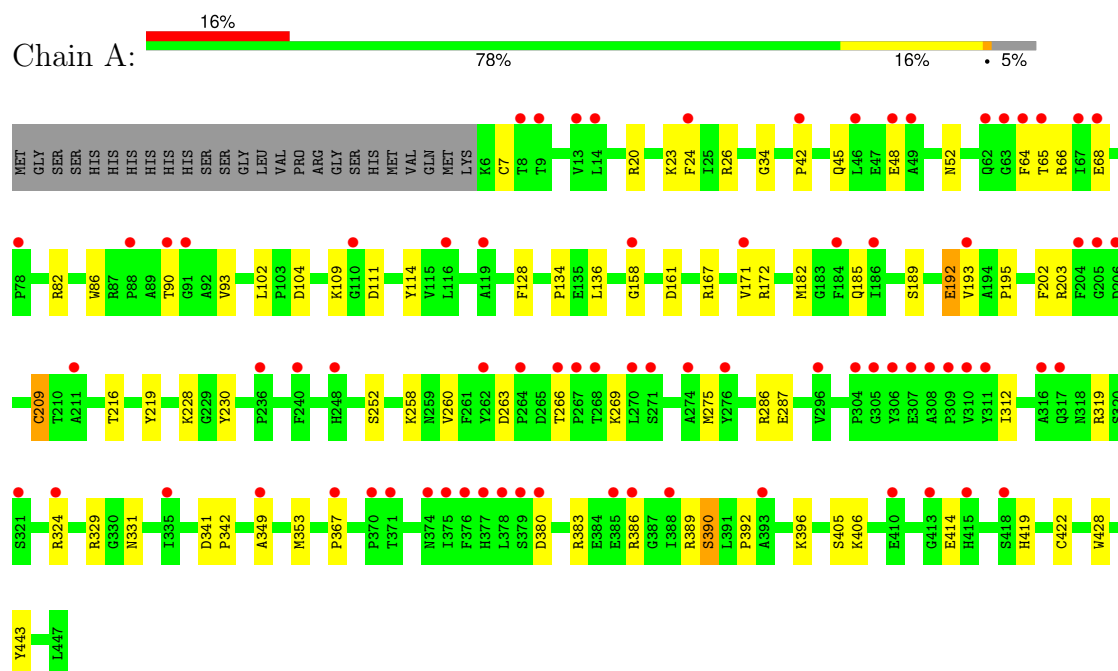
- Molecule 3 is water.

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

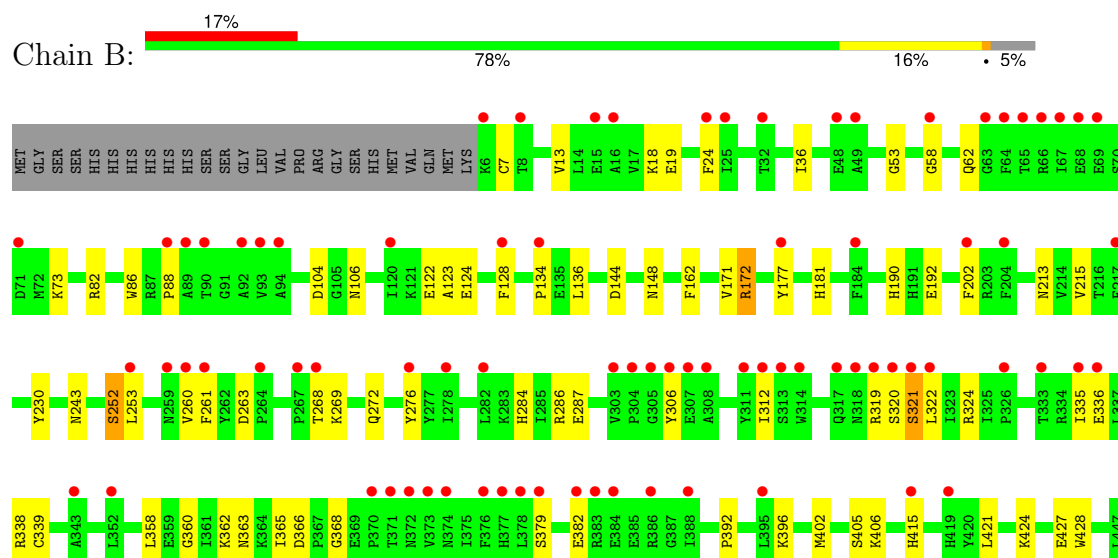
3 Residue-property plots [i](#)

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.

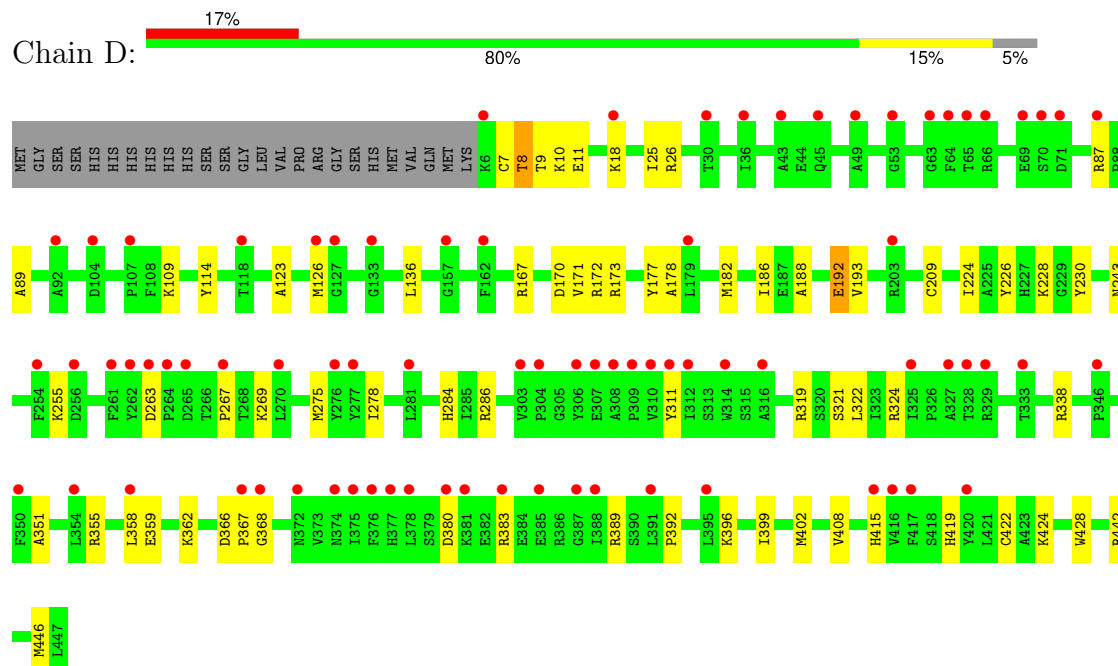
• Molecule 1: Glutamine synthetase



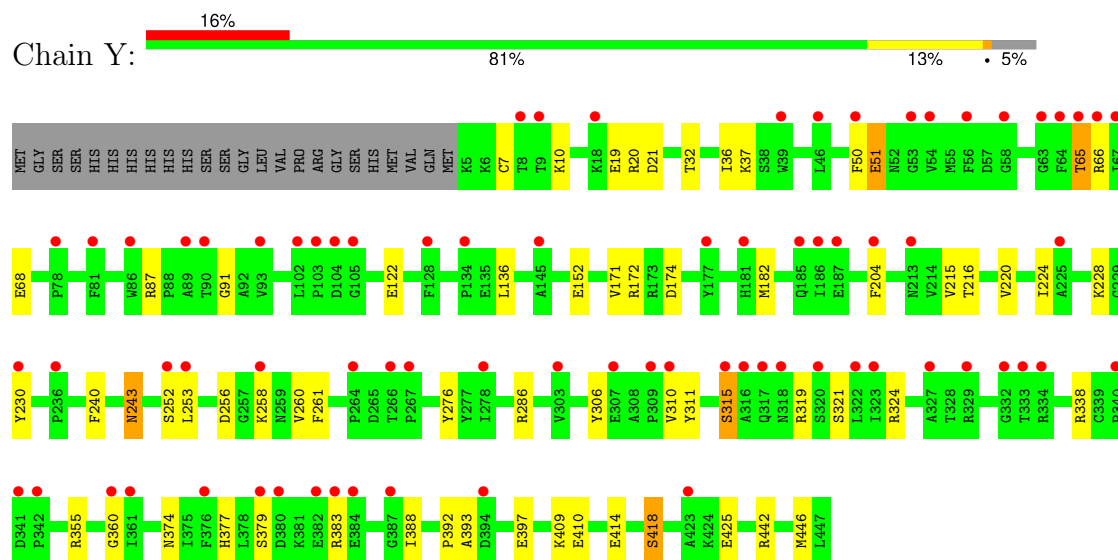
• Molecule 1: Glutamine synthetase



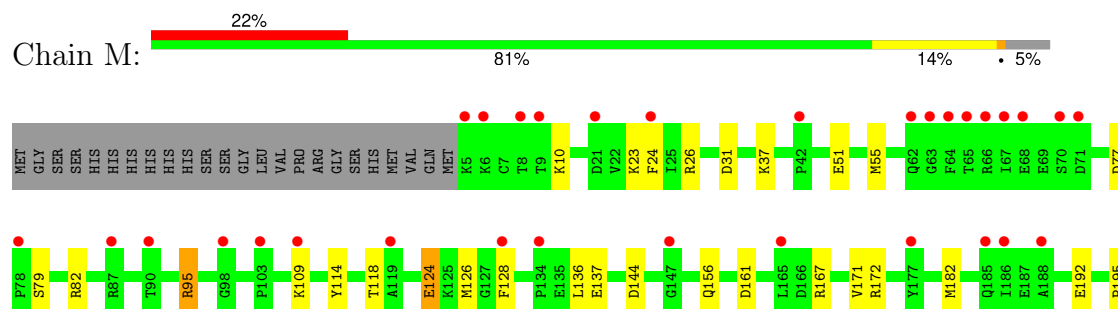
- Molecule 1: Glutamine synthetase

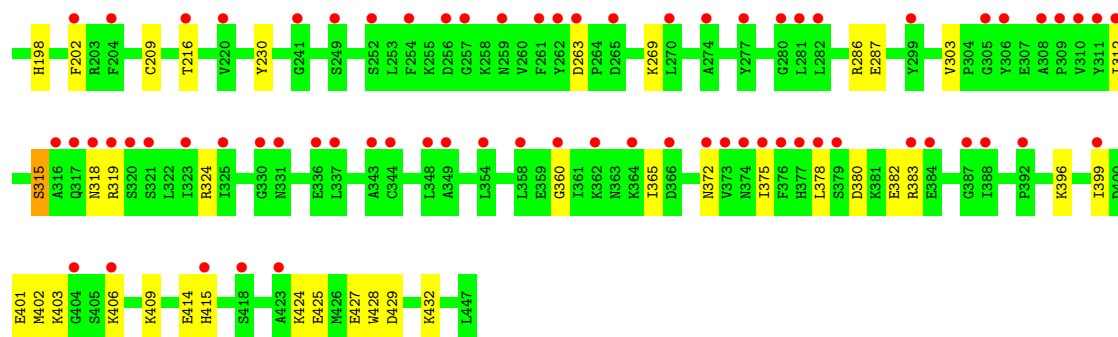


- Molecule 1: Glutamine synthetase

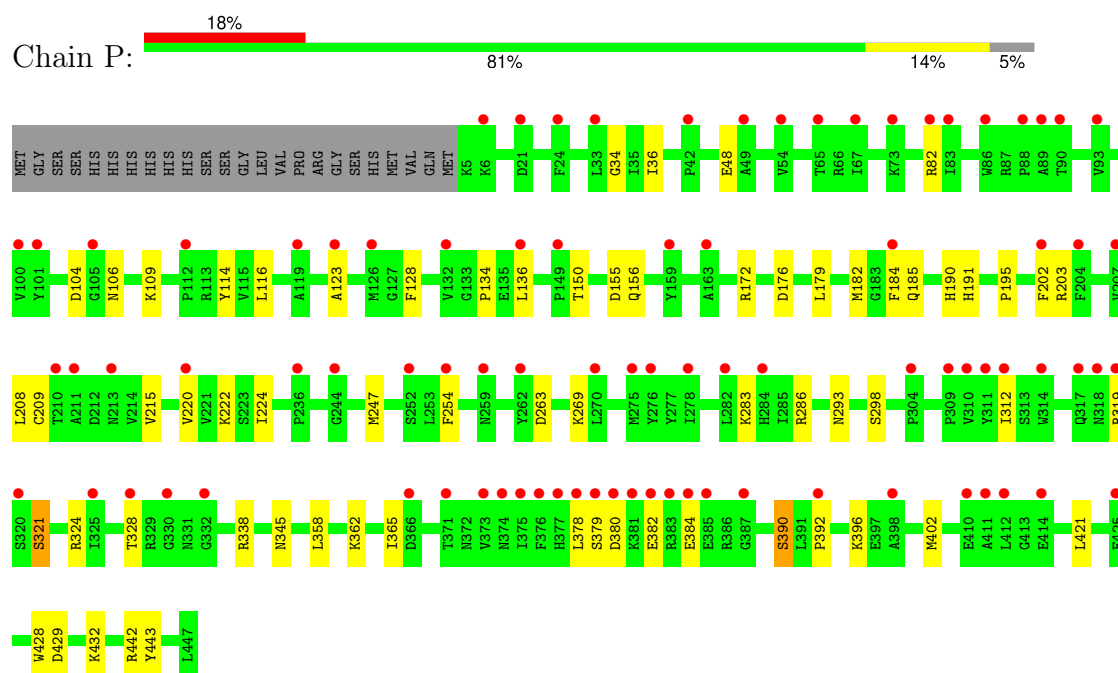


- Molecule 1: Glutamine synthetase

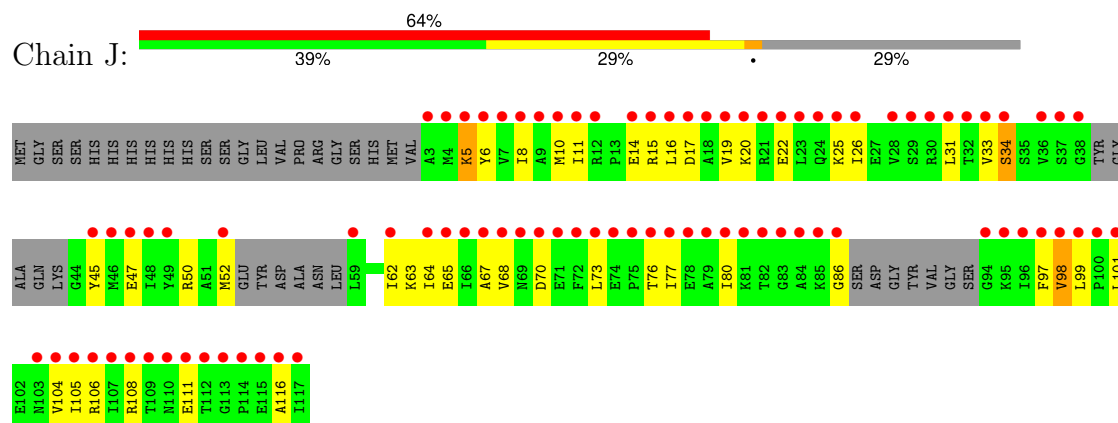




• Molecule 1: Glutamine synthetase

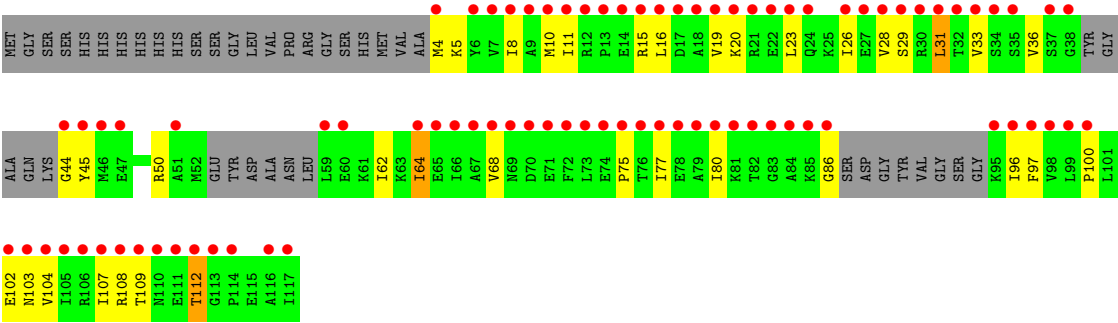


• Molecule 2: Nitrogen regulatory protein GlnK1

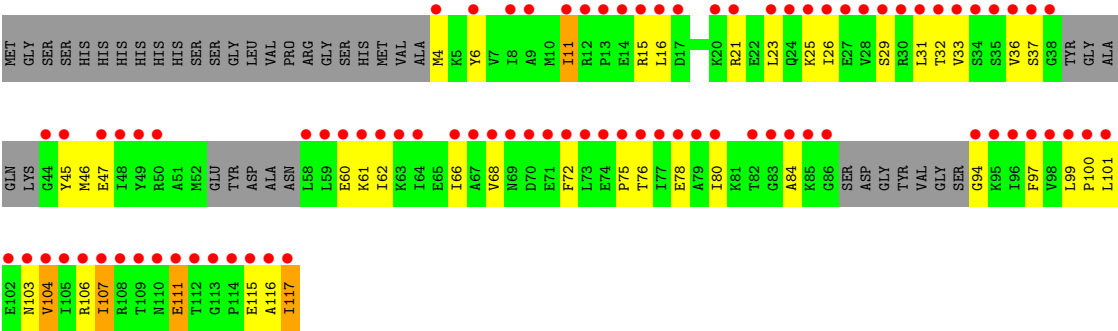


• Molecule 2: Nitrogen regulatory protein GlnK1





● Molecule 2: Nitrogen regulatory protein GlnK1



4 Data and refinement statistics

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 89.02 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (89.02-2.30) 98.1 (89.02-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	60.41 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.165 , 0.223 0.167 , 0.219	Depositor DCC
R_{free} test set	1997 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)	0.35 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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	0.85	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.33	0/3568	0.52	0/4837
1	B	0.34	0/3578	0.55	0/4849
1	D	0.35	0/3584	0.53	0/4857
1	M	0.36	0/3607	0.54	0/4883
1	P	0.34	0/3601	0.52	0/4876
1	Y	0.36	0/3595	0.56	0/4869
2	G	0.31	0/710	0.53	0/956
2	J	0.29	0/738	0.49	0/992
2	Z	0.34	0/736	0.52	0/991
All	All	0.34	0/23717	0.53	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3479	0	3377	53	1
1	B	3490	0	3388	51	2
1	D	3495	0	3393	40	1
1	M	3518	0	3439	45	0
1	P	3512	0	3428	44	0
1	Y	3506	0	3417	37	1
2	G	706	0	710	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	733	0	752	42	0
2	Z	731	0	745	30	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	347	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 8.

All (347) 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
1:P:104:ASP:OD2	1:P:106:ASN:ND2	2.17	0.78
1:D:167:ARG:NH2	1:D:228:LYS:O	2.18	0.77
2:Z:101:LEU:HD21	2:Z:104:VAL:HG23	1.66	0.77
1:M:10:LYS:NZ	1:M:51:GLU:OE2	2.18	0.76
2:Z:26:ILE:HG21	2:Z:75:PRO:HB3	1.68	0.76
1:B:319:ARG:HA	1:B:324:ARG:HD3	1.69	0.74
1:A:319:ARG:HA	1:A:324:ARG:HD2	1.69	0.74
1:M:286:ARG:NH1	1:M:401:GLU:OE1	2.19	0.74
1:Y:10:LYS:NZ	1:Y:51:GLU:OE2	2.21	0.73
1:Y:36:ILE:HG12	1:Y:215:VAL:HG13	1.70	0.73
2:J:97:PHE:HD1	2:Z:104:VAL:HG22	1.55	0.72
1:P:286:ARG:HG2	1:P:392:PRO:HD3	1.71	0.71
1:A:380:ASP:OD1	1:A:383:ARG:NH2	2.24	0.70
1:Y:66:ARG:NH2	1:Y:418:SER:OG	2.17	0.70
2:J:16:LEU:HD13	2:J:62:ILE:HG21	1.74	0.68
2:J:6:TYR:HB2	2:J:101:LEU:HG	1.75	0.68
1:P:402:MET:HE2	1:P:421:LEU:HG	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:102:GLU:HB2	2:Z:100:PRO:HD3	1.76	0.67
1:B:19:GLU:OE1	2:J:45:TYR:OH	2.10	0.67
1:M:403:LYS:NZ	1:M:425:GLU:OE1	2.28	0.67
1:P:380:ASP:O	1:P:384:GLU:HB2	1.95	0.66
1:B:392:PRO:O	3:B:501:HOH:O	2.14	0.66
1:B:213:ASN:ND2	3:B:507:HOH:O	2.25	0.66
1:B:104:ASP:OD2	1:B:106:ASN:ND2	2.29	0.65
1:A:34:GLY:O	3:A:501:HOH:O	2.13	0.65
1:Y:409:LYS:HE2	1:Y:414:GLU:HG2	1.77	0.65
2:J:14:GLU:HG2	2:J:15:ARG:HD3	1.79	0.65
1:A:111:ASP:OD2	3:A:502:HOH:O	2.15	0.64
1:B:336:GLU:OE2	3:B:502:HOH:O	2.14	0.64
1:A:7:CYS:SG	3:A:525:HOH:O	2.52	0.64
1:A:23:LYS:HZ3	2:J:50:ARG:HH12	1.44	0.64
1:A:286:ARG:HG2	1:A:392:PRO:HD3	1.79	0.64
1:Y:315:SER:HB3	1:Y:321:SER:OG	1.98	0.64
1:B:82:ARG:NH2	3:B:516:HOH:O	2.31	0.64
1:M:429:ASP:OD1	1:M:432:LYS:NZ	2.27	0.63
1:P:134:PRO:HD2	1:P:202:PHE:HB2	1.80	0.63
1:P:82:ARG:HG2	1:P:182:MET:HE2	1.79	0.63
2:G:44:GLY:N	3:G:201:HOH:O	2.30	0.63
1:B:136:LEU:HD13	1:B:202:PHE:CE1	2.33	0.63
1:P:36:ILE:HG12	1:P:215:VAL:HG13	1.81	0.63
2:J:33:VAL:HG22	2:J:64:ILE:HG13	1.79	0.63
1:P:396:LYS:HB2	1:P:428:TRP:CE2	2.33	0.62
1:A:65:THR:HG22	1:A:66:ARG:HG2	1.82	0.62
2:G:102:GLU:OE1	2:G:103:ASN:HB2	1.99	0.62
1:P:185:GLN:HB3	1:P:203:ARG:HG3	1.82	0.61
2:J:70:ASP:O	2:J:73:LEU:HB2	2.01	0.61
1:A:23:LYS:NZ	2:J:50:ARG:HH12	1.99	0.61
1:Y:252:SER:HB2	3:Y:505:HOH:O	1.98	0.61
1:B:321:SER:O	1:B:338:ARG:HD3	2.00	0.60
1:M:414:GLU:HA	3:M:551:HOH:O	2.01	0.60
1:A:48:GLU:OE2	1:A:52:ASN:ND2	2.33	0.60
2:J:80:ILE:HG22	2:Z:107:ILE:HD11	1.82	0.60
1:P:379:SER:H	1:P:382:GLU:HG3	1.67	0.60
2:J:68:VAL:HG11	2:J:76:THR:HG21	1.84	0.60
2:Z:15:ARG:HD3	2:Z:84:ALA:HA	1.84	0.60
1:B:13:VAL:HG23	3:B:531:HOH:O	2.03	0.59
1:B:86:TRP:O	3:B:503:HOH:O	2.16	0.59
2:J:15:ARG:O	2:J:19:VAL:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:34:SER:HB3	2:G:36:VAL:HG12	1.84	0.59
2:J:98:VAL:HG13	2:Z:103:ASN:HB3	1.83	0.59
1:Y:171:VAL:HG21	1:Y:230:TYR:CE2	2.37	0.59
1:A:82:ARG:HG2	1:A:182:MET:HE2	1.84	0.58
2:J:106:ARG:NH2	3:J:201:HOH:O	2.37	0.58
1:Y:321:SER:O	1:Y:338:ARG:HD3	2.04	0.58
1:Y:21:ASP:OD2	1:Y:87:ARG:NH2	2.36	0.57
1:D:26:ARG:NH2	3:D:509:HOH:O	2.29	0.57
1:Y:393:ALA:H	1:Y:397:GLU:CD	2.13	0.57
2:J:97:PHE:CD1	2:Z:104:VAL:HG22	2.39	0.57
1:Y:65:THR:HG23	1:Y:66:ARG:HG3	1.86	0.57
1:B:415:HIS:HB3	3:B:671:HOH:O	2.03	0.57
1:M:378:LEU:HD22	1:M:382:GLU:HB3	1.85	0.57
1:P:293:ASN:HB3	1:P:298:SER:HB3	1.87	0.56
2:J:20:LYS:HE2	3:J:204:HOH:O	2.05	0.56
1:P:442:ARG:HD3	1:P:443:TYR:CE1	2.40	0.56
1:D:171:VAL:HG21	1:D:230:TYR:CD2	2.41	0.56
1:D:170:ASP:OD1	1:D:173:ARG:NH2	2.38	0.56
1:Y:286:ARG:HG2	1:Y:392:PRO:HD3	1.88	0.56
1:Y:253:LEU:N	3:Y:505:HOH:O	2.32	0.56
1:M:23:LYS:NZ	2:Z:47:GLU:OE2	2.33	0.56
1:A:172:ARG:HH22	1:A:189:SER:HB2	1.71	0.55
1:P:338:ARG:NH2	3:P:517:HOH:O	2.39	0.55
2:G:15:ARG:NE	2:G:86:GLY:HA2	2.21	0.55
1:A:26:ARG:NH2	3:A:519:HOH:O	2.38	0.55
1:B:287:GLU:OE1	1:B:405:SER:OG	2.20	0.55
1:M:424:LYS:NZ	1:M:427:GLU:OE1	2.34	0.55
1:D:89:ALA:O	2:G:50:ARG:NH1	2.39	0.55
1:Y:182:MET:HE1	1:Y:216:THR:HG21	1.88	0.55
1:A:396:LYS:HB2	1:A:428:TRP:CE2	2.42	0.55
2:G:15:ARG:CZ	2:G:86:GLY:HA2	2.37	0.55
1:P:156:GLN:HA	1:P:195:PRO:HB3	1.89	0.54
1:D:275:MET:HE2	1:D:278:ILE:HD12	1.90	0.53
1:D:446:MET:O	3:D:501:HOH:O	2.18	0.53
2:J:22:GLU:HA	2:J:25:LYS:HG2	1.91	0.53
1:A:167:ARG:NH2	1:A:228:LYS:O	2.42	0.53
1:B:53:GLY:HA3	1:B:73:LYS:HD3	1.91	0.53
1:M:286:ARG:HG3	1:M:312:ILE:HD11	1.89	0.53
1:Y:171:VAL:HG21	1:Y:230:TYR:CD2	2.44	0.53
1:B:261:PHE:CE2	1:B:335:ILE:HD12	2.43	0.53
1:M:360:GLY:HA2	1:M:365:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:TYR:O	1:B:181:HIS:HD2	1.91	0.52
1:B:171:VAL:HG21	1:B:230:TYR:CE1	2.44	0.52
1:A:216:THR:HA	1:A:219:TYR:CE2	2.45	0.52
1:M:409:LYS:HG3	3:M:551:HOH:O	2.09	0.52
1:P:319:ARG:HA	1:P:324:ARG:CD	2.34	0.52
2:J:15:ARG:HH22	2:J:86:GLY:HA3	1.75	0.52
1:D:126:MET:O	1:D:255:LYS:NZ	2.41	0.52
1:D:389:ARG:HD3	3:D:676:HOH:O	2.10	0.52
1:Y:152:GLU:HG3	3:Y:740:HOH:O	2.09	0.52
1:M:263:ASP:O	1:M:269:LYS:HA	2.10	0.52
2:J:19:VAL:HG13	2:J:80:ILE:HA	1.92	0.51
1:D:123:ALA:HB2	1:D:358:LEU:HD11	1.92	0.51
1:M:406:LYS:HE3	3:M:630:HOH:O	2.10	0.51
1:A:263:ASP:O	1:A:269:LYS:HA	2.11	0.51
1:A:414:GLU:OE1	3:A:503:HOH:O	2.18	0.51
1:Y:7:CYS:SG	3:Y:708:HOH:O	2.59	0.51
1:M:109:LYS:HG2	1:M:114:TYR:CE2	2.45	0.51
2:J:10:MET:HE1	2:Z:32:THR:OG1	2.11	0.51
1:A:90:THR:O	2:J:50:ARG:NH1	2.44	0.51
1:A:286:ARG:HG3	1:A:312:ILE:HD11	1.92	0.51
1:D:321:SER:O	1:D:338:ARG:HD3	2.11	0.51
1:M:399:ILE:HD11	1:M:424:LYS:HB3	1.93	0.50
1:A:24:PHE:HB2	1:A:93:VAL:HG13	1.93	0.50
1:P:442:ARG:HD3	1:P:443:TYR:CZ	2.45	0.50
1:M:375:ILE:O	1:M:383:ARG:NH1	2.45	0.50
1:P:283:LYS:HD2	1:P:365:ILE:HD13	1.94	0.50
2:J:73:LEU:O	2:J:76:THR:OG1	2.27	0.50
1:D:396:LYS:HB2	1:D:428:TRP:CE2	2.47	0.50
2:G:5:LYS:HA	2:G:5:LYS:HE2	1.93	0.50
2:G:100:PRO:O	2:Z:100:PRO:HD2	2.12	0.50
1:B:252:SER:HA	1:B:261:PHE:CE2	2.47	0.50
1:A:286:ARG:NH1	1:A:390:SER:O	2.39	0.49
2:Z:104:VAL:HG11	2:Z:117:ILE:HG23	1.94	0.49
1:M:396:LYS:HB2	1:M:428:TRP:CE2	2.48	0.49
2:G:8:ILE:HG22	2:G:10:MET:HE2	1.94	0.49
1:P:220:VAL:O	1:P:224:ILE:HG12	2.12	0.49
1:D:366:ASP:CG	1:D:368:GLY:H	2.21	0.49
2:J:106:ARG:NH1	2:J:108:ARG:HD3	2.28	0.49
2:J:6:TYR:CZ	2:J:65:GLU:HB3	2.47	0.49
1:Y:243:ASN:ND2	1:Y:306:TYR:HB3	2.28	0.49
1:B:396:LYS:HB2	1:B:428:TRP:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:SER:OG	1:B:382:GLU:HG3	2.13	0.48
1:A:82:ARG:NH1	3:A:534:HOH:O	2.45	0.48
2:J:105:ILE:HA	2:J:111:GLU:O	2.13	0.48
1:Y:174:ASP:OD2	1:Y:228:LYS:NZ	2.43	0.48
1:M:303:VAL:HG23	3:M:509:HOH:O	2.13	0.48
1:D:9:THR:HB	1:D:11:GLU:OE2	2.13	0.48
1:Y:383:ARG:HG2	1:Y:388:ILE:HB	1.96	0.48
1:P:263:ASP:O	1:P:269:LYS:HA	2.14	0.48
2:J:10:MET:HA	2:J:62:ILE:O	2.13	0.48
2:Z:111:GLU:HG3	2:Z:115:GLU:HB3	1.94	0.48
1:B:36:ILE:HG12	1:B:215:VAL:HG13	1.95	0.48
2:G:20:LYS:HD3	2:G:31:LEU:HD21	1.96	0.48
2:Z:4:MET:HB3	2:Z:101:LEU:HD23	1.95	0.48
1:M:319:ARG:HA	1:M:324:ARG:HD2	1.96	0.48
1:A:349:ALA:O	1:A:353:MET:HG3	2.13	0.48
1:A:396:LYS:HD3	1:A:428:TRP:CD1	2.49	0.48
2:Z:11:ILE:O	2:Z:62:ILE:HG22	2.14	0.47
1:A:341:ASP:HB2	1:A:342:PRO:HD2	1.96	0.47
1:A:7:CYS:HB2	3:A:525:HOH:O	2.15	0.47
1:A:102:LEU:HB2	1:A:104:ASP:OD1	2.14	0.47
1:B:123:ALA:HB2	1:B:358:LEU:HD11	1.96	0.47
1:Y:122:GLU:OE1	3:Y:501:HOH:O	2.20	0.47
1:P:116:LEU:HD23	1:P:208:LEU:HD12	1.95	0.47
1:B:24:PHE:HZ	1:D:177:TYR:HB2	1.78	0.47
1:M:24:PHE:HB2	3:M:558:HOH:O	2.15	0.47
1:P:190:HIS:HD2	1:P:191:HIS:O	1.98	0.47
2:Z:45:TYR:CD2	2:Z:46:MET:HG2	2.50	0.47
1:Y:37:LYS:NZ	1:M:161:ASP:OD1	2.48	0.47
1:B:360:GLY:HA2	1:B:365:ILE:HD12	1.96	0.47
1:D:286:ARG:HG2	1:D:392:PRO:HD3	1.96	0.47
2:G:107:ILE:HG13	2:G:108:ARG:N	2.30	0.47
1:B:263:ASP:O	1:B:269:LYS:HA	2.15	0.47
1:D:192:GLU:OE1	1:D:193:VAL:HG23	2.16	0.47
1:M:137:GLU:HA	1:M:198:HIS:O	2.15	0.47
2:J:5:LYS:HB3	2:J:5:LYS:HE3	1.59	0.47
1:D:178:ALA:O	1:D:182:MET:HG3	2.15	0.46
1:Y:20:ARG:HH12	2:G:45:TYR:HA	1.79	0.46
1:A:68:GLU:OE1	1:A:419:HIS:HE1	1.99	0.46
1:B:322:LEU:HD11	1:B:339:CYS:HB3	1.96	0.46
1:P:136:LEU:HD22	1:P:247:MET:HG3	1.97	0.46
1:B:319:ARG:HA	1:B:324:ARG:CD	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:26:ILE:HG21	2:G:75:PRO:HB3	1.98	0.46
1:A:86:TRP:O	3:A:504:HOH:O	2.20	0.46
1:B:366:ASP:OD1	1:B:368:GLY:N	2.41	0.46
1:P:286:ARG:HG3	1:P:312:ILE:HD11	1.98	0.46
1:P:321:SER:O	1:P:338:ARG:HD3	2.16	0.46
1:P:429:ASP:OD1	1:P:432:LYS:NZ	2.43	0.46
2:G:20:LYS:HA	2:G:23:LEU:HD12	1.97	0.46
2:Z:25:LYS:C	2:Z:26:ILE:HD13	2.40	0.46
2:G:20:LYS:NZ	2:G:29:SER:HA	2.31	0.46
1:M:167:ARG:HG2	3:M:628:HOH:O	2.16	0.46
2:G:15:ARG:O	2:G:19:VAL:HG23	2.16	0.46
1:A:90:THR:HB	1:B:177:TYR:CD2	2.51	0.45
1:B:122:GLU:OE2	3:B:504:HOH:O	2.21	0.45
1:D:186:ILE:N	1:D:186:ILE:HD13	2.31	0.45
1:Y:10:LYS:HD2	1:Y:50:PHE:HB3	1.97	0.45
1:M:171:VAL:HG21	1:M:230:TYR:CD2	2.50	0.45
1:M:287:GLU:O	1:M:402:MET:HG3	2.15	0.45
2:G:108:ARG:HG3	2:G:109:THR:HG23	1.97	0.45
1:B:286:ARG:HG3	1:B:312:ILE:HD11	1.98	0.45
1:M:172:ARG:HA	1:M:172:ARG:HD2	1.76	0.45
1:P:155:ASP:CG	1:P:191:HIS:HE2	2.25	0.45
1:P:185:GLN:CB	1:P:203:ARG:HG3	2.44	0.45
2:J:67:ALA:HB2	2:G:97:PHE:HE1	1.82	0.45
1:B:7:CYS:HB3	3:B:531:HOH:O	2.16	0.45
1:M:378:LEU:HB3	1:M:382:GLU:HB2	1.99	0.45
2:G:23:LEU:O	2:G:28:VAL:HG22	2.17	0.45
1:B:362:LYS:HD3	1:B:363:ASN:OD1	2.16	0.45
1:Y:319:ARG:HA	1:Y:324:ARG:HD2	1.99	0.45
1:M:182:MET:HE1	1:M:216:THR:HG21	1.98	0.45
1:M:372:ASN:ND2	3:M:531:HOH:O	2.47	0.45
2:J:17:ASP:HA	2:J:20:LYS:HD2	1.99	0.45
1:A:64:PHE:HE1	3:A:710:HOH:O	2.00	0.45
1:A:275:MET:HE3	1:A:367:PRO:HG3	1.99	0.45
1:M:380:ASP:OD1	1:M:383:ARG:NH2	2.48	0.45
1:P:172:ARG:HA	1:P:172:ARG:HD2	1.73	0.45
1:B:177:TYR:OH	2:J:47:GLU:O	2.21	0.45
1:P:109:LYS:HA	1:P:114:TYR:CD1	2.52	0.45
2:J:104:VAL:HA	2:G:96:ILE:O	2.17	0.45
1:D:380:ASP:HA	1:D:383:ARG:NH1	2.32	0.45
1:A:389:ARG:NH2	3:A:542:HOH:O	2.49	0.45
1:B:58:GLY:O	1:B:62:GLN:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:61:LYS:HA	2:Z:61:LYS:HD3	1.80	0.45
1:B:162:PHE:HB3	3:B:547:HOH:O	2.17	0.44
1:D:263:ASP:O	1:D:269:LYS:HA	2.17	0.44
1:D:399:ILE:HD11	1:D:424:LYS:HB3	1.98	0.44
1:D:355:ARG:NH1	3:D:536:HOH:O	2.50	0.44
1:D:7:CYS:SG	3:D:740:HOH:O	2.53	0.44
1:D:351:ALA:O	1:D:355:ARG:HG2	2.17	0.44
1:Y:276:TYR:HB3	1:Y:360:GLY:O	2.17	0.44
2:G:10:MET:HA	2:G:62:ILE:O	2.17	0.44
2:Z:36:VAL:O	2:Z:60:GLU:HG2	2.17	0.44
1:Y:172:ARG:HD2	1:Y:172:ARG:HA	1.69	0.44
1:A:329:ARG:HD3	1:A:329:ARG:HA	1.82	0.44
1:Y:220:VAL:O	1:Y:224:ILE:HG12	2.18	0.44
1:Y:87:ARG:CZ	1:Y:91:GLY:HA2	2.47	0.44
2:J:15:ARG:HH12	2:J:86:GLY:HA2	1.82	0.44
1:A:185:GLN:O	1:A:203:ARG:HG3	2.17	0.44
1:D:172:ARG:HA	1:D:172:ARG:HD2	1.78	0.44
1:M:124:GLU:HG2	3:M:564:HOH:O	2.17	0.44
2:G:104:VAL:HG22	2:Z:97:PHE:HD1	1.83	0.43
1:A:386:ARG:NH1	3:A:545:HOH:O	2.50	0.43
1:D:319:ARG:HA	1:D:324:ARG:HD2	2.00	0.43
1:Y:252:SER:HA	1:Y:261:PHE:CE2	2.53	0.43
1:M:415:HIS:HB3	3:M:595:HOH:O	2.18	0.43
1:B:415:HIS:HB2	3:B:736:HOH:O	2.18	0.43
1:P:128:PHE:HA	1:P:254:PHE:O	2.18	0.43
1:B:134:PRO:HD2	1:B:202:PHE:HB2	2.00	0.43
1:M:24:PHE:CZ	1:P:176:ASP:HB3	2.54	0.43
1:M:156:GLN:HA	1:M:195:PRO:HB3	1.99	0.43
2:G:104:VAL:O	2:G:112:THR:HA	2.17	0.43
1:A:134:PRO:HG2	1:A:202:PHE:CD2	2.53	0.43
1:P:286:ARG:NH1	1:P:390:SER:O	2.48	0.43
2:J:73:LEU:O	2:J:77:ILE:HG13	2.18	0.43
1:D:366:ASP:OD1	1:D:367:PRO:HD2	2.19	0.43
2:J:34:SER:OG	2:J:63:LYS:HB3	2.17	0.43
2:G:4:MET:HE1	2:G:103:ASN:HA	2.00	0.43
1:D:311:TYR:O	1:D:322:LEU:HB2	2.17	0.43
1:Y:240:PHE:O	3:Y:502:HOH:O	2.21	0.43
1:M:26:ARG:O	1:M:95:ARG:HA	2.18	0.43
2:G:20:LYS:HZ3	2:G:29:SER:HA	1.83	0.43
1:B:144:ASP:OD2	1:B:148:ASN:HB2	2.19	0.43
1:P:48:GLU:HG3	3:P:525:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:123:ALA:HB2	1:P:358:LEU:HD11	2.01	0.43
2:Z:111:GLU:HB3	2:Z:116:ALA:HB2	2.00	0.43
1:M:126:MET:HE2	1:M:128:PHE:HE2	1.83	0.43
1:A:331:ASN:HB3	3:A:701:HOH:O	2.19	0.43
1:D:186:ILE:HG22	1:D:188:ALA:N	2.34	0.43
1:M:315:SER:OG	1:M:318:ASN:N	2.44	0.43
1:P:378:LEU:HB3	1:P:382:GLU:HB2	2.00	0.43
2:J:15:ARG:NH2	2:J:86:GLY:HA3	2.34	0.43
1:B:243:ASN:OD1	1:B:306:TYR:HB3	2.19	0.42
1:M:144:ASP:HB2	3:M:680:HOH:O	2.19	0.42
1:Y:355:ARG:NH2	1:Y:410:GLU:OE2	2.51	0.42
1:A:287:GLU:OE1	1:A:405:SER:OG	2.30	0.42
1:B:402:MET:HB3	1:B:421:LEU:HD21	2.01	0.42
1:D:442:ARG:O	1:D:446:MET:HE3	2.19	0.42
1:M:375:ILE:HG22	1:M:383:ARG:HD3	2.01	0.42
2:G:5:LYS:HB2	2:G:68:VAL:HG23	2.00	0.42
1:M:55:MET:HB3	3:M:570:HOH:O	2.19	0.42
1:B:172:ARG:HD2	1:B:172:ARG:HA	1.78	0.42
1:M:136:LEU:HD12	1:M:202:PHE:CZ	2.53	0.42
1:P:82:ARG:HG2	1:P:182:MET:CE	2.49	0.42
1:A:263:ASP:CG	1:A:266:THR:HG23	2.45	0.42
1:B:190:HIS:ND1	3:B:515:HOH:O	2.31	0.42
1:B:272:GLN:HG3	1:B:276:TYR:CZ	2.54	0.42
1:D:126:MET:HG3	1:D:362:LYS:NZ	2.34	0.42
1:Y:392:PRO:HB3	1:Y:397:GLU:HG2	2.00	0.42
1:P:179:LEU:O	1:P:184:PHE:HB2	2.19	0.42
2:G:19:VAL:HG13	2:G:80:ILE:HA	2.01	0.42
1:D:284:HIS:HE2	1:D:359:GLU:CD	2.25	0.42
1:Y:374:ASN:OD1	1:Y:377:HIS:N	2.37	0.42
1:A:128:PHE:CD1	1:A:260:VAL:HG21	2.55	0.42
1:P:34:GLY:HA2	1:P:345:ASN:HD22	1.85	0.42
2:G:107:ILE:HG12	2:Z:94:GLY:O	2.20	0.42
1:Y:442:ARG:O	1:Y:446:MET:HE3	2.19	0.42
2:Z:31:LEU:HD13	2:Z:33:VAL:HG23	2.01	0.42
1:A:172:ARG:HH22	1:A:189:SER:CB	2.33	0.42
2:J:104:VAL:HG23	2:J:116:ALA:HB3	2.01	0.42
2:Z:72:PHE:C	2:Z:75:PRO:HD2	2.45	0.42
1:Y:19:GLU:OE2	2:G:45:TYR:OH	2.38	0.41
1:M:114:TYR:O	1:M:118:THR:HG23	2.20	0.41
1:D:267:PRO:HG2	3:D:707:HOH:O	2.19	0.41
1:Y:310:VAL:HG23	1:Y:311:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:82:ARG:NH2	3:M:541:HOH:O	2.52	0.41
2:Z:76:THR:O	2:Z:80:ILE:HG13	2.20	0.41
1:A:171:VAL:HG21	1:A:230:TYR:CE2	2.55	0.41
1:B:406:LYS:HB2	1:B:406:LYS:HE2	1.86	0.41
2:Z:66:ILE:HG22	2:Z:68:VAL:HG13	2.01	0.41
2:Z:6:TYR:HB2	2:Z:101:LEU:HD13	2.02	0.41
2:Z:21:ARG:O	2:Z:25:LYS:HG2	2.21	0.41
1:A:42:PRO:O	1:A:45:GLN:N	2.48	0.41
1:B:177:TYR:O	1:B:181:HIS:CD2	2.72	0.41
1:B:424:LYS:NZ	3:B:514:HOH:O	2.30	0.41
1:P:134:PRO:HD2	1:P:202:PHE:CB	2.50	0.41
1:D:402:MET:HG3	1:D:408:VAL:HG11	2.02	0.41
1:M:31:ASP:HB3	1:M:37:LYS:HE2	2.01	0.41
2:J:8:ILE:HD12	2:J:99:LEU:HD23	2.02	0.41
2:J:16:LEU:HD21	3:J:204:HOH:O	2.19	0.41
2:G:16:LEU:CD1	2:G:64:ILE:HD11	2.51	0.41
1:A:192:GLU:OE2	1:A:193:VAL:HG23	2.20	0.41
2:Z:99:LEU:HD23	2:Z:100:PRO:C	2.45	0.41
2:Z:106:ARG:N	2:Z:116:ALA:HB1	2.35	0.41
1:A:258:LYS:HE2	3:A:507:HOH:O	2.21	0.41
1:D:87:ARG:HD3	1:D:87:ARG:HA	1.88	0.41
1:P:222:LYS:HE2	3:P:743:HOH:O	2.20	0.41
1:P:362:LYS:HB3	1:P:362:LYS:HE2	1.77	0.41
1:A:134:PRO:HD2	1:A:202:PHE:HB2	2.03	0.41
1:A:195:PRO:HG3	3:A:764:HOH:O	2.20	0.41
1:D:109:LYS:HA	1:D:114:TYR:CD2	2.56	0.41
1:B:88:PRO:HB3	1:D:173:ARG:NH1	2.36	0.40
1:A:202:PHE:CD1	1:A:202:PHE:N	2.87	0.40
1:B:284:HIS:ND1	1:B:287:GLU:OE2	2.50	0.40
1:D:415:HIS:CD2	1:D:419:HIS:CE1	3.09	0.40
2:G:20:LYS:HA	2:G:20:LYS:HD2	1.70	0.40
1:A:158:GLY:H	1:A:161:ASP:CG	2.30	0.40
1:B:86:TRP:HB3	2:J:52:MET:HG3	2.02	0.40
1:P:184:PHE:HE2	1:P:202:PHE:CE2	2.40	0.40
2:J:67:ALA:HB2	2:G:97:PHE:CE1	2.56	0.40
1:A:109:LYS:HA	1:A:114:TYR:CD2	2.57	0.40
1:B:128:PHE:CG	1:B:253:LEU:HD13	2.56	0.40
1:M:77:ASP:OD1	1:M:79:SER:OG	2.23	0.40

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%)	360 (98%)	8 (2%)	45	65
1	B	371/400 (93%)	363 (98%)	8 (2%)	45	65
1	D	372/400 (93%)	362 (97%)	10 (3%)	39	58
1	M	376/400 (94%)	371 (99%)	5 (1%)	61	77
1	P	375/400 (94%)	371 (99%)	4 (1%)	65	81
1	Y	374/400 (94%)	361 (96%)	13 (4%)	32	48
2	G	72/115 (63%)	66 (92%)	6 (8%)	10	14
2	J	76/115 (66%)	71 (93%)	5 (7%)	15	21
2	Z	76/115 (66%)	66 (87%)	10 (13%)	4	4
All	All	2460/2745 (90%)	2391 (97%)	69 (3%)	38	56

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	136	LEU
1	A	192	GLU
1	A	209	CYS
1	A	252	SER
1	A	390	SER
1	A	406	LYS
1	A	422	CYS
1	B	18	LYS
1	B	172	ARG
1	B	192	GLU
1	B	252	SER
1	B	260	VAL
1	B	268	THR
1	B	320	SER
1	B	321	SER
1	D	8	THR
1	D	10	LYS
1	D	18	LYS
1	D	25	ILE
1	D	136	LEU
1	D	192	GLU
1	D	209	CYS
1	D	224	ILE
1	D	243	ASN
1	D	422	CYS

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Mol	Chain	Res	Type
1	Y	32	THR
1	Y	51	GLU
1	Y	65	THR
1	Y	68	GLU
1	Y	136	LEU
1	Y	204	PHE
1	Y	243	ASN
1	Y	256	ASP
1	Y	260	VAL
1	Y	315	SER
1	Y	379	SER
1	Y	418	SER
1	Y	425	GLU
1	M	95	ARG
1	M	124	GLU
1	M	192	GLU
1	M	209	CYS
1	M	315	SER
1	P	150	THR
1	P	321	SER
1	P	328	THR
1	P	390	SER
2	J	5	LYS
2	J	26	ILE
2	J	31	LEU
2	J	34	SER
2	J	98	VAL
2	G	11	ILE
2	G	31	LEU
2	G	33	VAL
2	G	64	ILE
2	G	77	ILE
2	G	112	THR
2	Z	11	ILE
2	Z	16	LEU
2	Z	23	LEU
2	Z	29	SER
2	Z	37	SER
2	Z	78	GLU
2	Z	104	VAL
2	Z	107	ILE
2	Z	111	GLU

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Mol	Chain	Res	Type
2	Z	117	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	ASN
1	A	374	ASN
1	A	377	HIS
1	A	419	HIS
1	B	52	ASN
1	B	181	HIS
1	B	293	ASN
1	B	317	GLN
1	D	52	ASN
1	D	293	ASN
1	D	372	ASN
1	D	374	ASN
1	Y	272	GLN
1	Y	293	ASN
1	Y	331	ASN
1	Y	415	HIS
1	M	181	HIS
1	M	185	GLN
1	M	190	HIS
1	M	251	GLN
1	M	372	ASN
1	P	131	ASN
1	P	213	ASN
1	P	250	ASN
1	P	272	GLN
1	P	372	ASN
1	P	419	HIS
2	J	69	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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, 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(Å ²)	Q<0.9
1	A	442/467 (94%)	1.14	76 (17%) 4 4	17, 26, 49, 81	0
1	B	442/467 (94%)	1.16	81 (18%) 3 4	17, 27, 49, 97	0
1	D	442/467 (94%)	1.22	79 (17%) 3 4	17, 27, 46, 76	0
1	M	443/467 (94%)	1.25	101 (22%) 2 2	17, 27, 54, 83	0
1	P	443/467 (94%)	1.28	86 (19%) 3 3	17, 27, 47, 90	0
1	Y	443/467 (94%)	1.13	75 (16%) 4 5	16, 26, 47, 97	0
2	G	95/137 (69%)	3.32	83 (87%) 0 0	38, 76, 105, 124	0
2	J	97/137 (70%)	3.23	87 (89%) 0 0	37, 75, 103, 125	0
2	Z	97/137 (70%)	3.37	86 (88%) 0 0	38, 84, 113, 133	0
All	All	2944/3213 (91%)	1.40	754 (25%) 1 2	16, 28, 78, 133	0

All (754) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	84	ALA	8.5
2	Z	104	VAL	7.7
2	J	22	GLU	6.5
2	G	26	ILE	6.3
1	P	65	THR	6.0
2	Z	95	LYS	5.9
2	Z	29	SER	5.8
2	G	84	ALA	5.7
1	A	90	THR	5.6
2	Z	94	GLY	5.5
2	J	94	GLY	5.4
1	D	63	GLY	5.4
2	J	98	VAL	5.3
2	Z	114	PRO	5.3
1	Y	316	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
2	G	16	LEU	5.2
2	J	83	GLY	5.2
1	B	320	SER	5.1
2	G	83	GLY	5.1
2	Z	59	LEU	5.1
2	G	23	LEU	5.0
2	G	99	LEU	5.0
2	Z	44	GLY	4.9
2	Z	6	TYR	4.9
2	J	64	ILE	4.9
2	Z	69	ASN	4.9
2	J	82	THR	4.9
2	G	30	ARG	4.8
2	J	99	LEU	4.8
2	Z	103	ASN	4.8
1	D	368	GLY	4.8
2	G	104	VAL	4.8
2	Z	109	THR	4.8
2	Z	28	VAL	4.8
2	J	24	GLN	4.7
2	J	69	ASN	4.7
1	P	380	ASP	4.7
2	G	97	PHE	4.7
2	G	72	PHE	4.7
2	J	38	GLY	4.7
2	J	104	VAL	4.6
2	J	95	LYS	4.6
2	Z	33	VAL	4.6
2	G	38	GLY	4.6
2	J	96	ILE	4.6
2	J	23	LEU	4.5
1	A	376	PHE	4.5
2	G	105	ILE	4.5
2	Z	80	ILE	4.5
2	Z	100	PRO	4.5
1	A	308	ALA	4.5
2	Z	71	GLU	4.5
1	Y	67	ILE	4.5
1	M	376	PHE	4.5
2	Z	67	ALA	4.5
2	G	69	ASN	4.5
1	P	373	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
2	G	29	SER	4.4
2	J	4	MET	4.4
2	Z	84	ALA	4.4
2	G	75	PRO	4.4
1	Y	64	PHE	4.4
2	J	31	LEU	4.4
1	B	71	ASP	4.3
2	J	109	THR	4.3
2	G	107	ILE	4.3
2	G	68	VAL	4.2
2	G	9	ALA	4.2
2	G	117	ILE	4.2
2	Z	45	TYR	4.2
1	B	376	PHE	4.2
1	M	65	THR	4.2
2	G	31	LEU	4.2
1	P	332	GLY	4.2
2	Z	61	LYS	4.2
2	Z	76	THR	4.2
2	Z	111	GLU	4.2
2	J	86	GLY	4.1
2	G	28	VAL	4.1
1	A	264	PRO	4.1
2	Z	85	LYS	4.1
2	Z	79	ALA	4.1
2	J	59	LEU	4.1
2	Z	16	LEU	4.1
2	G	95	LYS	4.0
1	A	379	SER	4.0
2	J	101	LEU	4.0
1	B	65	THR	4.0
2	Z	86	GLY	4.0
1	A	276	TYR	4.0
2	G	45	TYR	4.0
1	P	270	LEU	4.0
1	D	333	THR	4.0
2	Z	97	PHE	4.0
2	G	71	GLU	4.0
2	G	66	ILE	4.0
1	B	326	PRO	4.0
1	Y	66	ARG	4.0
2	Z	82	THR	4.0

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Mol	Chain	Res	Type	RSRZ
2	J	49	TYR	4.0
2	J	77	ILE	4.0
2	G	81	LYS	3.9
1	Y	309	PRO	3.9
1	P	317	GLN	3.9
1	A	91	GLY	3.9
2	G	70	ASP	3.9
2	G	20	LYS	3.9
1	P	375	ILE	3.9
2	G	24	GLN	3.9
2	Z	99	LEU	3.9
1	M	8	THR	3.9
1	Y	264	PRO	3.9
1	Y	177	TYR	3.9
1	M	282	LEU	3.9
2	G	59	LEU	3.9
1	Y	8	THR	3.9
2	J	72	PHE	3.8
2	G	100	PRO	3.8
2	Z	31	LEU	3.8
2	Z	110	ASN	3.8
2	Z	105	ILE	3.8
1	M	321	SER	3.8
2	G	15	ARG	3.8
2	J	110	ASN	3.8
1	A	413	GLY	3.8
1	A	266	THR	3.7
2	G	82	THR	3.7
2	G	114	PRO	3.7
1	P	376	PHE	3.7
2	J	97	PHE	3.7
2	G	11	ILE	3.7
2	J	28	VAL	3.7
1	B	318	ASN	3.7
2	Z	106	ARG	3.7
2	J	26	ILE	3.7
2	G	86	GLY	3.7
2	Z	83	GLY	3.7
1	B	373	VAL	3.7
1	D	308	ALA	3.7
1	A	388	ILE	3.7
1	P	100	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	309	PRO	3.7
1	Y	50	PHE	3.6
1	Y	46	LEU	3.6
1	P	310	VAL	3.6
2	G	17	ASP	3.6
1	P	398	ALA	3.6
2	G	18	ALA	3.6
2	J	37	SER	3.6
1	M	348	LEU	3.6
2	Z	98	VAL	3.6
2	G	116	ALA	3.6
1	Y	317	GLN	3.6
1	D	375	ILE	3.6
1	M	330	GLY	3.6
2	Z	17	ASP	3.6
2	Z	32	THR	3.6
2	J	79	ALA	3.6
2	G	79	ALA	3.6
2	Z	4	MET	3.6
1	M	375	ILE	3.6
2	Z	26	ILE	3.6
2	Z	107	ILE	3.6
1	D	64	PHE	3.6
2	Z	30	ARG	3.5
2	G	77	ILE	3.5
1	B	377	HIS	3.5
1	Y	225	ALA	3.5
1	M	317	GLN	3.5
2	Z	15	ARG	3.5
2	J	29	SER	3.5
1	A	306	TYR	3.5
2	Z	96	ILE	3.5
1	A	184	PHE	3.5
1	B	64	PHE	3.5
1	M	349	ALA	3.5
2	G	67	ALA	3.5
2	G	96	ILE	3.5
1	D	376	PHE	3.5
2	Z	23	LEU	3.5
2	J	114	PRO	3.5
1	P	220	VAL	3.5
2	G	33	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	321	SER	3.5
2	Z	63	LYS	3.5
2	G	47	GLU	3.5
2	G	44	GLY	3.4
2	G	111	GLU	3.4
1	A	375	ILE	3.4
2	G	64	ILE	3.4
2	G	80	ILE	3.4
2	Z	64	ILE	3.4
1	M	311	TYR	3.4
2	G	110	ASN	3.4
2	G	4	MET	3.4
2	G	46	MET	3.4
2	G	7	VAL	3.4
2	Z	68	VAL	3.4
2	Z	62	ILE	3.4
2	Z	117	ILE	3.4
2	G	19	VAL	3.4
1	Y	63	GLY	3.4
2	J	11	ILE	3.4
2	J	20	LYS	3.4
2	J	73	LEU	3.4
1	M	306	TYR	3.4
2	G	76	THR	3.4
2	Z	11	ILE	3.3
2	Z	48	ILE	3.3
1	P	90	THR	3.3
1	P	371	THR	3.3
1	P	385	GLU	3.3
2	Z	27	GLU	3.3
1	D	70	SER	3.3
1	P	330	GLY	3.3
2	Z	73	LEU	3.3
1	A	262	TYR	3.3
1	B	69	GLU	3.3
1	Y	379	SER	3.3
1	M	373	VAL	3.3
2	G	98	VAL	3.3
1	M	318	ASN	3.3
2	J	62	ILE	3.3
2	J	105	ILE	3.3
1	Y	65	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	6	LYS	3.3
1	Y	54	VAL	3.3
1	B	25	ILE	3.3
2	J	80	ILE	3.3
2	Z	21	ARG	3.3
2	Z	102	GLU	3.3
1	D	65	THR	3.3
1	D	45	GLN	3.3
2	J	7	VAL	3.3
2	Z	36	VAL	3.3
1	Y	387	GLY	3.2
1	M	331	ASN	3.2
1	D	388	ILE	3.2
2	J	85	LYS	3.2
2	J	100	PRO	3.2
1	M	90	THR	3.2
2	Z	72	PHE	3.2
2	Z	49	TYR	3.2
1	B	48	GLU	3.2
1	A	116	LEU	3.2
1	Y	102	LEU	3.2
1	P	282	LEU	3.2
2	Z	75	PRO	3.2
2	J	48	ILE	3.2
1	A	305	GLY	3.2
1	B	6	LYS	3.2
2	J	5	LYS	3.2
2	Z	14	GLU	3.2
1	M	67	ILE	3.2
1	D	133	GLY	3.2
1	P	163	ALA	3.2
1	P	411	ALA	3.2
2	J	36	VAL	3.2
2	G	73	LEU	3.2
2	G	8	ILE	3.2
1	Y	266	THR	3.2
2	J	108	ARG	3.1
1	Y	315	SER	3.1
2	Z	112	THR	3.1
2	G	14	GLU	3.1
1	B	24	PHE	3.1
2	J	18	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	Y	329	ARG	3.1
2	J	12	ARG	3.1
1	A	65	THR	3.1
2	Z	35	SER	3.1
1	B	261	PHE	3.1
1	M	265	ASP	3.1
2	Z	101	LEU	3.1
2	J	107	ILE	3.1
1	A	415	HIS	3.1
1	B	308	ALA	3.1
1	A	78	PRO	3.1
1	M	383	ARG	3.1
2	J	78	GLU	3.0
1	P	325	ILE	3.0
1	D	387	GLY	3.0
1	D	329	ARG	3.0
1	A	309	PRO	3.0
2	Z	13	PRO	3.0
1	B	384	GLU	3.0
2	G	112	THR	3.0
1	D	380	ASP	3.0
1	B	370	PRO	3.0
1	B	378	LEU	3.0
1	D	311	TYR	3.0
1	M	252	SER	3.0
2	Z	38	GLY	3.0
1	D	254	PHE	3.0
2	Z	58	LEU	3.0
1	A	9	THR	3.0
1	M	9	THR	3.0
1	Y	39	TRP	3.0
1	Y	307	GLU	3.0
2	J	14	GLU	3.0
2	J	16	LEU	2.9
2	Z	8	ILE	2.9
1	B	311	TYR	2.9
2	G	34	SER	2.9
1	Y	303	VAL	2.9
2	G	85	LYS	2.9
1	A	67	ILE	2.9
1	M	186	ILE	2.9
1	A	321	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	264	PRO	2.9
1	M	364	LYS	2.9
2	J	15	ARG	2.9
2	J	19	VAL	2.9
1	D	30	THR	2.9
2	J	71	GLU	2.9
2	Z	78	GLU	2.9
2	J	30	ARG	2.9
1	P	136	LEU	2.9
1	M	344	CYS	2.9
2	G	74	GLU	2.9
1	D	71	ASP	2.9
1	P	320	SER	2.8
1	B	267	PRO	2.8
1	Y	267	PRO	2.8
1	P	159	TYR	2.8
1	A	24	PHE	2.8
2	Z	9	ALA	2.8
1	B	314	TRP	2.8
1	A	377	HIS	2.8
1	P	378	LEU	2.8
2	J	3	ALA	2.8
2	J	68	VAL	2.8
1	M	388	ILE	2.8
1	P	328	THR	2.8
1	D	385	GLU	2.8
1	M	204	PHE	2.8
1	D	415	HIS	2.8
2	G	35	SER	2.8
1	A	304	PRO	2.8
1	M	309	PRO	2.8
1	P	384	GLU	2.8
2	J	65	GLU	2.8
1	P	89	ALA	2.8
1	M	24	PHE	2.8
1	D	377	HIS	2.7
1	M	325	ILE	2.7
1	P	318	ASN	2.7
2	Z	70	ASP	2.7
1	M	387	GLY	2.7
1	P	314	TRP	2.7
2	J	34	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	134	PRO	2.7
1	A	68	GLU	2.7
1	P	412	LEU	2.7
1	Y	423	ALA	2.7
1	A	380	ASP	2.7
1	Y	90	THR	2.7
2	J	66	ILE	2.7
2	G	103	ASN	2.7
1	M	379	SER	2.7
1	A	236	PRO	2.7
1	M	103	PRO	2.7
1	M	384	GLU	2.7
1	D	270	LEU	2.7
1	D	281	LEU	2.7
1	M	87	ARG	2.7
2	Z	12	ARG	2.7
1	D	327	ALA	2.7
2	J	33	VAL	2.7
1	Y	213	ASN	2.7
1	Y	318	ASN	2.7
2	J	70	ASP	2.7
1	M	360	GLY	2.7
2	J	25	LYS	2.7
2	G	22	GLU	2.7
1	D	49	ALA	2.7
2	J	67	ALA	2.7
1	B	306	TYR	2.7
2	J	45	TYR	2.7
2	G	6	TYR	2.7
1	M	366	ASP	2.7
1	D	69	GLU	2.7
1	D	307	GLU	2.7
1	A	186	ILE	2.7
1	A	335	ILE	2.7
2	J	117	ILE	2.7
1	D	107	PRO	2.7
1	Y	236	PRO	2.7
1	P	304	PRO	2.7
1	Y	327	ALA	2.6
1	M	316	ALA	2.6
1	P	49	ALA	2.6
2	Z	24	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	64	PHE	2.6
1	B	260	VAL	2.6
1	B	374	ASN	2.6
2	J	47	GLU	2.6
1	P	319	ARG	2.6
2	J	21	ARG	2.6
1	Y	181	HIS	2.6
1	Y	89	ALA	2.6
1	D	277	TYR	2.6
2	J	113	GLY	2.6
1	P	88	PRO	2.6
1	M	378	LEU	2.6
1	M	5	LYS	2.6
1	B	307	GLU	2.6
1	A	211	ALA	2.6
1	B	89	ALA	2.6
1	P	123	ALA	2.6
1	A	374	ASN	2.6
1	B	372	ASN	2.6
1	A	371	THR	2.6
1	D	303	VAL	2.6
1	Y	9	THR	2.6
1	Y	105	GLY	2.6
1	Y	333	THR	2.6
1	Y	360	GLY	2.6
1	P	244	GLY	2.6
2	J	52	MET	2.6
1	M	377	HIS	2.6
1	P	284	HIS	2.6
1	B	282	LEU	2.6
1	B	336	GLU	2.6
1	D	66	ARG	2.6
2	G	108	ARG	2.6
1	M	308	ALA	2.6
1	M	263	ASP	2.6
1	P	213	ASN	2.6
1	Y	186	ILE	2.6
1	Y	320	SER	2.6
1	M	70	SER	2.6
2	J	6	TYR	2.6
1	M	354	LEU	2.5
2	Z	47	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	Z	116	ALA	2.5
1	Y	380	ASP	2.5
1	B	305	GLY	2.5
1	A	64	PHE	2.5
1	P	392	PRO	2.5
1	A	171	VAL	2.5
1	B	303	VAL	2.5
1	P	379	SER	2.5
2	J	8	ILE	2.5
1	A	317	GLN	2.5
1	M	277	TYR	2.5
1	D	92	ALA	2.5
1	A	88	PRO	2.5
2	J	81	LYS	2.5
2	Z	113	GLY	2.5
1	B	204	PHE	2.5
1	B	217	PHE	2.5
2	G	37	SER	2.5
1	B	312	ILE	2.5
1	A	307	GLU	2.5
1	P	382	GLU	2.5
2	J	74	GLU	2.5
1	B	319	ARG	2.5
1	M	66	ARG	2.5
2	Z	108	ARG	2.5
1	A	270	LEU	2.5
2	G	10	MET	2.5
1	D	265	ASP	2.5
1	D	381	LYS	2.5
1	M	362	LYS	2.5
2	J	103	ASN	2.5
2	G	113	GLY	2.5
1	A	418	SER	2.5
1	B	15	GLU	2.5
1	Y	252	SER	2.5
2	J	115	GLU	2.5
1	A	311	TYR	2.5
1	P	311	TYR	2.5
1	M	6	LYS	2.5
1	A	316	ALA	2.5
1	P	377	HIS	2.5
1	M	280	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	385	GLU	2.4
2	J	112	THR	2.4
2	G	65	GLU	2.4
1	B	184	PHE	2.4
1	M	261	PHE	2.4
1	M	312	ILE	2.4
1	P	67	ILE	2.4
1	D	262	TYR	2.4
1	M	270	LEU	2.4
1	M	299	TYR	2.4
1	M	337	LEU	2.4
1	A	206	ASP	2.4
1	M	256	ASP	2.4
1	M	372	ASN	2.4
1	P	366	ASP	2.4
1	P	374	ASN	2.4
1	A	410	GLU	2.4
1	B	382	GLU	2.4
1	B	383	ARG	2.4
2	J	106	ARG	2.4
2	G	51	ALA	2.4
1	Y	58	GLY	2.4
2	G	60	GLU	2.4
1	D	118	THR	2.4
1	D	328	THR	2.4
2	J	76	THR	2.4
1	A	271	SER	2.4
1	A	204	PHE	2.4
1	B	67	ILE	2.4
1	Y	376	PHE	2.4
1	D	126	MET	2.4
2	J	46	MET	2.4
1	A	46	LEU	2.4
1	D	391	LEU	2.4
1	P	101	TYR	2.4
1	B	415	HIS	2.4
2	G	106	ARG	2.4
1	A	48	GLU	2.4
1	P	309	PRO	2.4
1	P	387	GLY	2.4
2	G	32	THR	2.4
1	B	388	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	417	PHE	2.4
1	P	86	TRP	2.4
2	G	21	ARG	2.4
1	Y	341	ASP	2.4
1	M	188	ALA	2.4
1	M	404	GLY	2.4
1	B	90	THR	2.4
1	D	18	LYS	2.4
2	Z	34	SER	2.4
1	B	128	PHE	2.4
1	Y	93	VAL	2.4
1	Y	323	ILE	2.4
1	P	126	MET	2.4
2	Z	66	ILE	2.4
1	A	14	LEU	2.4
1	Y	253	LEU	2.4
1	Y	334	ARG	2.4
1	M	62	GLN	2.4
1	D	263	ASP	2.3
1	P	276	TYR	2.3
1	D	267	PRO	2.3
1	B	49	ALA	2.3
1	Y	145	ALA	2.3
2	Z	37	SER	2.3
1	A	13	VAL	2.3
1	B	278	ILE	2.3
1	D	36	ILE	2.3
1	B	66	ARG	2.3
1	B	386	ARG	2.3
2	Z	74	GLU	2.3
1	P	21	ASP	2.3
1	D	306	TYR	2.3
1	P	236	PRO	2.3
1	A	49	ALA	2.3
1	A	274	ALA	2.3
2	J	116	ALA	2.3
1	A	8	THR	2.3
1	M	249	SER	2.3
1	B	335	ILE	2.3
1	B	93	VAL	2.3
1	M	68	GLU	2.3
1	D	104	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	259	ASN	2.3
1	Y	342	PRO	2.3
1	A	393	ALA	2.3
1	B	94	ALA	2.3
1	D	43	ALA	2.3
1	D	316	ALA	2.3
1	M	343	ALA	2.3
2	J	9	ALA	2.3
1	P	383	ARG	2.3
2	Z	115	GLU	2.3
1	Y	310	VAL	2.3
1	A	378	LEU	2.3
1	Y	322	LEU	2.3
1	M	281	LEU	2.3
1	P	381	LYS	2.3
1	D	346	PRO	2.3
1	P	149	PRO	2.3
1	Y	332	GLY	2.3
1	M	257	GLY	2.3
1	P	105	GLY	2.3
1	B	276	TYR	2.3
1	D	420	TYR	2.3
1	A	119	ALA	2.3
1	B	16	ALA	2.3
1	D	203	ARG	2.3
1	P	119	ALA	2.3
2	Z	50	ARG	2.3
2	J	32	THR	2.3
1	B	317	GLN	2.3
2	J	111	GLU	2.3
1	B	120	ILE	2.3
1	Y	56	PHE	2.2
1	P	24	PHE	2.2
1	P	207	VAL	2.3
1	Y	394	ASP	2.2
2	J	17	ASP	2.2
1	A	267	PRO	2.2
1	D	367	PRO	2.2
1	Y	78	PRO	2.2
2	G	13	PRO	2.2
1	A	110	GLY	2.2
1	M	305	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	10	MET	2.2
1	B	92	ALA	2.2
1	M	262	TYR	2.2
1	P	410	GLU	2.2
2	Z	20	LYS	2.2
2	Z	77	ILE	2.2
1	B	352	LEU	2.2
1	B	395	LEU	2.2
1	D	179	LEU	2.2
1	A	240	PHE	2.2
1	Y	204	PHE	2.2
1	P	54	VAL	2.2
1	A	42	PRO	2.2
1	Y	103	PRO	2.2
1	M	78	PRO	2.2
1	P	42	PRO	2.2
1	B	58	GLY	2.2
1	A	248	HIS	2.2
1	Y	382	GLU	2.2
1	M	336	GLU	2.2
2	G	78	GLU	2.2
1	A	349	ALA	2.2
1	M	216	THR	2.2
1	P	211	ALA	2.2
1	Y	86	TRP	2.2
1	P	83	ILE	2.2
1	D	354	LEU	2.2
1	M	358	LEU	2.2
1	P	33	LEU	2.2
1	Y	128	PHE	2.2
1	A	386	ARG	2.2
1	M	374	ASN	2.2
1	P	259	ASN	2.2
1	B	304	PRO	2.2
1	D	157	GLY	2.2
1	M	147	GLY	2.2
1	P	6	LYS	2.2
1	B	333	THR	2.2
1	M	177	TYR	2.2
1	P	262	TYR	2.2
1	D	395	LEU	2.2
1	M	323	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	310	VAL	2.2
1	M	220	VAL	2.2
1	D	304	PRO	2.2
1	P	414	GLU	2.2
1	P	425	GLU	2.2
1	A	62	GLN	2.2
1	M	63	GLY	2.2
1	B	8	THR	2.2
1	B	268	THR	2.2
1	A	324	ARG	2.1
1	D	325	ILE	2.1
1	D	358	LEU	2.1
1	A	296	VAL	2.1
1	D	261	PHE	2.1
1	Y	134	PRO	2.1
1	M	128	PHE	2.1
1	P	204	PHE	2.1
1	B	419	HIS	2.1
1	A	63	GLY	2.1
1	B	63	GLY	2.1
1	B	379	SER	2.1
1	M	119	ALA	2.1
1	M	319	ARG	2.1
1	Y	230	TYR	2.1
1	Y	361	ILE	2.1
1	B	68	GLU	2.1
1	D	374	ASN	2.1
2	G	27	GLU	2.1
1	B	88	PRO	2.1
1	B	264	PRO	2.1
1	D	416	VAL	2.1
1	M	134	PRO	2.1
1	M	310	VAL	2.1
1	A	158	GLY	2.1
1	D	127	GLY	2.1
1	Y	53	GLY	2.1
1	M	98	GLY	2.1
1	M	241	GLY	2.1
1	M	274	ALA	2.1
1	M	320	SER	2.1
1	D	256	ASP	2.1
1	D	312	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	378	LEU	2.1
1	M	71	ASP	2.1
1	Y	185	GLN	2.1
1	A	193	VAL	2.1
1	A	310	VAL	2.1
1	P	93	VAL	2.1
1	B	202	PHE	2.1
1	D	162	PHE	2.1
1	D	314	TRP	2.1
1	P	202	PHE	2.1
1	P	254	PHE	2.1
1	Y	383	ARG	2.1
2	G	12	ARG	2.1
1	B	313	SER	2.1
1	M	418	SER	2.1
1	P	252	SER	2.1
1	M	109	LYS	2.1
2	Z	25	LYS	2.1
2	G	102	GLU	2.1
1	B	322	LEU	2.1
1	M	21	ASP	2.1
1	M	185	GLN	2.1
1	M	415	HIS	2.1
1	B	177	TYR	2.1
1	D	276	TYR	2.1
1	D	350	PHE	2.1
1	Y	81	PHE	2.1
1	M	254	PHE	2.1
1	P	184	PHE	2.1
1	D	383	ARG	2.1
1	Y	258	LYS	2.0
1	M	406	LYS	2.0
1	A	268	THR	2.0
1	B	371	THR	2.0
1	B	343	ALA	2.0
1	Y	187	GLU	2.0
1	Y	384	GLU	2.0
1	M	423	ALA	2.0
2	Z	60	GLU	2.0
1	D	372	ASN	2.0
1	Y	104	ASP	2.0
1	M	165	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	Y	278	ILE	2.0
1	M	399	ILE	2.0
1	P	278	ILE	2.0
1	P	312	ILE	2.0
1	A	370	PRO	2.0
1	P	112	PRO	2.0
2	J	75	PRO	2.0
1	D	87	ARG	2.0
1	P	82	ARG	2.0
1	P	132	VAL	2.0
1	A	205	GLY	2.0
1	D	53	GLY	2.0
1	M	202	PHE	2.0
1	Y	18	LYS	2.0
1	P	73	LYS	2.0
1	P	275	MET	2.0
1	B	32	THR	2.0
1	P	210	THR	2.0
2	G	109	THR	2.0
1	B	253	LEU	2.0
1	B	259	ASN	2.0
1	A	367	PRO	2.0
1	Y	340	PRO	2.0
1	M	42	PRO	2.0
1	M	392	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.