



Full wwPDB X-ray Structure Validation Report i

Nov 7, 2023 – 07:26 PM EST

PDB ID : 8TGE
Title : Crystal structure of the Methanoscincus 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 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](#) i) 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 (Gargroves)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

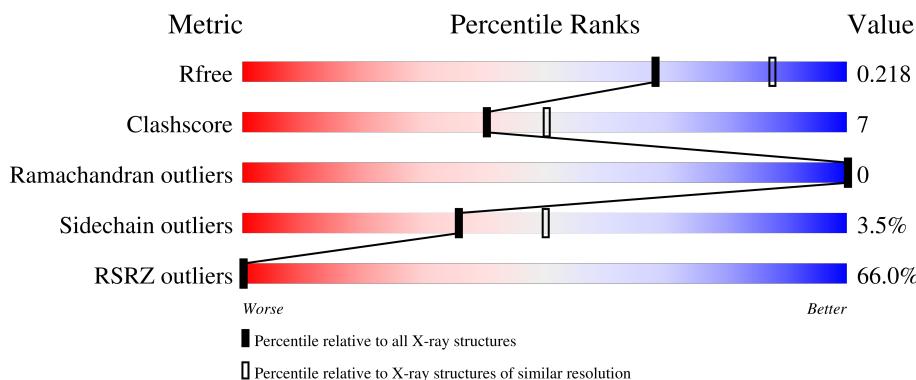
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

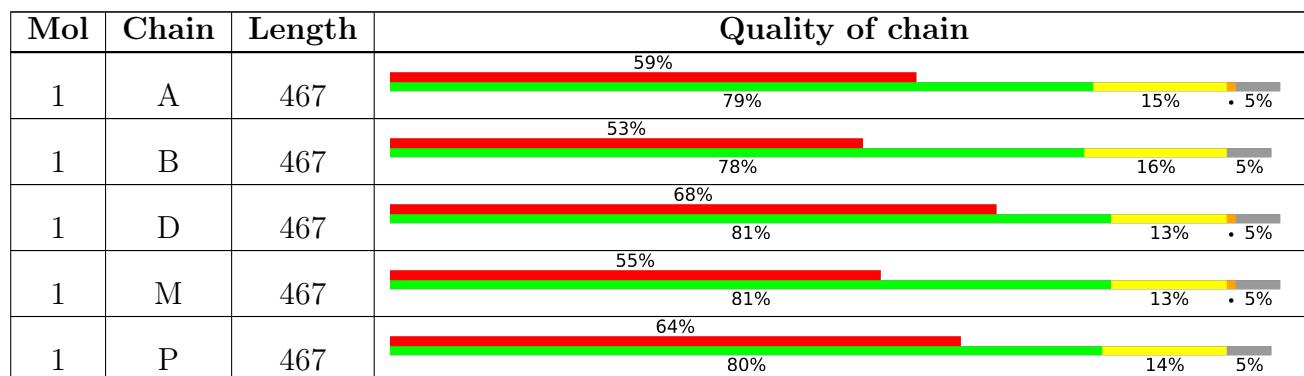
The reported resolution of this entry is 2.30 Å.

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.



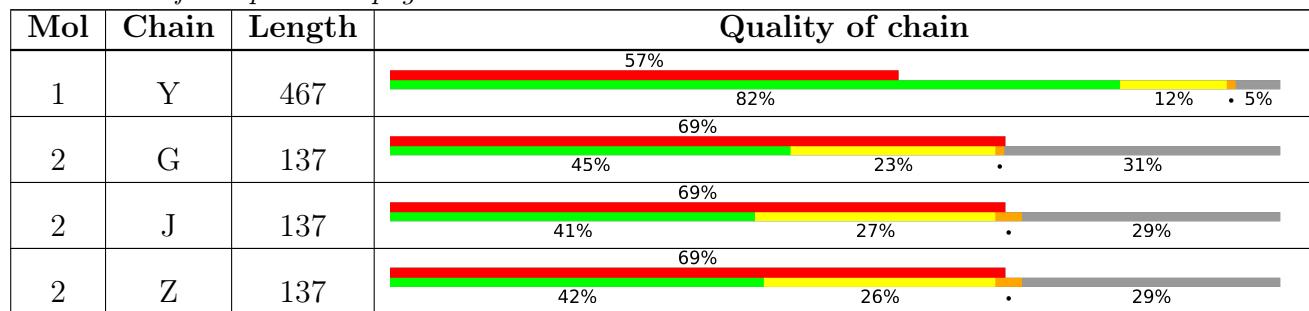
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 $\leq 5\%$. 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.



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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 3479	N 2225	O 588	S 649	17	0	0
1	B	442	Total	C 3490	N 2230	O 586	S 657	17	0	0
1	D	442	Total	C 3495	N 2233	O 588	S 657	17	0	0
1	Y	443	Total	C 3506	N 2242	O 589	S 658	17	0	0
1	M	443	Total	C 3518	N 2248	O 595	S 658	17	0	0
1	P	443	Total	C 3512	N 2245	O 592	S 658	17	0	0

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

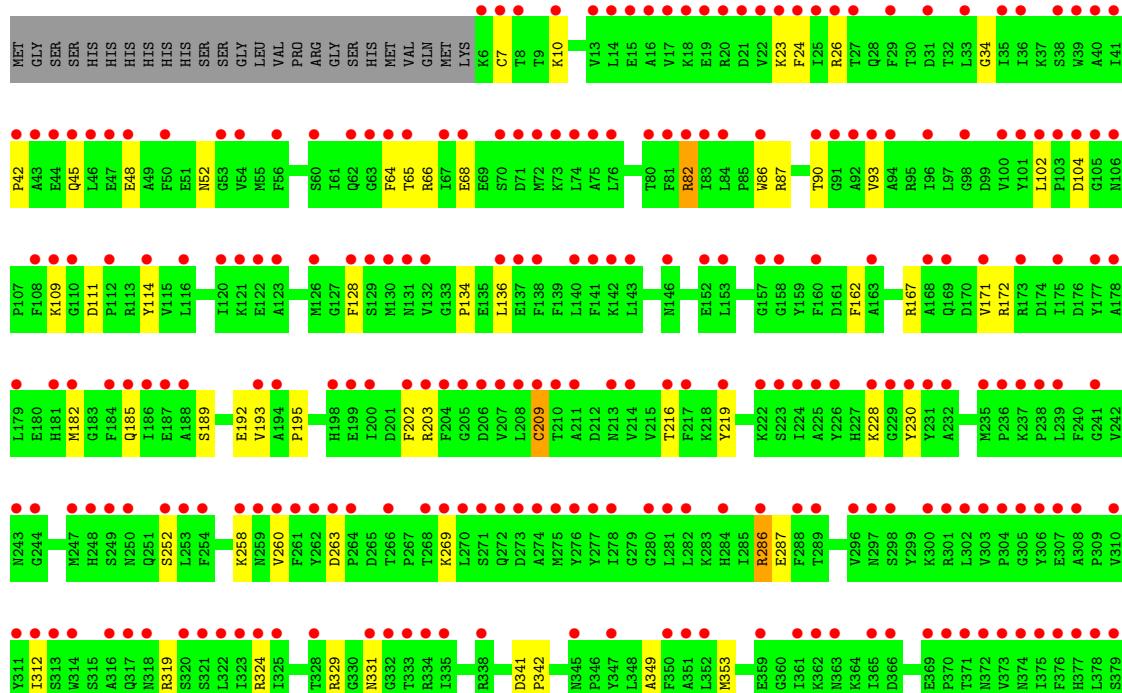
- Molecule 3 is water.

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

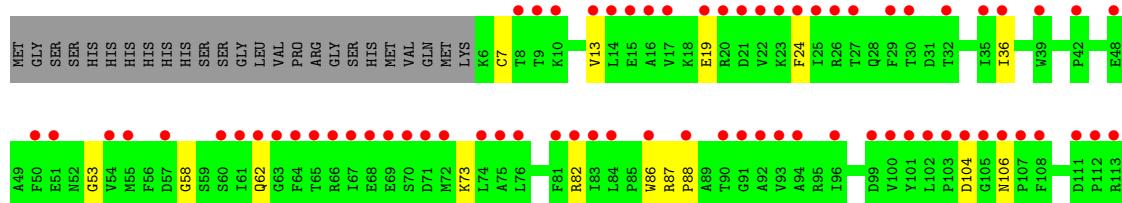
3 Residue-property plots

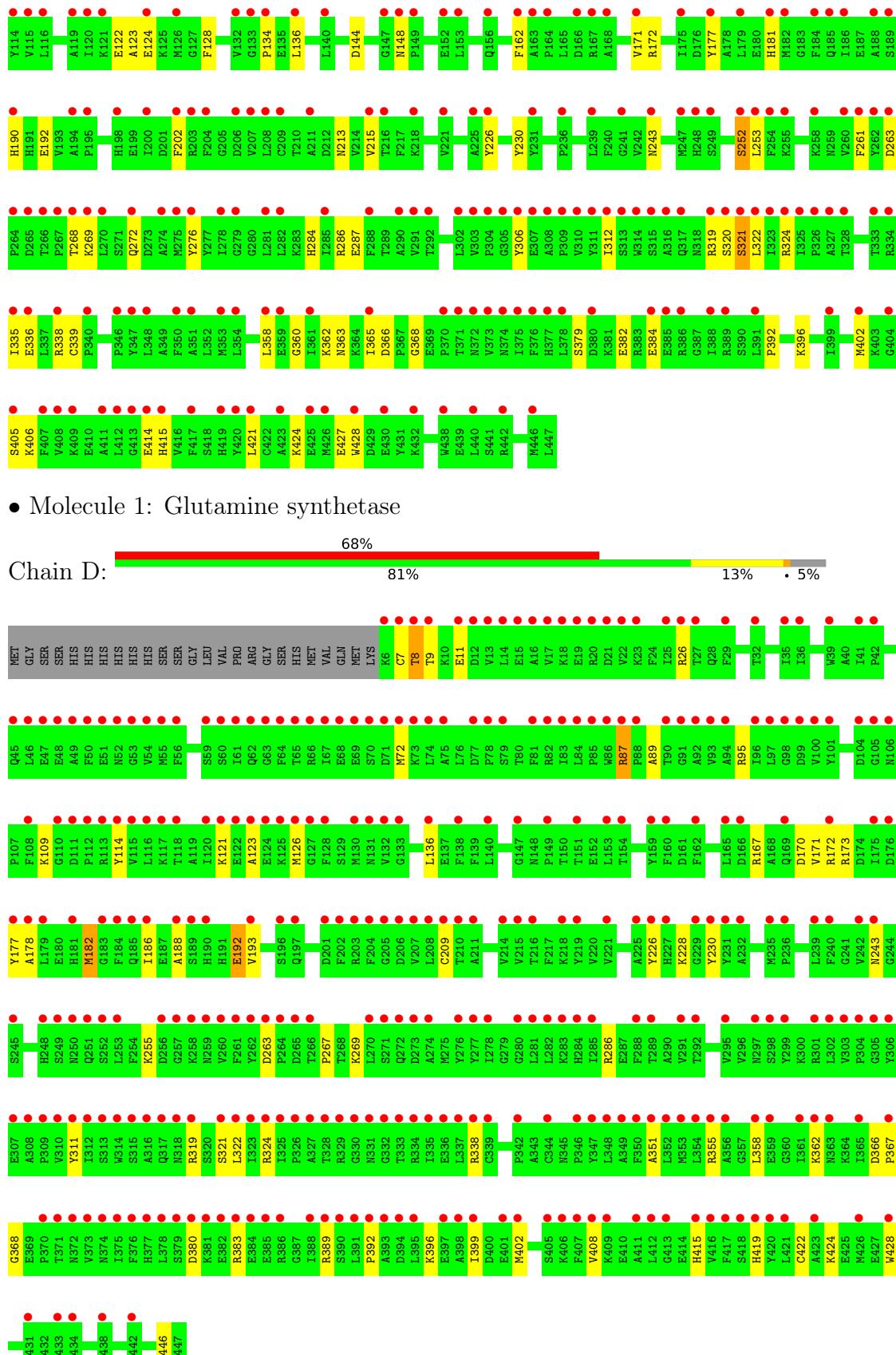
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

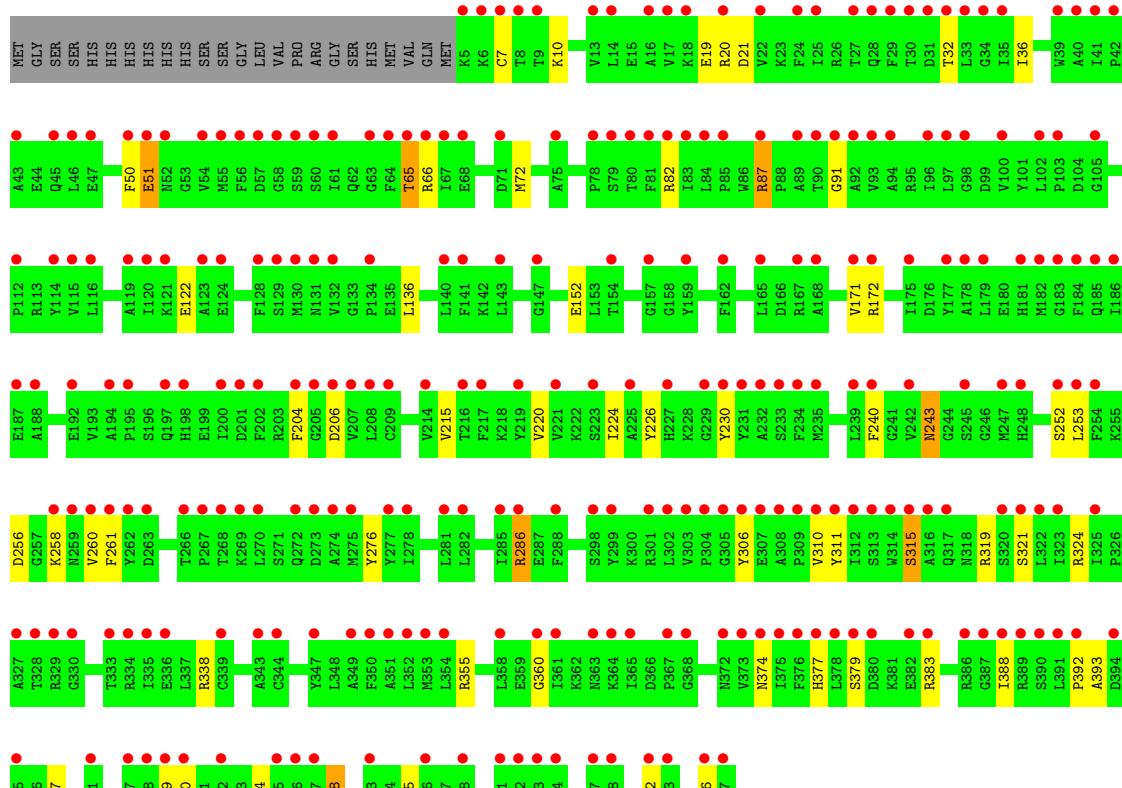
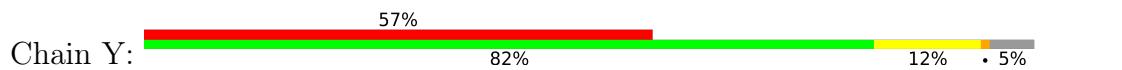


- Molecule 1: Glutamine synthetase

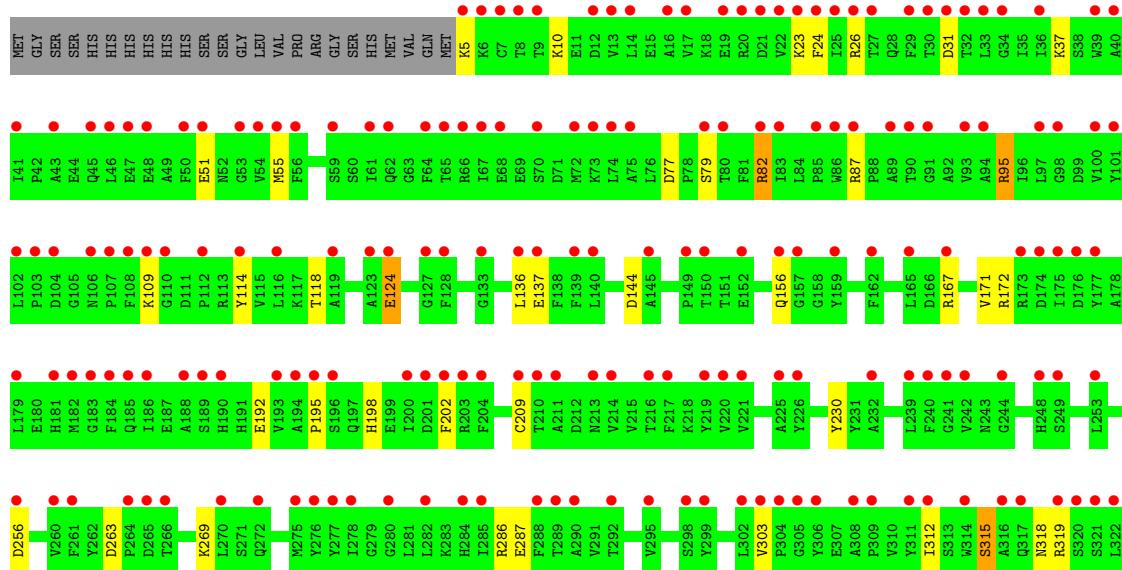
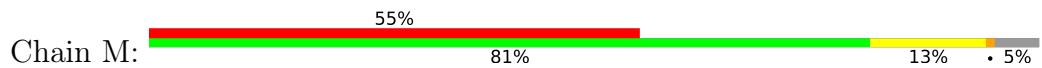




- Molecule 1: Glutamine synthetase

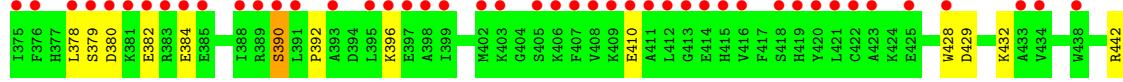
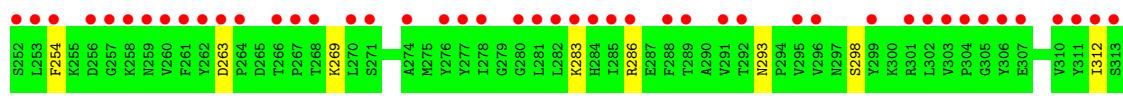
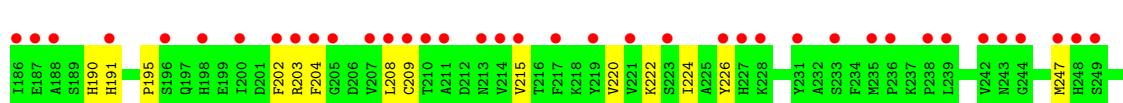
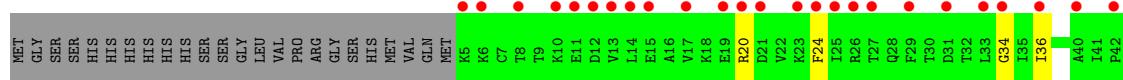
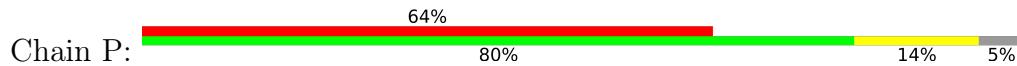


- Molecule 1: Glutamine synthetase

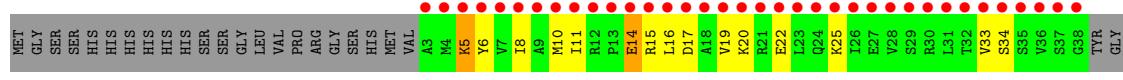




- Molecule 1: Glutamine synthetase

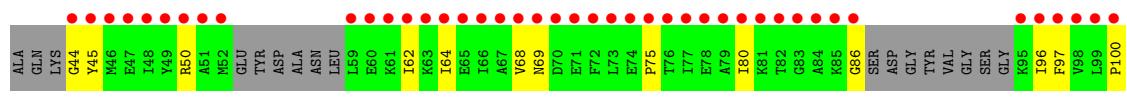
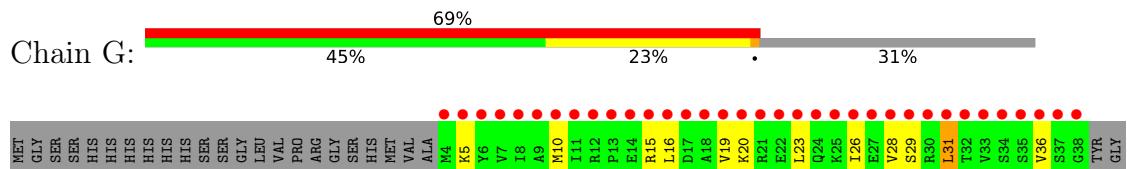


- Molecule 2: Nitrogen regulatory protein GlnK1

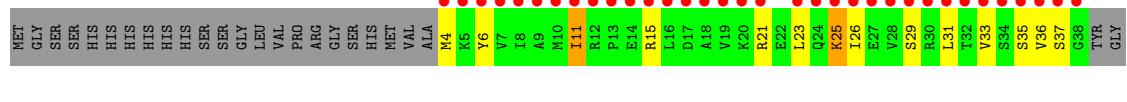




- Molecule 2: Nitrogen regulatory protein GlnK1



- 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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 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	0.41	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 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	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.

All (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
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
2:G:102:GLU:HB2	2:Z:100:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:P:82:ARG:HG2	1:P:182:MET:HE2	1.80	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
2:J:34:SER:HB3	2:G:36:VAL:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:D:89:ALA:O	2:G:50:ARG:NH1	2.39	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: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
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:Y:393:ALA:H	1:Y:397:GLU:CD	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:P:220:VAL:O	1:P:224:ILE:HG12	2.12	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
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
2:Z:109:THR:OG1	2:Z:111:GLU:OE1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:23:LYS:NZ	2:Z:47:GLU:OE2	2.33	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:M:77:ASP:OD1	1:M:79:SER:OG	2.23	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
2:Z:61:LYS:HA	2:Z:61:LYS:HD3	1.80	0.45
1:A:24:PHE:HE1	1:A:90:THR:HG1	1.64	0.44
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:D:366:ASP:CG	1:D:368:GLY:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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:M:375:ILE:HG22	1:M:383:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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:A:82:ARG:HG2	1:A:182:MET:HE2	2.02	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
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:287:GLU:OE1	1:B:405:SER:OG	2.20	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
2:Z:25:LYS:C	2:Z:26:ILE:HD13	2.40	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
1:M:424:LYS:NZ	1:M:427:GLU:OE1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:P:155:ASP:CG	1:P:191:HIS:HE2	2.25	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: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:Y:442:ARG:O	1:Y:446:MET:HE3	2.22	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%)	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
All	All	2460/2745 (90%)	2374 (96%)	86 (4%)	36 50

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	82	ARG
1	A	87	ARG
1	A	136	LEU
1	A	162	PHE
1	A	209	CYS
1	A	252	SER
1	A	286	ARG
1	A	384	GLU
1	A	390	SER
1	A	406	LYS
1	A	422	CYS
1	B	87	ARG
1	B	192	GLU
1	B	226	TYR
1	B	252	SER
1	B	268	THR
1	B	320	SER
1	B	321	SER
1	B	384	GLU
1	B	414	GLU
1	D	8	THR
1	D	72	MET
1	D	87	ARG
1	D	95	ARG
1	D	121	LYS
1	D	136	LEU
1	D	182	MET
1	D	192	GLU
1	D	209	CYS
1	D	243	ASN
1	D	422	CYS
1	Y	32	THR
1	Y	51	GLU
1	Y	65	THR
1	Y	72	MET
1	Y	82	ARG
1	Y	87	ARG
1	Y	136	LEU
1	Y	204	PHE
1	Y	206	ASP
1	Y	226	TYR
1	Y	243	ASN

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Mol	Chain	Res	Type
1	Y	256	ASP
1	Y	260	VAL
1	Y	286	ARG
1	Y	315	SER
1	Y	379	SER
1	Y	418	SER
1	Y	425	GLU
1	M	5	LYS
1	M	82	ARG
1	M	87	ARG
1	M	95	ARG
1	M	124	GLU
1	M	192	GLU
1	M	209	CYS
1	M	256	ASP
1	M	315	SER
1	M	406	LYS
1	P	20	ARG
1	P	24	PHE
1	P	87	ARG
1	P	162	PHE
1	P	204	PHE
1	P	226	TYR
1	P	321	SER
1	P	390	SER
1	P	410	GLU
2	J	5	LYS
2	J	14	GLU
2	J	98	VAL
2	J	106	ARG
2	G	31	LEU
2	G	69	ASN
2	G	106	ARG
2	G	112	THR
2	Z	11	ILE
2	Z	23	LEU
2	Z	25	LYS
2	Z	29	SER
2	Z	35	SER
2	Z	37	SER
2	Z	78	GLU
2	Z	106	ARG

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Mol	Chain	Res	Type
2	Z	111	GLU

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 i

6.1 Protein, DNA and RNA chains i

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%)	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

All (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
2	Z	59	LEU	20.0
2	G	73	LEU	18.9
2	Z	69	ASN	17.9
2	G	107	ILE	16.9
2	Z	17	ASP	15.8
2	J	96	ILE	15.6
2	J	31	LEU	15.4
2	J	4	MET	15.1
2	Z	98	VAL	14.7
2	Z	16	LEU	14.6

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Mol	Chain	Res	Type	RSRZ
2	J	105	ILE	14.6
2	G	86	GLY	14.2
2	J	94	GLY	14.0
2	Z	9	ALA	13.8
2	J	52	MET	13.7
2	Z	82	THR	13.0
2	G	7	VAL	13.0
2	G	28	VAL	13.0
2	J	30	ARG	13.0
2	J	101	LEU	13.0
2	G	97	PHE	12.8
2	Z	30	ARG	12.8
2	J	3	ALA	12.8
2	Z	67	ALA	12.7
2	G	72	PHE	12.6
2	Z	109	THR	12.2
2	G	38	GLY	12.1
2	J	38	GLY	12.1
2	J	59	LEU	12.0
2	J	26	ILE	11.9
2	G	20	LYS	11.8
2	J	23	LEU	11.8
2	G	33	VAL	11.6
2	G	4	MET	11.6
2	Z	28	VAL	11.5
2	Z	4	MET	11.5
2	J	49	TYR	11.4
2	G	59	LEU	11.3
1	A	171	VAL	11.3
2	Z	58	LEU	11.3
2	J	95	LYS	11.2
2	J	104	VAL	11.1
2	J	85	LYS	11.0
2	Z	104	VAL	10.8
2	Z	60	GLU	10.7
2	G	106	ARG	10.7
2	G	99	LEU	10.6
2	Z	97	PHE	10.6
2	J	86	GLY	10.6
2	G	68	VAL	10.5
2	J	98	VAL	10.5
2	J	8	ILE	10.5

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Mol	Chain	Res	Type	RSRZ
2	J	7	VAL	10.3
2	G	14	GLU	10.3
2	Z	68	VAL	10.3
2	G	31	LEU	10.3
2	Z	63	LYS	10.3
2	Z	64	ILE	10.2
2	J	25	LYS	10.2
2	G	61	LYS	10.1
2	G	32	THR	10.0
1	P	100	VAL	10.0
2	Z	11	ILE	10.0
2	Z	80	ILE	10.0
2	J	117	ILE	9.9
2	Z	114	PRO	9.8
1	A	178	ALA	9.8
2	Z	46	MET	9.6
2	J	83	GLY	9.6
2	Z	71	GLU	9.6
2	J	113	GLY	9.5
1	D	63	GLY	9.5
1	Y	102	LEU	9.5
2	Z	21	ARG	9.4
2	G	65	GLU	9.4
2	Z	115	GLU	9.4
2	Z	31	LEU	9.4
2	G	77	ILE	9.3
2	Z	99	LEU	9.3
1	M	317	GLN	9.3
2	G	104	VAL	9.2
1	B	326	PRO	9.2
2	G	12	ARG	9.2
2	G	11	ILE	9.2
2	Z	107	ILE	9.2
2	Z	111	GLU	9.1
2	Z	113	GLY	9.0
2	J	84	ALA	8.9
2	G	101	LEU	8.9
2	G	83	GLY	8.9
2	G	6	TYR	8.8
2	G	44	GLY	8.7
2	Z	106	ARG	8.7
2	J	70	ASP	8.7

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Mol	Chain	Res	Type	RSRZ
2	Z	94	GLY	8.7
2	G	70	ASP	8.6
2	G	23	LEU	8.6
2	G	108	ARG	8.6
1	A	94	ALA	8.5
2	J	18	ALA	8.5
2	Z	112	THR	8.5
2	J	99	LEU	8.5
1	B	184	PHE	8.4
2	J	110	ASN	8.4
2	Z	20	LYS	8.4
2	Z	70	ASP	8.3
2	G	84	ALA	8.3
2	Z	101	LEU	8.2
2	J	78	GLU	8.2
1	A	261	PHE	8.2
2	Z	105	ILE	8.1
2	Z	8	ILE	8.1
2	G	15	ARG	8.1
2	J	66	ILE	8.1
2	J	36	VAL	8.0
2	Z	110	ASN	8.0
1	Y	90	THR	7.9
2	J	10	MET	7.9
1	B	308	ALA	7.9
2	J	97	PHE	7.8
2	G	96	ILE	7.8
1	A	93	VAL	7.7
1	B	310	VAL	7.7
2	G	81	LYS	7.7
1	B	76	LEU	7.6
2	Z	49	TYR	7.6
1	Y	177	TYR	7.5
2	J	45	TYR	7.5
2	G	29	SER	7.5
2	J	77	ILE	7.5
1	D	308	ALA	7.5
1	D	358	LEU	7.5
2	G	69	ASN	7.5
2	Z	48	ILE	7.5
2	G	51	ALA	7.4
1	A	90	THR	7.4

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Mol	Chain	Res	Type	RSRZ
2	Z	61	LYS	7.4
2	J	32	THR	7.4
1	D	350	PHE	7.4
2	G	30	ARG	7.4
1	D	126	MET	7.3
1	P	126	MET	7.3
2	Z	95	LYS	7.3
2	G	18	ALA	7.3
2	Z	100	PRO	7.3
2	Z	73	LEU	7.3
1	A	312	ILE	7.2
2	J	15	ARG	7.2
2	J	35	SER	7.2
1	Y	39	TRP	7.1
1	A	378	LEU	7.1
2	J	21	ARG	7.1
2	J	19	VAL	7.1
2	Z	84	ALA	7.1
2	Z	52	MET	7.1
2	Z	86	GLY	7.1
2	Z	37	SER	7.0
2	Z	108	ARG	7.0
2	Z	75	PRO	7.0
1	D	303	VAL	7.0
2	Z	13	PRO	7.0
2	G	85	LYS	7.0
1	M	280	GLY	7.0
1	B	261	PHE	7.0
2	Z	117	ILE	7.0
1	A	446	MET	6.9
2	J	48	ILE	6.9
2	J	71	GLU	6.9
1	P	202	PHE	6.9
2	G	63	LYS	6.9
2	J	6	TYR	6.9
1	P	270	LEU	6.9
1	P	261	PHE	6.8
1	B	325	ILE	6.8
1	A	184	PHE	6.8
2	Z	24	GLN	6.8
2	Z	14	GLU	6.8
2	Z	96	ILE	6.7

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Mol	Chain	Res	Type	RSRZ
1	P	356	ALA	6.7
1	D	86	TRP	6.7
2	Z	15	ARG	6.7
1	B	92	ALA	6.7
2	G	67	ALA	6.6
2	Z	35	SER	6.6
2	Z	6	TYR	6.6
2	G	110	ASN	6.6
2	J	109	THR	6.6
2	G	26	ILE	6.6
2	J	34	SER	6.5
1	P	98	GLY	6.5
1	A	67	ILE	6.5
1	D	41	ILE	6.5
2	J	33	VAL	6.5
2	J	64	ILE	6.5
1	D	36	ILE	6.4
2	G	48	ILE	6.4
2	G	105	ILE	6.4
2	J	16	LEU	6.4
2	Z	27	GLU	6.4
1	P	327	ALA	6.4
2	G	82	THR	6.4
1	D	309	PRO	6.4
1	P	317	GLN	6.4
2	Z	76	THR	6.3
1	A	321	SER	6.3
1	B	376	PHE	6.3
1	A	14	LEU	6.3
1	A	202	PHE	6.3
1	A	101	TYR	6.3
2	J	37	SER	6.3
1	M	83	ILE	6.3
2	J	22	GLU	6.3
2	G	19	VAL	6.2
2	J	82	THR	6.2
1	D	330	GLY	6.2
2	J	68	VAL	6.2
1	P	103	PRO	6.2
1	D	116	LEU	6.2
1	D	385	GLU	6.1
1	M	378	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
2	J	50	ARG	6.1
2	J	106	ARG	6.1
2	J	51	ALA	6.1
2	Z	79	ALA	6.1
2	J	114	PRO	6.0
1	A	73	LYS	6.0
1	D	277	TYR	6.0
1	M	186	ILE	6.0
1	P	296	VAL	6.0
1	D	131	ASN	6.0
1	P	136	LEU	6.0
1	B	350	PHE	6.0
1	M	219	TYR	6.0
1	A	325	ILE	5.9
2	J	20	LYS	5.9
1	Y	205	GLY	5.9
1	D	204	PHE	5.9
1	M	149	PRO	5.9
1	B	65	THR	5.9
1	A	307	GLU	5.9
1	A	310	VAL	5.9
1	Y	260	VAL	5.9
1	D	361	ILE	5.9
1	P	112	PRO	5.8
2	G	114	PRO	5.8
2	Z	38	GLY	5.8
1	P	314	TRP	5.8
2	J	72	PHE	5.8
1	D	78	PRO	5.8
1	P	82	ARG	5.8
1	M	325	ILE	5.8
1	B	70	SER	5.8
1	B	101	TYR	5.8
2	J	80	ILE	5.8
1	P	376	PHE	5.7
1	Y	281	LEU	5.7
2	J	46	MET	5.7
2	Z	103	ASN	5.7
2	G	21	ARG	5.7
1	P	91	GLY	5.7
2	J	103	ASN	5.7
1	M	319	ARG	5.7

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Mol	Chain	Res	Type	RSRZ
1	M	327	ALA	5.7
1	P	373	VAL	5.7
2	G	103	ASN	5.7
2	Z	85	LYS	5.6
1	M	408	VAL	5.6
2	J	76	THR	5.6
2	Z	36	VAL	5.6
2	J	111	GLU	5.6
1	A	375	ILE	5.6
1	P	278	ILE	5.6
1	Y	303	VAL	5.6
1	Y	239	LEU	5.6
1	D	331	ASN	5.5
1	P	311	TYR	5.5
1	P	352	LEU	5.5
1	M	393	ALA	5.5
1	A	186	ILE	5.5
1	M	202	PHE	5.5
1	M	387	GLY	5.5
1	A	306	TYR	5.5
1	Y	162	PHE	5.5
1	B	30	THR	5.5
2	Z	26	ILE	5.5
1	P	207	VAL	5.5
1	Y	311	TYR	5.5
1	D	333	THR	5.4
1	M	183	GLY	5.4
1	A	103	PRO	5.4
1	D	347	TYR	5.4
1	D	260	VAL	5.4
1	M	165	LEU	5.4
1	D	379	SER	5.4
1	Y	25	ILE	5.4
1	B	104	ASP	5.4
2	J	29	SER	5.4
1	B	82	ARG	5.4
1	M	67	ILE	5.3
1	D	395	LEU	5.3
1	D	362	LYS	5.3
1	M	289	THR	5.3
1	P	132	VAL	5.3
2	J	100	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
2	J	47	GLU	5.3
1	D	312	ILE	5.3
1	P	188	ALA	5.3
1	A	371	THR	5.3
1	D	314	TRP	5.3
1	P	374	ASN	5.3
1	P	254	PHE	5.3
2	J	116	ALA	5.3
1	A	65	THR	5.3
1	Y	22	VAL	5.3
2	G	98	VAL	5.3
1	M	316	ALA	5.3
1	A	376	PHE	5.3
1	P	67	ILE	5.3
1	M	20	ARG	5.3
1	D	25	ILE	5.2
1	D	391	LEU	5.2
1	B	71	ASP	5.2
1	P	182	MET	5.2
1	Y	350	PHE	5.2
2	Z	72	PHE	5.2
1	P	186	ILE	5.2
2	G	64	ILE	5.2
1	Y	181	HIS	5.2
1	A	132	VAL	5.2
1	P	209	CYS	5.2
1	B	335	ILE	5.2
1	Y	358	LEU	5.2
1	A	26	ARG	5.2
1	B	320	SER	5.2
1	Y	204	PHE	5.2
1	P	349	ALA	5.2
1	B	64	PHE	5.2
2	G	49	TYR	5.2
1	A	380	ASP	5.2
1	Y	334	ARG	5.1
2	G	117	ILE	5.1
2	Z	102	GLU	5.1
1	D	88	PRO	5.1
1	D	399	ILE	5.1
2	G	62	ILE	5.1
2	Z	62	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
2	Z	44	GLY	5.1
1	A	381	LYS	5.1
1	D	380	ASP	5.1
1	M	90	THR	5.1
1	Y	47	GLU	5.1
2	Z	50	ARG	5.1
1	B	288	PHE	5.1
1	M	335	ILE	5.1
1	P	24	PHE	5.1
2	G	8	ILE	5.1
1	P	282	LEU	5.1
2	J	60	GLU	5.1
1	A	254	PHE	5.1
1	A	42	PRO	5.0
1	D	365	ILE	5.1
1	M	65	THR	5.0
1	M	331	ASN	5.0
1	D	407	PHE	5.0
1	D	65	THR	5.0
1	B	314	TRP	5.0
1	Y	378	LEU	5.0
1	M	239	LEU	5.0
1	A	211	ALA	5.0
1	P	332	GLY	5.0
2	Z	7	VAL	5.0
2	J	11	ILE	5.0
1	M	116	LEU	5.0
1	P	208	LEU	5.0
1	A	393	ALA	5.0
1	D	92	ALA	5.0
2	J	9	ALA	5.0
1	P	248	HIS	5.0
1	P	271	SER	5.0
1	P	390	SER	5.0
1	A	81	PHE	5.0
1	P	345	ASN	5.0
1	P	380	ASP	5.0
1	Y	230	TYR	5.0
1	D	128	PHE	5.0
1	M	24	PHE	5.0
1	M	375	ILE	5.0
1	D	351	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	Y	66	ARG	4.9
1	D	276	TYR	4.9
1	D	398	ALA	4.9
1	P	365	ILE	4.9
1	M	447	LEU	4.9
1	M	26	ARG	4.9
1	D	98	GLY	4.9
1	P	295	VAL	4.9
2	J	5	LYS	4.9
1	D	93	VAL	4.9
1	Y	248	HIS	4.9
1	P	312	ILE	4.9
1	Y	56	PHE	4.9
1	P	89	ALA	4.9
1	D	311	TYR	4.9
1	P	310	VAL	4.9
1	D	183	GLY	4.9
1	A	276	TYR	4.9
1	D	281	LEU	4.9
1	P	337	LEU	4.9
1	A	130	MET	4.9
1	P	316	ALA	4.8
1	A	270	LEU	4.8
2	Z	45	TYR	4.8
1	P	393	ALA	4.8
1	P	253	LEU	4.8
1	D	50	PHE	4.8
1	D	377	HIS	4.8
1	P	328	THR	4.8
1	A	260	VAL	4.8
2	G	46	MET	4.8
1	Y	347	TYR	4.8
1	D	256	ASP	4.8
1	P	343	ALA	4.8
1	B	269	LYS	4.8
1	Y	46	LEU	4.8
1	D	209	CYS	4.7
2	J	14	GLU	4.7
1	D	29	PHE	4.7
1	D	310	VAL	4.7
1	P	26	ARG	4.7
1	Y	96	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	M	379	SER	4.7
1	M	103	PRO	4.7
2	J	102	GLU	4.7
1	D	316	ALA	4.7
1	B	389	ARG	4.7
1	D	72	MET	4.7
1	P	321	SER	4.7
1	Y	67	ILE	4.7
1	P	108	PHE	4.7
1	M	181	HIS	4.7
2	G	10	MET	4.7
1	Y	307	GLU	4.7
2	G	71	GLU	4.7
1	Y	302	LEU	4.7
2	G	75	PRO	4.7
1	M	306	TYR	4.7
1	P	178	ALA	4.7
1	Y	32	THR	4.6
1	A	410	GLU	4.6
2	Z	66	ILE	4.6
1	M	59	SER	4.6
1	P	284	HIS	4.6
1	D	45	GLN	4.6
1	D	389	ARG	4.6
1	Y	41	ILE	4.6
2	G	45	TYR	4.6
1	D	285	ILE	4.6
1	B	407	PHE	4.6
1	P	313	SER	4.5
2	J	24	GLN	4.5
2	Z	47	GLU	4.5
1	P	83	ILE	4.5
1	A	63	GLY	4.5
1	P	302	LEU	4.5
1	A	301	ARG	4.5
1	D	402	MET	4.5
1	D	8	THR	4.5
1	M	19	GLU	4.5
1	P	242	VAL	4.5
1	P	101	TYR	4.5
1	A	64	PHE	4.5
1	M	384	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	304	PRO	4.5
1	P	134	PRO	4.5
1	D	271	SER	4.5
1	P	128	PHE	4.5
1	P	252	SER	4.5
1	B	140	LEU	4.5
1	A	264	PRO	4.5
1	D	262	TYR	4.5
2	G	24	GLN	4.4
1	P	289	THR	4.4
1	P	371	THR	4.4
1	P	92	ALA	4.4
2	G	13	PRO	4.4
1	Y	317	GLN	4.4
1	A	385	GLU	4.4
2	G	27	GLU	4.4
1	Y	240	PHE	4.4
1	D	434	VAL	4.4
1	P	408	VAL	4.4
1	Y	223	SER	4.4
1	M	66	ARG	4.4
1	Y	65	THR	4.4
1	Y	24	PHE	4.4
1	P	130	MET	4.4
1	B	69	GLU	4.4
1	P	433	ALA	4.4
2	G	74	GLU	4.4
1	A	17	VAL	4.4
1	P	303	VAL	4.4
1	A	335	ILE	4.4
1	A	226	TYR	4.4
1	B	276	TYR	4.4
1	P	262	TYR	4.4
1	P	129	SER	4.4
1	Y	61	ILE	4.4
1	D	138	PHE	4.4
1	D	243	ASN	4.4
2	G	34	SER	4.4
1	D	14	LEU	4.3
1	Y	360	GLY	4.3
1	M	221	VAL	4.3
1	B	285	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	182	MET	4.3
1	B	317	GLN	4.3
1	P	357	GLY	4.3
2	G	109	THR	4.3
1	A	407	PHE	4.3
2	G	79	ALA	4.3
1	A	313	SER	4.3
1	M	107	PRO	4.3
1	A	182	MET	4.3
1	A	311	TYR	4.3
1	B	307	GLU	4.3
1	M	119	ALA	4.3
1	P	184	PHE	4.3
1	D	66	ARG	4.3
1	P	412	LEU	4.3
1	B	386	ARG	4.3
2	Z	12	ARG	4.3
2	G	100	PRO	4.3
1	M	156	GLN	4.3
1	B	348	LEU	4.3
1	M	74	LEU	4.3
1	P	14	LEU	4.3
1	M	54	VAL	4.3
2	J	62	ILE	4.2
1	A	274	ALA	4.2
1	P	410	GLU	4.2
1	D	371	THR	4.2
2	G	35	SER	4.2
2	Z	34	SER	4.2
1	A	203	ARG	4.2
1	M	365	ILE	4.2
1	D	315	SER	4.2
1	M	311	TYR	4.2
1	P	10	LYS	4.2
2	J	63	LYS	4.2
1	D	374	ASN	4.2
1	A	179	LEU	4.2
1	A	379	SER	4.2
1	D	324	ARG	4.2
1	P	54	VAL	4.2
1	A	96	ILE	4.2
1	A	414	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	81	PHE	4.2
1	D	282	LEU	4.2
1	P	76	LEU	4.2
1	Y	231	TYR	4.2
1	P	367	PRO	4.2
1	M	419	HIS	4.2
1	B	204	PHE	4.2
1	M	184	PHE	4.2
1	B	100	VAL	4.2
1	P	87	ARG	4.2
2	J	79	ALA	4.2
1	Y	305	GLY	4.2
1	M	265	ASP	4.2
1	Y	304	PRO	4.1
1	M	376	PHE	4.1
1	D	12	ASP	4.1
1	M	366	ASP	4.1
1	B	323	ILE	4.1
1	M	348	LEU	4.1
1	B	290	ALA	4.1
1	A	284	HIS	4.1
1	A	365	ILE	4.1
1	B	414	GLU	4.1
2	Z	23	LEU	4.1
1	D	202	PHE	4.1
1	Y	202	PHE	4.1
1	D	416	VAL	4.1
1	D	388	ILE	4.1
1	P	304	PRO	4.1
1	D	208	LEU	4.1
1	A	332	GLY	4.1
1	B	305	GLY	4.1
1	A	137	GLU	4.1
1	B	324	ARG	4.1
1	Y	382	GLU	4.1
1	Y	267	PRO	4.1
1	A	268	THR	4.1
1	M	136	LEU	4.1
1	M	360	GLY	4.1
1	P	258	LYS	4.1
2	J	73	LEU	4.1
1	A	24	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	64	PHE	4.1
1	M	204	PHE	4.1
1	B	25	ILE	4.1
1	A	48	GLU	4.1
1	P	73	LYS	4.1
1	B	413	GLY	4.1
1	M	329	ARG	4.1
1	D	249	SER	4.1
1	Y	245	SER	4.1
1	Y	50	PHE	4.1
1	M	64	PHE	4.1
1	M	190	HIS	4.1
2	G	5	LYS	4.0
2	G	111	GLU	4.0
1	D	328	THR	4.0
1	A	21	ASP	4.0
1	A	297	ASN	4.0
1	B	81	PHE	4.0
1	P	204	PHE	4.0
1	D	367	PRO	4.0
1	Y	134	PRO	4.0
2	Z	33	VAL	4.0
1	P	210	THR	4.0
1	B	74	LEU	4.0
1	A	108	PHE	4.0
1	P	403	LYS	4.0
2	J	107	ILE	4.0
1	D	318	ASN	4.0
2	Z	10	MET	4.0
1	M	97	LEU	4.0
1	M	304	PRO	4.0
1	Y	183	GLY	4.0
1	A	323	ILE	4.0
1	D	438	TRP	4.0
1	B	421	LEU	4.0
1	A	194	ALA	4.0
1	M	392	PRO	4.0
1	P	368	GLY	4.0
1	P	90	THR	4.0
1	P	260	VAL	4.0
1	A	200	ILE	4.0
1	Y	323	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	86	TRP	4.0
1	A	163	ALA	4.0
2	G	9	ALA	4.0
1	D	319	ARG	4.0
1	A	320	SER	4.0
1	A	275	MET	3.9
2	J	112	THR	3.9
1	D	264	PRO	3.9
1	M	109	LYS	3.9
1	M	277	TYR	3.9
1	P	277	TYR	3.9
1	D	354	LEU	3.9
1	B	26	ARG	3.9
1	M	214	VAL	3.9
1	P	13	VAL	3.9
1	M	388	ILE	3.9
1	M	195	PRO	3.9
1	A	76	LEU	3.9
1	M	47	GLU	3.9
2	J	108	ARG	3.9
1	Y	159	TYR	3.9
1	B	90	THR	3.9
1	D	184	PHE	3.9
1	P	280	GLY	3.9
1	M	426	MET	3.9
1	P	181	HIS	3.9
1	P	33	LEU	3.9
1	Y	83	ILE	3.9
1	Y	285	ILE	3.9
1	M	200	ILE	3.9
1	B	420	TYR	3.8
1	D	307	GLU	3.8
1	M	266	THR	3.8
1	Y	114	TYR	3.8
1	A	128	PHE	3.8
1	Y	329	ARG	3.8
1	B	171	VAL	3.8
1	D	335	ILE	3.8
1	Y	154	THR	3.8
1	A	317	GLN	3.8
1	D	82	ARG	3.8
1	M	383	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	240	PHE	3.8
1	B	15	GLU	3.8
1	P	214	VAL	3.8
1	A	331	ASN	3.8
1	D	94	ALA	3.8
1	M	72	MET	3.8
2	G	52	MET	3.8
1	B	268	THR	3.8
1	P	391	LEU	3.8
2	Z	32	THR	3.8
1	P	375	ILE	3.8
1	A	7	CYS	3.8
1	A	82	ARG	3.8
1	B	203	ARG	3.8
1	A	352	LEU	3.8
1	D	124	GLU	3.8
1	M	412	LEU	3.8
1	P	187	GLU	3.8
1	B	264	PRO	3.8
1	D	299	TYR	3.8
1	P	219	TYR	3.8
1	D	408	VAL	3.8
1	Y	89	ALA	3.8
1	Y	178	ALA	3.8
1	P	325	ILE	3.8
1	D	6	LYS	3.8
1	B	249	SER	3.8
1	D	342	PRO	3.8
1	M	85	PRO	3.8
1	Y	376	PHE	3.8
1	A	110	GLY	3.8
1	M	305	GLY	3.8
1	M	364	LYS	3.8
1	A	308	ALA	3.8
1	Y	179	LEU	3.8
1	Y	68	GLU	3.8
2	J	69	ASN	3.8
1	Y	201	ASP	3.7
1	D	17	VAL	3.7
1	Y	216	THR	3.7
1	P	96	ILE	3.7
1	D	405	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	P	384	GLU	3.7
1	Y	16	ALA	3.7
1	Y	351	ALA	3.7
1	D	27	THR	3.7
1	A	247	MET	3.7
1	M	13	VAL	3.7
1	A	372	ASN	3.7
1	D	104	ASP	3.7
1	Y	328	THR	3.7
1	Y	252	SER	3.7
1	P	342	PRO	3.7
1	B	20	ARG	3.7
1	B	163	ALA	3.7
1	D	288	PHE	3.7
1	P	306	TYR	3.7
1	A	377	HIS	3.7
1	A	322	LEU	3.7
1	D	327	ALA	3.7
1	D	411	ALA	3.7
1	P	94	ALA	3.7
1	P	274	ALA	3.7
1	B	252	SER	3.7
1	A	205	GLY	3.7
1	Y	383	ARG	3.7
1	P	156	GLN	3.7
1	M	82	ARG	3.7
1	B	88	PRO	3.7
1	B	36	ILE	3.7
1	B	281	LEU	3.6
1	B	372	ASN	3.6
1	D	190	HIS	3.6
1	A	359	GLU	3.6
1	M	413	GLY	3.6
1	Y	306	TYR	3.6
1	P	347	TYR	3.6
1	Y	54	VAL	3.6
1	B	385	GLU	3.6
1	M	415	HIS	3.6
1	A	318	ASN	3.6
1	D	323	ILE	3.6
1	B	313	SER	3.6
1	D	415	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	409	LYS	3.6
2	G	116	ALA	3.6
1	A	304	PRO	3.6
1	D	355	ARG	3.6
1	B	426	MET	3.6
1	M	446	MET	3.6
1	D	132	VAL	3.6
1	P	443	TYR	3.6
1	Y	390	SER	3.6
1	B	279	GLY	3.6
1	M	241	GLY	3.6
1	D	90	THR	3.6
1	M	211	ALA	3.6
2	J	75	PRO	3.6
1	D	235	MET	3.6
1	Y	375	ILE	3.6
1	A	248	HIS	3.6
1	B	179	LEU	3.6
1	D	291	VAL	3.6
1	M	260	VAL	3.6
1	D	39	TRP	3.6
1	M	404	GLY	3.6
1	P	334	ARG	3.6
2	G	112	THR	3.6
2	Z	51	ALA	3.6
1	B	116	LEU	3.6
1	D	13	VAL	3.6
1	D	207	VAL	3.6
1	Y	5	LYS	3.6
2	Z	116	ALA	3.5
1	A	152	GLU	3.5
1	A	419	HIS	3.5
1	M	321	SER	3.5
1	P	315	SER	3.5
1	P	320	SER	3.5
1	P	389	ARG	3.5
1	B	278	ILE	3.5
1	B	306	TYR	3.5
1	Y	377	HIS	3.5
1	Y	432	LYS	3.5
1	A	33	LEU	3.5
1	B	22	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	411	ALA	3.5
1	A	334	ARG	3.5
1	D	87	ARG	3.5
1	Y	314	TRP	3.5
2	J	17	ASP	3.5
1	D	421	LEU	3.5
1	P	116	LEU	3.5
1	A	206	ASP	3.5
1	A	271	SER	3.5
1	B	428	TRP	3.5
1	A	286	ARG	3.5
1	D	83	ILE	3.5
1	D	278	ILE	3.5
1	Y	309	PRO	3.5
1	P	421	LEU	3.5
1	B	373	VAL	3.5
1	P	177	TYR	3.5
1	P	276	TYR	3.5
1	B	358	LEU	3.5
1	B	399	ILE	3.5
2	J	13	PRO	3.5
1	A	54	VAL	3.5
1	Y	13	VAL	3.5
1	P	65	THR	3.5
1	D	114	TYR	3.5
1	Y	18	LYS	3.5
1	Y	315	SER	3.5
1	P	414	GLU	3.5
2	G	102	GLU	3.5
1	A	72	MET	3.4
1	D	353	MET	3.4
1	D	97	LEU	3.4
1	B	292	THR	3.4
1	Y	229	GLY	3.4
1	M	418	SER	3.4
1	B	334	ARG	3.4
1	M	101	TYR	3.4
1	M	425	GLU	3.4
1	B	10	LYS	3.4
1	A	314	TRP	3.4
1	B	312	ILE	3.4
1	M	175	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	312	ILE	3.4
1	P	175	ILE	3.4
1	A	445	SER	3.4
1	B	351	ALA	3.4
1	Y	87	ARG	3.4
1	Y	434	VAL	3.4
1	P	119	ALA	3.4
1	D	99	ASP	3.4
1	P	364	LYS	3.4
1	Y	103	PRO	3.4
1	A	187	GLU	3.4
1	P	247	MET	3.4
1	A	120	ILE	3.4
1	A	421	LEU	3.4
1	B	412	LEU	3.4
1	Y	200	ILE	3.4
1	A	123	ALA	3.4
1	Y	93	VAL	3.4
1	P	331	ASN	3.4
1	A	129	SER	3.4
1	A	300	LYS	3.4
1	Y	233	SER	3.4
1	M	5	LYS	3.4
1	A	399	ILE	3.4
1	D	61	ILE	3.4
1	P	50	PHE	3.4
1	D	106	ASN	3.4
1	A	236	PRO	3.4
2	G	113	GLY	3.4
1	B	402	MET	3.4
1	P	72	MET	3.4
1	A	16	ALA	3.4
1	B	48	GLU	3.4
1	B	50	PHE	3.4
1	B	186	ILE	3.4
1	B	378	LEU	3.4
1	D	51	GLU	3.4
1	Y	322	LEU	3.4
1	M	322	LEU	3.4
1	P	84	LEU	3.4
1	P	319	ARG	3.4
2	G	36	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	P	6	LYS	3.4
1	Y	58	GLY	3.4
1	M	445	SER	3.4
1	P	159	TYR	3.4
1	P	154	THR	3.4
2	G	76	THR	3.4
1	D	423	ALA	3.4
1	M	89	ALA	3.4
1	A	83	ILE	3.4
1	Y	325	ILE	3.4
2	J	12	ARG	3.4
1	A	62	GLN	3.3
1	M	193	VAL	3.3
1	B	133	GLY	3.3
1	B	241	GLY	3.3
1	D	205	GLY	3.3
1	P	21	ASP	3.3
2	G	78	GLU	3.3
2	G	25	LYS	3.3
1	B	168	ALA	3.3
1	D	123	ALA	3.3
1	B	202	PHE	3.3
1	M	323	ILE	3.3
1	D	71	ASP	3.3
1	P	215	VAL	3.3
1	A	249	SER	3.3
1	M	298	SER	3.3
1	A	15	GLU	3.3
1	Y	40	ALA	3.3
1	M	275	MET	3.3
1	P	49	ALA	3.3
1	Y	391	LEU	3.3
1	B	29	PHE	3.3
1	B	83	ILE	3.3
1	M	112	PRO	3.3
1	P	301	ARG	3.3
1	Y	339	CYS	3.3
1	Y	131	ASN	3.3
1	B	384	GLU	3.3
1	D	15	GLU	3.3
2	J	74	GLU	3.3
1	D	118	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	337	LEU	3.3
1	P	358	LEU	3.3
1	D	105	GLY	3.3
1	A	338	ARG	3.3
1	D	56	PHE	3.3
1	D	203	ARG	3.3
1	D	383	ARG	3.3
1	M	162	PHE	3.3
1	B	62	GLN	3.3
1	P	11	GLU	3.3
1	Y	428	TRP	3.3
1	M	334	ARG	3.3
1	B	248	HIS	3.3
1	D	11	GLU	3.3
1	A	112	PRO	3.3
1	P	388	ILE	3.3
1	M	390	SER	3.3
1	P	12	ASP	3.3
1	Y	316	ALA	3.3
1	D	253	LEU	3.3
1	M	182	MET	3.3
1	P	318	ASN	3.3
1	B	200	ILE	3.3
1	B	375	ILE	3.3
1	D	60	SER	3.3
1	P	285	ILE	3.3
1	B	132	VAL	3.3
1	D	292	THR	3.3
1	M	150	THR	3.3
1	B	354	LEU	3.2
1	D	226	TYR	3.2
1	M	285	ILE	3.2
2	Z	65	GLU	3.2
1	A	296	VAL	3.2
1	Y	310	VAL	3.2
1	B	272	GLN	3.2
1	Y	80	THR	3.2
2	J	44	GLY	3.2
1	M	16	ALA	3.2
1	D	390	SER	3.2
1	B	167	ARG	3.2
1	D	302	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	P	344	CYS	3.2
1	B	175	ILE	3.2
1	B	254	PHE	3.2
1	A	373	VAL	3.2
1	M	23	LYS	3.2
1	M	303	VAL	3.2
1	P	221	VAL	3.2
1	M	284	HIS	3.2
1	B	206	ASP	3.2
1	D	136	LEU	3.2
1	Y	354	LEU	3.2
1	M	302	LEU	3.2
1	P	322	LEU	3.2
1	P	444	LEU	3.2
1	D	261	PHE	3.2
1	P	217	PHE	3.2
1	A	333	THR	3.2
1	D	111	ASP	3.2
1	Y	206	ASP	3.2
1	M	256	ASP	3.2
1	D	393	ALA	3.2
1	D	18	LYS	3.2
1	D	378	LEU	3.2
1	D	384	GLU	3.2
1	D	120	ILE	3.2
1	P	323	ILE	3.2
1	A	422	CYS	3.2
1	Y	78	PRO	3.2
1	Y	327	ALA	3.2
1	P	102	LEU	3.2
1	A	36	ILE	3.2
1	A	361	ILE	3.2
1	B	319	ARG	3.2
1	A	204	PHE	3.2
1	A	217	PHE	3.2
1	B	377	HIS	3.2
1	Y	184	PHE	3.2
1	B	408	VAL	3.2
1	M	422	CYS	3.2
1	P	233	SER	3.2
1	D	349	ALA	3.2
1	P	351	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	273	ASP	3.2
1	B	23	LYS	3.2
1	B	121	LYS	3.2
1	B	270	LEU	3.2
1	M	53	GLY	3.2
1	M	381	LYS	3.2
1	A	175	ILE	3.1
1	B	124	GLU	3.1
1	A	38	SER	3.1
1	D	295	VAL	3.1
1	M	22	VAL	3.1
1	A	86	TRP	3.1
1	A	121	LYS	3.1
1	D	259	ASN	3.1
1	Y	273	ASP	3.1
1	Y	380	ASP	3.1
1	D	110	GLY	3.1
1	Y	98	GLY	3.1
1	M	330	GLY	3.1
1	D	337	LEU	3.1
1	D	426	MET	3.1
1	D	216	THR	3.1
1	Y	365	ILE	3.1
1	M	328	THR	3.1
1	P	335	ILE	3.1
1	D	376	PHE	3.1
1	P	350	PHE	3.1
1	B	347	TYR	3.1
1	D	406	LYS	3.1
1	D	232	ALA	3.1
1	A	158	GLY	3.1
1	B	181	HIS	3.1
1	B	247	MET	3.1
1	P	419	HIS	3.1
1	A	23	LYS	3.1
1	M	320	SER	3.1
1	Y	82	ARG	3.1
1	Y	71	ASP	3.1
1	Y	195	PRO	3.1
1	D	219	TYR	3.1
1	D	231	TYR	3.1
1	M	100	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	P	415	HIS	3.1
1	D	26	ARG	3.1
1	P	74	LEU	3.1
1	M	380	ASP	3.1
1	P	8	THR	3.1
1	A	131	ASN	3.1
1	M	217	PHE	3.1
1	B	115	VAL	3.1
1	D	215	VAL	3.1
1	M	225	ALA	3.1
1	Y	116	LEU	3.1
2	G	17	ASP	3.1
1	B	61	ILE	3.1
1	B	67	ILE	3.1
1	B	417	PHE	3.1
1	P	283	LYS	3.1
1	Y	274	ALA	3.1
1	P	383	ARG	3.1
1	D	245	SER	3.1
1	M	79	SER	3.1
1	Y	6	LYS	3.1
1	D	42	PRO	3.1
1	D	325	ILE	3.1
1	P	399	ILE	3.1
1	B	188	ALA	3.1
1	P	411	ALA	3.1
1	P	366	ASP	3.0
1	Y	121	LYS	3.0
2	J	61	LYS	3.0
1	Y	97	LEU	3.0
1	M	326	PRO	3.0
1	M	370	PRO	3.0
1	P	413	GLY	3.0
1	D	338	ARG	3.0
1	A	43	ALA	3.0
1	A	71	ASP	3.0
1	Y	92	ALA	3.0
1	D	125	LYS	3.0
1	B	63	GLY	3.0
1	A	35	ILE	3.0
1	D	258	LYS	3.0
1	Y	433	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	P	407	PHE	3.0
1	D	100	VAL	3.0
1	Y	147	GLY	3.0
1	B	9	THR	3.0
1	B	32	THR	3.0
1	B	136	LEU	3.0
1	D	84	LEU	3.0
1	D	352	LEU	3.0
1	M	179	LEU	3.0
2	G	22	GLU	3.0
1	M	248	HIS	3.0
1	B	94	ALA	3.0
1	B	243	ASN	3.0
1	D	75	ALA	3.0
1	P	398	ALA	3.0
1	D	22	VAL	3.0
1	Y	17	VAL	3.0
1	Y	221	VAL	3.0
1	P	17	VAL	3.0
1	D	257	GLY	3.0
1	A	27	THR	3.0
1	Y	266	THR	3.0
1	M	27	THR	3.0
1	M	68	GLU	3.0
1	P	378	LEU	3.0
1	A	278	ILE	3.0
1	D	274	ALA	3.0
1	M	70	SER	3.0
1	B	17	VAL	3.0
1	Y	63	GLY	3.0
1	D	176	ASP	3.0
1	M	30	THR	3.0
1	Y	426	MET	3.0
1	A	383	ARG	3.0
1	M	386	ARG	3.0
1	M	349	ALA	3.0
1	Y	361	ILE	3.0
2	Z	74	GLU	3.0
1	P	257	GLY	3.0
1	A	22	VAL	3.0
1	B	107	PRO	3.0
1	D	370	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	J	28	VAL	3.0
1	Y	9	THR	3.0
1	Y	227	HIS	3.0
1	A	219	TYR	2.9
1	D	322	LEU	2.9
1	Y	7	CYS	2.9
1	A	223	SER	2.9
1	D	79	SER	2.9
1	Y	387	GLY	2.9
1	B	162	PHE	2.9
1	A	39	TRP	2.9
1	D	326	PRO	2.9
1	Y	367	PRO	2.9
1	D	9	THR	2.9
1	B	14	LEU	2.9
1	Y	379	SER	2.9
1	D	344	CYS	2.9
1	D	96	ILE	2.9
1	D	186	ILE	2.9
1	P	125	LYS	2.9
1	A	100	VAL	2.9
1	A	198	HIS	2.9
1	A	214	VAL	2.9
1	A	328	THR	2.9
1	B	93	VAL	2.9
1	D	317	GLN	2.9
1	M	185	GLN	2.9
1	B	60	SER	2.9
1	B	391	LEU	2.9
1	P	348	LEU	2.9
1	B	51	GLU	2.9
1	P	211	ALA	2.9
1	B	338	ARG	2.9
1	A	224	ILE	2.9
1	B	388	ILE	2.9
1	P	78	PRO	2.9
1	P	326	PRO	2.9
1	D	272	GLN	2.9
1	D	108	PHE	2.9
1	Y	242	VAL	2.9
1	A	362	LYS	2.9
2	J	65	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	270	LEU	2.9
1	Y	253	LEU	2.9
1	Y	395	LEU	2.9
1	M	354	LEU	2.9
1	D	101	TYR	2.9
1	B	267	PRO	2.9
1	B	380	ASP	2.9
1	P	5	LYS	2.9
1	Y	417	PHE	2.9
2	Z	19	VAL	2.9
1	D	280	GLY	2.9
1	A	391	LEU	2.9
1	M	282	LEU	2.9
1	D	159	TYR	2.9
1	D	420	TYR	2.9
1	M	443	TYR	2.9
1	A	382	GLU	2.9
1	M	436	HIS	2.9
2	G	60	GLU	2.9
1	A	388	ILE	2.9
1	D	375	ILE	2.9
1	P	172	ARG	2.9
1	P	324	ARG	2.9
1	D	252	SER	2.9
1	Y	234	PHE	2.9
1	Y	288	PHE	2.9
1	Y	115	VAL	2.9
1	A	136	LEU	2.9
1	B	102	LEU	2.9
1	D	117	LYS	2.9
1	D	283	LYS	2.9
1	B	275	MET	2.9
1	Y	168	ALA	2.9
1	Y	410	GLU	2.9
1	M	351	ALA	2.9
1	P	307	GLU	2.9
1	P	428	TRP	2.9
1	B	346	PRO	2.9
1	B	442	ARG	2.9
1	Y	219	TYR	2.9
1	P	420	TYR	2.9
1	M	9	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	196	SER	2.8
1	D	147	GLY	2.8
1	D	250	ASN	2.8
1	A	47	GLU	2.8
1	M	108	PHE	2.8
1	A	102	LEU	2.8
1	B	440	LEU	2.8
1	P	203	ARG	2.8
1	Y	438	TRP	2.8
1	A	10	LYS	2.8
1	D	418	SER	2.8
1	Y	269	LYS	2.8
1	P	185	GLN	2.8
1	P	445	SER	2.8
1	B	423	ALA	2.8
1	B	134	PRO	2.8
1	P	236	PRO	2.8
1	M	177	TYR	2.8
1	P	405	SER	2.8
1	P	20	ARG	2.8
1	M	50	PHE	2.8
1	D	54	VAL	2.8
1	A	75	ALA	2.8
1	Y	51	GLU	2.8
1	M	6	LYS	2.8
1	Y	94	ALA	2.8
1	D	239	LEU	2.8
1	Y	14	LEU	2.8
1	P	42	PRO	2.8
1	P	346	PRO	2.8
1	B	105	GLY	2.8
1	M	189	SER	2.8
1	B	361	ILE	2.8
1	P	231	TYR	2.8
1	D	336	GLU	2.8
1	M	417	PHE	2.8
1	Y	408	VAL	2.8
1	Y	308	ALA	2.8
1	M	423	ALA	2.8
1	B	282	LEU	2.8
1	B	322	LEU	2.8
1	M	253	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	P	106	ASN	2.8
1	D	413	GLY	2.8
1	D	32	THR	2.8
2	Z	81	LYS	2.8
1	A	262	TYR	2.8
1	B	120	ILE	2.8
1	B	311	TYR	2.8
1	D	417	PHE	2.8
1	Y	29	PHE	2.8
1	Y	43	ALA	2.8
2	J	67	ALA	2.8
1	A	53	GLY	2.8
1	A	369	GLU	2.8
1	B	218	LYS	2.8
1	D	121	LYS	2.8
1	D	321	SER	2.8
1	D	332	GLY	2.8
1	Y	321	SER	2.8
1	P	223	SER	2.8
1	P	338	ARG	2.8
1	A	8	THR	2.8
1	A	185	GLN	2.8
1	Y	28	GLN	2.8
1	P	120	ILE	2.8
1	Y	259	ASN	2.8
1	Y	374	ASN	2.8
1	D	16	ALA	2.7
1	Y	119	ALA	2.7
1	Y	128	PHE	2.7
1	M	87	ARG	2.8
1	P	19	GLU	2.8
1	P	56	PHE	2.7
1	A	241	GLY	2.7
1	M	244	GLY	2.7
1	P	53	GLY	2.7
1	B	208	LEU	2.7
1	B	239	LEU	2.7
1	Y	84	LEU	2.7
1	Y	247	MET	2.7
1	M	270	LEU	2.7
1	P	235	MET	2.7
1	P	268	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	363	ASN	2.7
1	D	52	ASN	2.7
1	P	61	ILE	2.7
1	P	382	GLU	2.7
1	M	400	ASP	2.7
1	B	316	ALA	2.7
1	D	313	SER	2.7
1	Y	225	ALA	2.7
1	B	13	VAL	2.7
1	Y	45	GLN	2.7
1	Y	270	LEU	2.7
1	P	140	LEU	2.7
1	B	55	MET	2.7
1	B	126	MET	2.7
1	M	80	THR	2.7
1	M	409	LYS	2.7
2	Z	25	LYS	2.7
1	B	419	HIS	2.7
1	P	66	ARG	2.7
1	Y	298	SER	2.7
1	P	70	SER	2.7
1	P	249	SER	2.7
1	A	350	PHE	2.7
1	M	29	PHE	2.7
1	D	19	GLU	2.7
1	P	122	GLU	2.7
1	P	434	VAL	2.7
1	A	116	LEU	2.7
1	D	179	LEU	2.7
1	M	33	LEU	2.7
1	M	358	LEU	2.7
1	M	32	THR	2.7
1	M	31	ASP	2.7
1	B	91	GLY	2.7
1	P	205	GLY	2.7
1	D	392	PRO	2.7
1	A	18	LYS	2.7
1	A	298	SER	2.7
1	Y	313	SER	2.7
1	P	267	PRO	2.7
1	B	255	LYS	2.7
1	P	381	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	262	TYR	2.7
1	M	114	TYR	2.7
1	P	123	ALA	2.7
1	A	141	PHE	2.7
1	D	242	VAL	2.7
1	Y	214	VAL	2.7
1	A	444	LEU	2.7
1	D	266	THR	2.7
1	Y	8	THR	2.7
1	Y	263	ASP	2.7
1	P	266	THR	2.7
1	P	330	GLY	2.7
2	G	115	GLU	2.7
1	B	177	TYR	2.7
1	A	243	ASN	2.7
1	A	281	LEU	2.7
1	Y	207	VAL	2.7
1	M	56	PHE	2.7
1	M	295	VAL	2.7
1	D	47	GLU	2.7
1	A	305	GLY	2.7
1	D	91	GLY	2.7
1	Y	175	ILE	2.7
1	P	200	ILE	2.7
1	P	131	ASN	2.7
1	A	231	TYR	2.7
1	B	185	GLN	2.7
1	D	306	TYR	2.7
1	P	114	TYR	2.7
1	A	84	LEU	2.7
1	A	143	LEU	2.7
1	A	253	LEU	2.7
1	A	408	VAL	2.7
1	M	46	LEU	2.7
1	P	93	VAL	2.7
1	B	446	MET	2.7
1	D	386	ARG	2.6
1	P	286	ARG	2.6
1	P	48	GLU	2.6
1	P	256	ASP	2.6
1	P	259	ASN	2.6
1	A	277	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	239	LEU	2.6
1	B	215	VAL	2.6
1	B	371	THR	2.6
1	D	46	LEU	2.6
1	D	160	PHE	2.6
1	D	177	TYR	2.6
1	D	442	ARG	2.6
1	Y	64	PHE	2.6
1	Y	55	MET	2.6
1	P	402	MET	2.6
1	Y	112	PRO	2.6
1	B	438	TRP	2.6
1	D	363	ASN	2.6
1	B	327	ALA	2.6
1	Y	194	ALA	2.6
1	Y	349	ALA	2.6
1	Y	423	ALA	2.6
1	D	248	HIS	2.6
1	B	216	THR	2.6
1	Y	34	GLY	2.6
1	A	50	PHE	2.6
1	D	382	GLU	2.6
1	A	207	VAL	2.6
1	B	108	PHE	2.6
1	Y	412	LEU	2.6
1	P	379	SER	2.6
1	Y	372	ASN	2.6
1	P	238	PRO	2.6
1	D	225	ALA	2.6
1	Y	20	ARG	2.6
1	Y	312	ILE	2.6
2	Z	83	GLY	2.6
1	Y	268	THR	2.6
1	Y	235	MET	2.6
1	B	75	ALA	2.6
1	B	194	ALA	2.6
1	Y	232	ALA	2.6
1	M	377	HIS	2.6
1	A	280	GLY	2.6
1	A	428	TRP	2.6
1	Y	368	GLY	2.6
1	M	428	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	374	ASN	2.6
1	B	321	SER	2.6
1	B	340	PRO	2.6
1	Y	437	PRO	2.6
1	Y	447	LEU	2.6
1	D	359	GLU	2.6
1	M	94	ALA	2.6
1	A	273	ASP	2.6
1	M	39	TRP	2.6
1	M	374	ASN	2.6
1	A	44	GLU	2.6
1	P	385	GLU	2.6
1	A	302	LEU	2.6
1	D	149	PRO	2.6
1	A	193	VAL	2.6
1	Y	132	VAL	2.6
1	M	17	VAL	2.6
1	B	57	ASP	2.6
1	D	166	ASP	2.6
1	D	263	ASP	2.6
1	Y	105	GLY	2.6
1	Y	123	ALA	2.6
1	B	148	ASN	2.6
1	P	336	GLU	2.6
1	P	59	SER	2.5
1	P	113	ARG	2.5
1	D	348	LEU	2.5
1	B	353	MET	2.5
1	D	419	HIS	2.5
1	A	114	TYR	2.5
1	Y	443	TYR	2.5
1	A	92	ALA	2.5
1	D	334	ARG	2.5
1	Y	301	ARG	2.5
1	P	118	THR	2.5
1	M	62	GLN	2.5
1	M	314	TRP	2.5
1	P	239	LEU	2.5
1	D	130	MET	2.5
1	D	181	HIS	2.5
1	M	55	MET	2.5
1	M	73	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	362	LYS	2.5
1	Y	157	GLY	2.5
1	A	250	ASN	2.5
1	Y	277	TYR	2.5
2	Z	18	ALA	2.5
1	D	70	SER	2.5
2	G	37	SER	2.5
1	B	253	LEU	2.5
1	Y	165	LEU	2.5
1	M	14	LEU	2.5
1	M	86	TRP	2.5
1	A	29	PHE	2.5
1	M	232	ALA	2.5
1	B	425	GLU	2.5
1	D	265	ASP	2.5
1	M	167	ARG	2.5
1	M	389	ARG	2.5
1	A	213	ASN	2.5
1	B	207	VAL	2.5
1	D	69	GLU	2.5
1	D	221	VAL	2.5
1	D	428	TRP	2.5
1	Y	407	PHE	2.5
2	J	27	GLU	2.5
1	A	188	ALA	2.5
1	D	298	SER	2.5
1	B	114	TYR	2.5
1	A	216	THR	2.5
1	B	333	THR	2.5
1	D	339	CYS	2.5
1	P	27	THR	2.5
1	B	164	PRO	2.5
1	B	304	PRO	2.5
1	Y	85	PRO	2.5
1	A	25	ILE	2.5
1	P	36	ILE	2.5
1	B	432	LYS	2.5
1	D	165	LEU	2.5
1	Y	140	LEU	2.5
1	D	193	VAL	2.5
1	D	214	VAL	2.5
1	Y	79	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	Y	261	PHE	2.5
1	P	418	SER	2.5
1	P	43	ALA	2.5
1	A	324	ARG	2.5
1	B	113	ARG	2.5
1	D	154	THR	2.5
1	M	159	TYR	2.5
1	B	336	GLU	2.5
1	M	439	GLU	2.5
1	D	133	GLY	2.5
1	M	91	GLY	2.5
1	M	339	CYS	2.5
1	P	23	LYS	2.5
1	P	158	GLY	2.5
1	P	244	GLY	2.5
1	A	45	GLN	2.5
1	A	208	LEU	2.5
1	A	68	GLU	2.4
1	A	228	LYS	2.4
1	D	210	THR	2.4
1	D	218	LYS	2.4
1	D	289	THR	2.4
1	Y	52	ASN	2.4
1	M	438	TRP	2.4
1	B	226	TYR	2.4
1	M	36	ILE	2.4
1	D	7	CYS	2.4
1	Y	167	ARG	2.4
1	Y	172	ARG	2.4
1	Y	386	ARG	2.4
1	B	19	GLU	2.4
1	D	401	GLU	2.4
1	P	153	LEU	2.4
1	D	115	VAL	2.4
1	Y	373	VAL	2.4
1	D	85	PRO	2.4
1	Y	57	ASP	2.4
1	M	276	TYR	2.4
1	M	137	GLU	2.4
1	M	173	ARG	2.4
1	P	355	ARG	2.4
1	P	406	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	213	ASN	2.4
1	B	24	PHE	2.4
1	Y	81	PHE	2.4
1	B	266	THR	2.4
1	M	157	GLY	2.4
1	A	366	ASP	2.4
1	B	430	GLU	2.4
1	M	203	ARG	2.4
1	M	278	ILE	2.4
1	D	196	SER	2.4
1	P	97	LEU	2.4
1	D	229	GLY	2.4
1	Y	401	GLU	2.4
1	M	124	GLU	2.4
1	P	198	HIS	2.4
1	D	113	ARG	2.4
1	Y	30	THR	2.4
1	P	263	ASP	2.4
1	A	345	ASN	2.4
1	D	412	LEU	2.4
1	M	201	ASP	2.4
1	B	103	PRO	2.4
1	M	242	VAL	2.4
1	P	422	CYS	2.4
1	P	44	GLU	2.4
1	D	431	TYR	2.4
1	Y	258	LYS	2.4
1	M	347	TYR	2.4
1	M	362	LYS	2.4
1	B	211	ALA	2.4
1	P	353	MET	2.4
1	A	417	PHE	2.4
1	B	291	VAL	2.4
1	M	152	GLU	2.4
1	P	180	GLU	2.4
1	B	209	CYS	2.4
1	B	374	ASN	2.4
1	D	297	ASN	2.4
1	A	20	ARG	2.3
1	B	66	ARG	2.3
1	D	329	ARG	2.3
1	B	365	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	157	GLY	2.3
1	A	244	GLY	2.3
1	M	299	TYR	2.3
1	A	238	PRO	2.3
1	M	367	PRO	2.3
1	P	438	TRP	2.3
1	A	272	GLN	2.3
1	Y	275	MET	2.3
1	A	288	PHE	2.3
1	B	260	VAL	2.3
1	M	373	VAL	2.3
1	Y	286	ARG	2.3
1	P	139	PHE	2.3
1	D	77	ASP	2.3
1	Y	31	ASP	2.3
1	A	19	GLU	2.3
1	A	181	HIS	2.3
1	D	35	ILE	2.3
1	Y	120	ILE	2.3
1	Y	192	GLU	2.3
1	Y	278	ILE	2.3
1	Y	388	ILE	2.3
1	M	226	TYR	2.3
1	A	153	LEU	2.3
1	A	282	LEU	2.3
1	Y	188	ALA	2.3
1	M	194	ALA	2.3
1	M	308	ALA	2.3
1	P	40	ALA	2.3
1	P	354	LEU	2.3
1	D	21	ASP	2.3
1	P	416	VAL	2.3
1	M	48	GLU	2.3
1	D	305	GLY	2.3
1	A	415	HIS	2.3
1	B	190	HIS	2.3
1	B	258	LYS	2.3
1	D	169	GLN	2.3
1	M	272	GLN	2.3
2	Z	77	ILE	2.3
1	B	149	PRO	2.3
1	D	346	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	140	LEU	2.3
1	D	140	LEU	2.3
1	Y	352	LEU	2.3
1	M	145	ALA	2.3
1	M	338	ARG	2.3
1	P	46	LEU	2.3
1	P	423	ALA	2.3
1	A	266	THR	2.3
1	Y	320	SER	2.3
1	P	55	MET	2.3
1	M	93	VAL	2.3
1	M	110	GLY	2.3
1	M	133	GLY	2.3
1	P	396	LYS	2.3
1	A	122	GLU	2.3
1	D	49	ALA	2.3
1	P	69	GLU	2.3
1	P	369	GLU	2.3
1	A	46	LEU	2.3
1	A	347	TYR	2.3
1	Y	143	LEU	2.3
1	D	59	SER	2.3
1	A	6	LYS	2.3
1	D	55	MET	2.3
1	P	409	LYS	2.3
1	A	303	VAL	2.3
1	A	434	VAL	2.3
1	B	415	HIS	2.3
1	P	162	PHE	2.3
1	A	259	ASN	2.3
1	P	77	ASP	2.3
1	A	269	LYS	2.3
1	A	225	ALA	2.3
1	B	153	LEU	2.3
1	P	80	THR	2.3
1	A	431	TYR	2.3
1	Y	431	TYR	2.3
1	M	98	GLY	2.3
1	B	198	HIS	2.3
1	D	20	ARG	2.3
1	D	122	GLU	2.3
1	Y	100	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	138	PHE	2.3
1	D	206	ASP	2.3
1	Y	394	ASP	2.3
1	M	104	ASP	2.3
1	M	174	ASP	2.3
1	A	316	ALA	2.3
1	B	274	ALA	2.3
1	D	189	SER	2.3
1	B	8	THR	2.2
1	D	397	GLU	2.2
1	M	34	GLY	2.2
1	P	15	GLU	2.2
1	P	133	GLY	2.2
1	Y	262	TYR	2.2
1	Y	446	MET	2.2
1	Y	209	CYS	2.2
1	Y	364	LYS	2.2
1	B	265	ASP	2.2
1	Y	217	PHE	2.2
1	B	39	TRP	2.2
1	B	236	PRO	2.2
1	M	309	PRO	2.2
1	D	185	GLN	2.2
1	Y	336	GLU	2.2
1	P	397	GLU	2.2
1	B	16	ALA	2.2
1	D	211	ALA	2.2
1	Y	75	ALA	2.2
1	M	188	ALA	2.2
1	A	105	GLY	2.2
1	Y	27	THR	2.2
1	Y	330	GLY	2.2
1	Y	333	THR	2.2
1	D	153	LEU	2.2
1	A	106	ASN	2.2
1	B	166	ASP	2.2
1	D	251	GLN	2.2
1	M	7	CYS	2.2
1	B	309	PRO	2.2
1	D	68	GLU	2.2
1	D	112	PRO	2.2
1	B	405	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	301	ARG	2.2
1	Y	60	SER	2.2
1	Y	442	ARG	2.2
1	B	27	THR	2.2
1	B	225	ALA	2.2
1	P	333	THR	2.2
1	P	360	GLY	2.2
1	D	372	ASN	2.2
1	A	230	TYR	2.2
1	M	51	GLU	2.2
1	B	112	PRO	2.2
1	A	222	LYS	2.2
1	A	258	LYS	2.2
1	A	252	SER	2.2
1	Y	254	PHE	2.2
1	Y	344	CYS	2.2
1	M	128	PHE	2.2
1	A	210	THR	2.2
1	B	21	ASP	2.2
1	D	433	ALA	2.2
1	B	35	ILE	2.2
1	D	67	ILE	2.2
1	Y	186	ILE	2.2
1	M	25	ILE	2.2
1	M	216	THR	2.2
1	A	169	GLN	2.2
1	M	45	GLN	2.2
1	M	336	GLU	2.2
1	A	440	LEU	2.2
1	M	402	MET	2.2
1	B	195	PRO	2.2
1	B	303	VAL	2.2
1	M	127	GLY	2.2
1	A	209	CYS	2.2
1	B	119	ALA	2.2
1	D	197	GLN	2.2
1	Y	343	ALA	2.2
1	M	41	ILE	2.2
1	A	74	LEU	2.2
1	D	172	ARG	2.2
1	D	381	LYS	2.2
1	Y	33	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	Y	353	MET	2.2
1	A	60	SER	2.2
1	A	177	TYR	2.2
1	P	60	SER	2.2
1	P	299	TYR	2.2
1	A	416	VAL	2.2
1	D	373	VAL	2.2
1	Y	91	GLY	2.2
1	P	305	GLY	2.2
1	A	142	LYS	2.2
1	D	73	LYS	2.2
1	M	123	ALA	2.2
1	Y	389	ARG	2.2
1	P	425	GLU	2.2
1	A	126	MET	2.2
1	A	418	SER	2.2
1	B	189	SER	2.2
1	M	21	ASP	2.2
1	D	62	GLN	2.2
1	Y	272	GLN	2.2
1	P	110	GLY	2.2
1	B	231	TYR	2.1
1	D	284	HIS	2.1
1	Y	141	PHE	2.1
1	Y	415	HIS	2.1
1	Y	35	ILE	2.1
1	P	395	LEU	2.1
1	B	72	MET	2.1
1	B	315	SER	2.1
1	Y	409	LYS	2.1
1	D	53	GLY	2.1
1	M	106	ASN	2.1
1	M	420	TYR	2.1
1	P	191	HIS	2.1
1	B	54	VAL	2.1
1	Y	171	VAL	2.1
1	Y	416	VAL	2.1
1	A	56	PHE	2.1
1	A	138	PHE	2.1
1	D	188	ALA	2.1
1	M	240	PHE	2.1
1	M	292	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	237	LYS	2.1
1	D	394	ASP	2.1
1	A	41	ILE	2.1
1	Y	42	PRO	2.1
1	M	140	LEU	2.1
1	P	52	ASN	2.1
1	P	243	ASN	2.1
1	P	264	PRO	2.1
1	Y	130	MET	2.1
1	Y	182	MET	2.1
1	D	48	GLU	2.1
1	A	13	VAL	2.1
1	A	232	ALA	2.1
1	D	151	THR	2.1
1	A	263	ASP	2.1
1	B	99	ASP	2.1
1	D	162	PHE	2.1
1	D	356	ALA	2.1
1	Y	185	GLN	2.1
1	P	29	PHE	2.1
1	P	288	PHE	2.1
1	P	25	ILE	2.1
2	G	50	ARG	2.1
1	A	229	GLY	2.1
1	D	236	PRO	2.1
1	P	105	GLY	2.1
1	A	235	MET	2.1
1	P	339	CYS	2.1
1	A	394	ASP	2.1
1	D	201	ASP	2.1
1	A	351	ALA	2.1
1	B	221	VAL	2.1
1	D	230	TYR	2.1
1	Y	299	TYR	2.1
1	A	160	PHE	2.1
2	G	47	GLU	2.1
1	A	370	PRO	2.1
1	B	42	PRO	2.1
1	B	370	PRO	2.1
1	A	109	LYS	2.1
1	D	409	LYS	2.1
1	B	263	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	31	ASP	2.1
1	B	359	GLU	2.1
1	A	40	ALA	2.1
1	A	168	ALA	2.1
1	B	328	THR	2.1
1	M	8	THR	2.1
1	M	43	ALA	2.1
1	M	75	ALA	2.1
1	P	292	THR	2.1
1	B	106	ASN	2.1
1	M	213	ASN	2.1
1	P	363	ASN	2.1
1	P	34	GLY	2.1
1	Y	392	PRO	2.1
1	Y	335	ILE	2.1
1	Y	197	GLN	2.1
1	Y	198	HIS	2.1
1	B	68	GLU	2.1
1	M	176	ASP	2.1
1	A	146	ASN	2.1
1	M	210	THR	2.1
1	M	343	ALA	2.1
1	B	147	GLY	2.1
1	Y	59	SER	2.1
1	M	209	CYS	2.1
1	M	249	SER	2.1
1	P	291	VAL	2.1
1	A	420	TYR	2.1
1	B	152	GLU	2.0
1	B	156	GLN	2.0
1	B	96	ILE	2.0
1	Y	282	LEU	2.0
1	M	102	LEU	2.0
1	M	395	LEU	2.0
1	A	91	GLY	2.0
1	A	98	GLY	2.0
1	M	290	ALA	2.0
1	A	199	GLU	2.0
1	Y	129	SER	2.0
1	M	12	ASP	2.0
1	M	139	PHE	2.0
1	M	288	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	P	86	TRP	2.0
1	P	227	HIS	2.0
1	A	406	LYS	2.0
1	D	23	LYS	2.0
1	P	228	LYS	2.0
1	Y	208	LEU	2.0
1	Y	363	ASN	2.0
1	Y	187	GLU	2.0
1	P	152	GLU	2.0
1	D	127	GLY	2.0
1	D	178	ALA	2.0
1	P	196	SER	2.0
1	A	31	ASP	2.0
1	A	389	ARG	2.0
1	M	264	PRO	2.0
1	M	220	VAL	2.0
1	M	406	LYS	2.0
2	Z	5	LYS	2.0
1	D	227	HIS	2.0
1	M	261	PHE	2.0
1	M	372	ASN	2.0
1	P	226	TYR	2.0
1	B	84	LEU	2.0
1	B	302	LEU	2.0
1	D	74	LEU	2.0
1	D	175	ILE	2.0
1	Y	124	GLU	2.0
1	M	61	ILE	2.0
1	P	281	LEU	2.0
1	B	404	GLY	2.0
1	A	70	SER	2.0
1	A	80	THR	2.0
1	A	104	ASP	2.0
1	A	173	ARG	2.0
1	A	289	THR	2.0
1	B	111	ASP	2.0
1	P	155	ASP	2.0
1	M	40	ALA	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 monosaccharides 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.