Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 04:22 AM EDT

PDB ID	:	4WJ3
Title	:	Crystal structure of the asparagine transamidosome from Pseudomonas aeruginosa
Authors	:	Suzuki, T.; Nakamura, A.; Kato, K.; Tanaka, I.; Yao, M.
Deposited on	:	2014-09-29
Resolution	:	3.71 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:

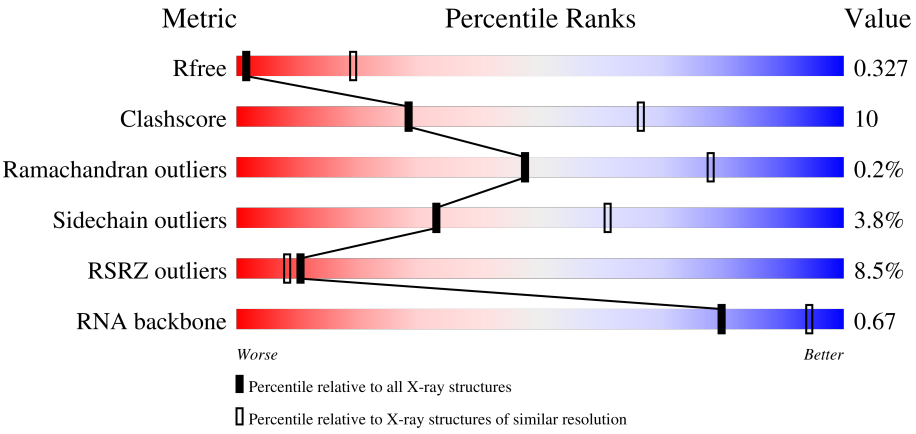
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	484	3% 77% 23%
1	D	484	% 76% 23%
1	G	484	27% 70% 28%
1	J	484	35% 76% 22%

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Mol	Chain	Length	Quality of chain
2	B	481	2% 74% 20% 5%
2	E	481	3% 74% 20% 5%
2	H	481	6% 77% 17% 5%
2	K	481	7% 71% 22% 5%
3	C	104	8% 68% 24% 8%
3	F	104	3% 62% 31% 8%
3	I	104	12% 68% 22% 8%
3	L	104	12% 68% 21% 8%
4	M	599	5% 69% 27%
4	N	599	2% 68% 28%
4	O	599	7% 71% 25%
4	P	599	2% 66% 30%
5	Q	76	4% 72% 20% 7%
5	R	76	5% 64% 33%
5	S	76	3% 67% 26% 7%
5	T	76	4% 70% 25% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 56045 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 Glutamyl-tRNA(Gln) amidotransferase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3639	2290	633	702	14			
1	D	483	Total	C	N	O	S	0	0	0
			3639	2290	633	702	14			
1	G	483	Total	C	N	O	S	0	0	0
			3639	2290	633	702	14			
1	J	483	Total	C	N	O	S	0	0	0
			3639	2290	633	702	14			

- Molecule 2 is a protein called Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	456	Total	C	N	O	S	0	0	0
			3372	2103	595	657	17			
2	E	455	Total	C	N	O	S	0	0	0
			3367	2100	594	656	17			
2	H	455	Total	C	N	O	S	0	0	0
			3367	2100	594	656	17			
2	K	455	Total	C	N	O	S	0	0	0
			3367	2100	594	656	17			

- Molecule 3 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	96	Total	C	N	O	S	0	0	0
			738	458	128	150	2			
3	F	96	Total	C	N	O	S	0	0	0
			738	458	128	150	2			
3	I	96	Total	C	N	O	S	0	0	0
			738	458	128	150	2			
3	L	96	Total	C	N	O	S	0	0	0
			738	458	128	150	2			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	MET	-	expression tag	UNP Q9HVT9
C	-6	GLY	-	expression tag	UNP Q9HVT9
C	-5	HIS	-	expression tag	UNP Q9HVT9
C	-4	HIS	-	expression tag	UNP Q9HVT9
C	-3	HIS	-	expression tag	UNP Q9HVT9
C	-2	HIS	-	expression tag	UNP Q9HVT9
C	-1	HIS	-	expression tag	UNP Q9HVT9
C	0	HIS	-	expression tag	UNP Q9HVT9
F	-7	MET	-	expression tag	UNP Q9HVT9
F	-6	GLY	-	expression tag	UNP Q9HVT9
F	-5	HIS	-	expression tag	UNP Q9HVT9
F	-4	HIS	-	expression tag	UNP Q9HVT9
F	-3	HIS	-	expression tag	UNP Q9HVT9
F	-2	HIS	-	expression tag	UNP Q9HVT9
F	-1	HIS	-	expression tag	UNP Q9HVT9
F	0	HIS	-	expression tag	UNP Q9HVT9
I	-7	MET	-	expression tag	UNP Q9HVT9
I	-6	GLY	-	expression tag	UNP Q9HVT9
I	-5	HIS	-	expression tag	UNP Q9HVT9
I	-4	HIS	-	expression tag	UNP Q9HVT9
I	-3	HIS	-	expression tag	UNP Q9HVT9
I	-2	HIS	-	expression tag	UNP Q9HVT9
I	-1	HIS	-	expression tag	UNP Q9HVT9
I	0	HIS	-	expression tag	UNP Q9HVT9
L	-7	MET	-	expression tag	UNP Q9HVT9
L	-6	GLY	-	expression tag	UNP Q9HVT9
L	-5	HIS	-	expression tag	UNP Q9HVT9
L	-4	HIS	-	expression tag	UNP Q9HVT9
L	-3	HIS	-	expression tag	UNP Q9HVT9
L	-2	HIS	-	expression tag	UNP Q9HVT9
L	-1	HIS	-	expression tag	UNP Q9HVT9
L	0	HIS	-	expression tag	UNP Q9HVT9

- Molecule 4 is a protein called Aspartate--tRNA(Asp/Asn) ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	589	Total	C	N	O	S	0	0	0
			4644	2943	816	865	20			
4	N	589	Total	C	N	O	S	0	0	0
			4644	2943	816	865	20			
4	O	589	Total	C	N	O	S	0	0	0
			4644	2943	816	865	20			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	589	Total	C	N	O	S	0	0	0
			4644	2943	816	865	20			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-7	MET	-	expression tag	UNP Q51422
M	-6	GLY	-	expression tag	UNP Q51422
M	-5	HIS	-	expression tag	UNP Q51422
M	-4	HIS	-	expression tag	UNP Q51422
M	-3	HIS	-	expression tag	UNP Q51422
M	-2	HIS	-	expression tag	UNP Q51422
M	-1	HIS	-	expression tag	UNP Q51422
M	0	HIS	-	expression tag	UNP Q51422
N	-7	MET	-	expression tag	UNP Q51422
N	-6	GLY	-	expression tag	UNP Q51422
N	-5	HIS	-	expression tag	UNP Q51422
N	-4	HIS	-	expression tag	UNP Q51422
N	-3	HIS	-	expression tag	UNP Q51422
N	-2	HIS	-	expression tag	UNP Q51422
N	-1	HIS	-	expression tag	UNP Q51422
N	0	HIS	-	expression tag	UNP Q51422
O	-7	MET	-	expression tag	UNP Q51422
O	-6	GLY	-	expression tag	UNP Q51422
O	-5	HIS	-	expression tag	UNP Q51422
O	-4	HIS	-	expression tag	UNP Q51422
O	-3	HIS	-	expression tag	UNP Q51422
O	-2	HIS	-	expression tag	UNP Q51422
O	-1	HIS	-	expression tag	UNP Q51422
O	0	HIS	-	expression tag	UNP Q51422
P	-7	MET	-	expression tag	UNP Q51422
P	-6	GLY	-	expression tag	UNP Q51422
P	-5	HIS	-	expression tag	UNP Q51422
P	-4	HIS	-	expression tag	UNP Q51422
P	-3	HIS	-	expression tag	UNP Q51422
P	-2	HIS	-	expression tag	UNP Q51422
P	-1	HIS	-	expression tag	UNP Q51422
P	0	HIS	-	expression tag	UNP Q51422

- Molecule 5 is a RNA chain called 76mer-tRNA.

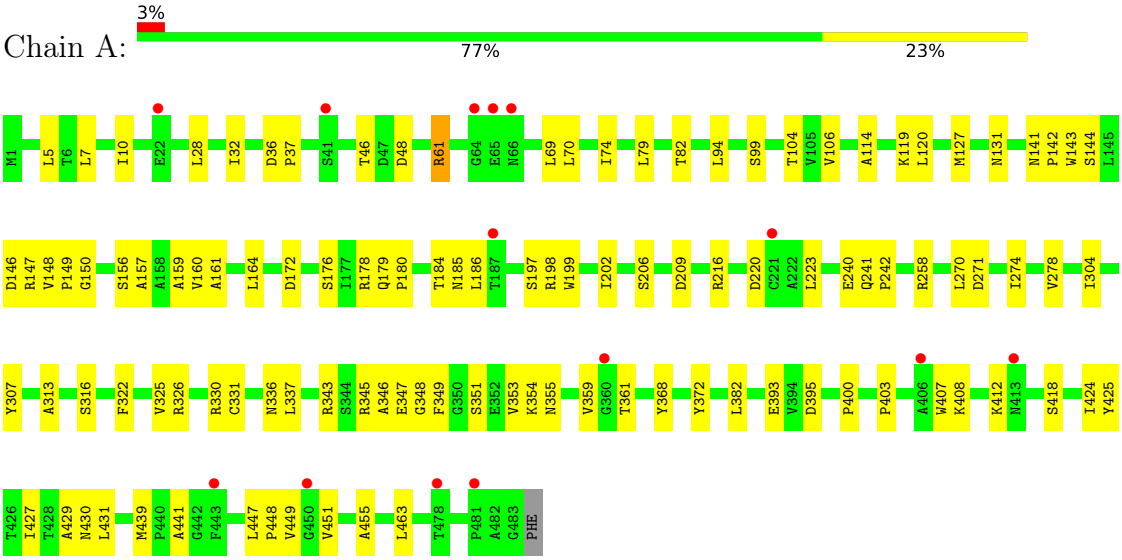
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	76	Total	C	N	O	P	0	0	0
			1622	723	288	535	76			
5	R	76	Total	C	N	O	P	0	0	0
			1622	723	288	535	76			
5	S	76	Total	C	N	O	P	0	0	0
			1622	723	288	535	76			
5	T	76	Total	C	N	O	P	0	0	0
			1622	723	288	535	76			

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.

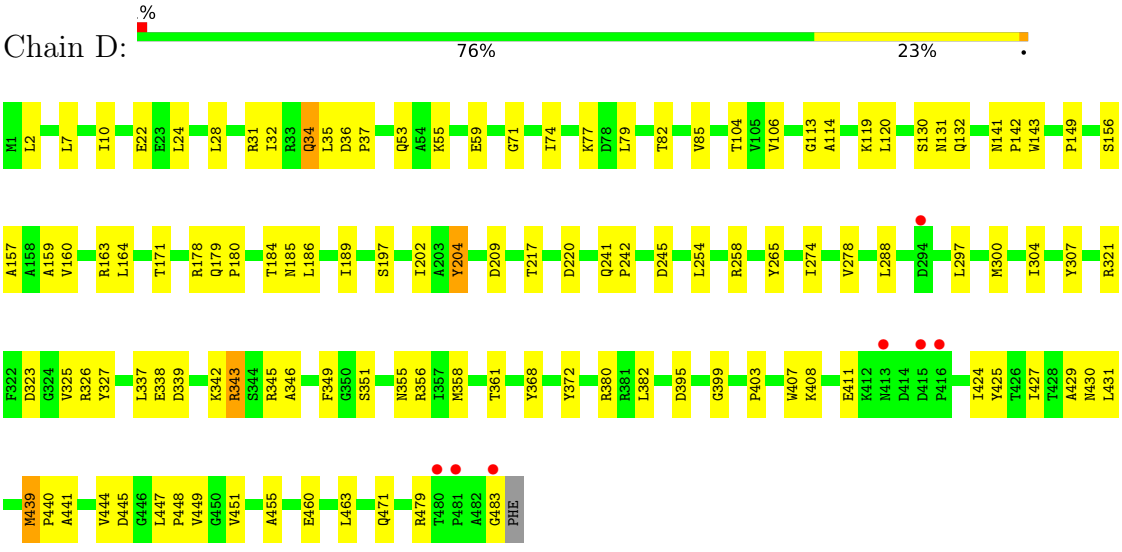
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain A:



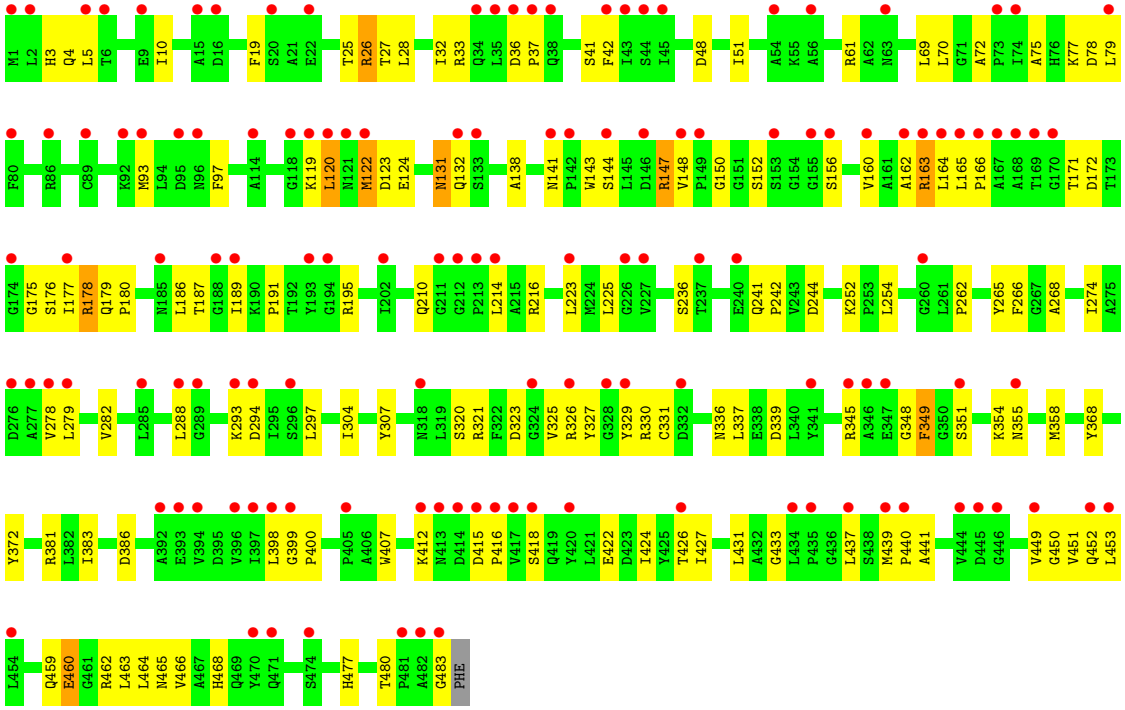
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain D:



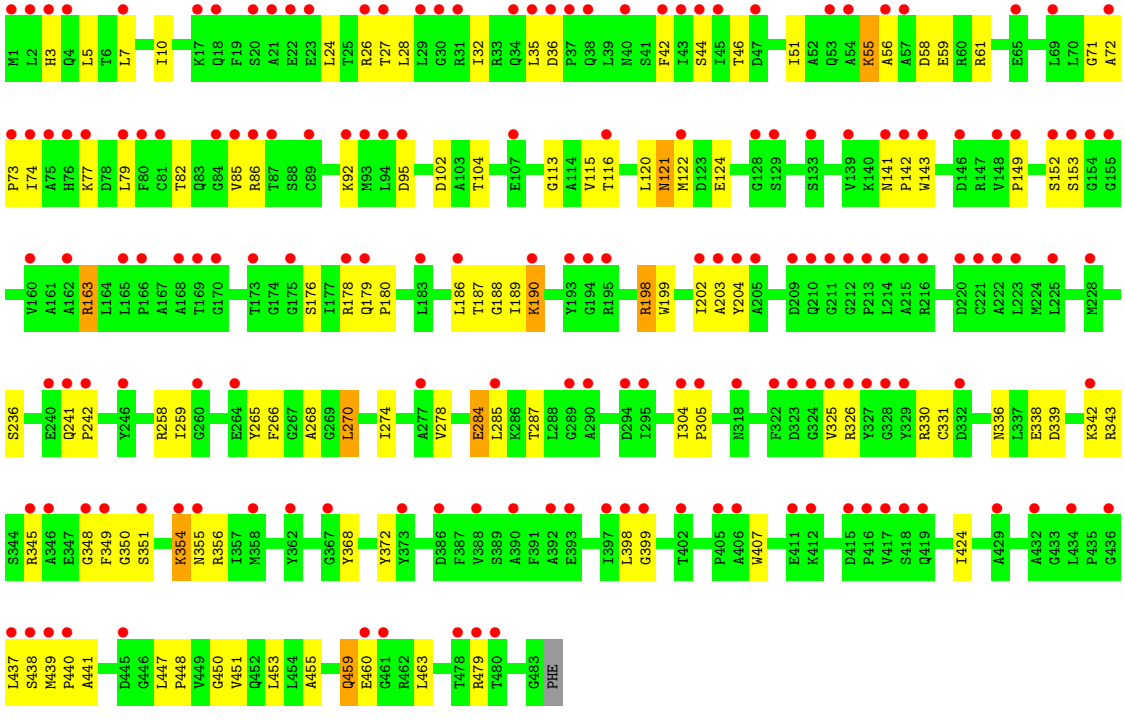
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain G:



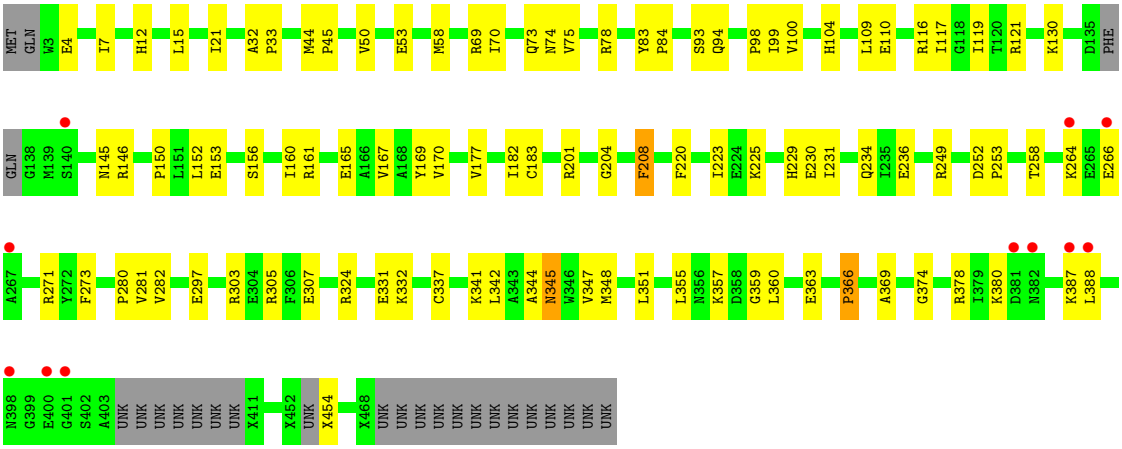
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain J:



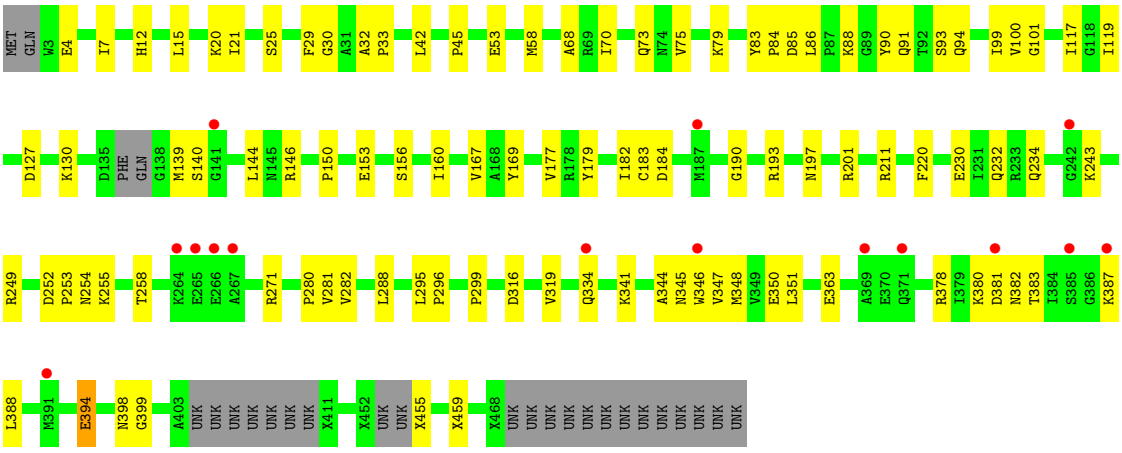
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain B:



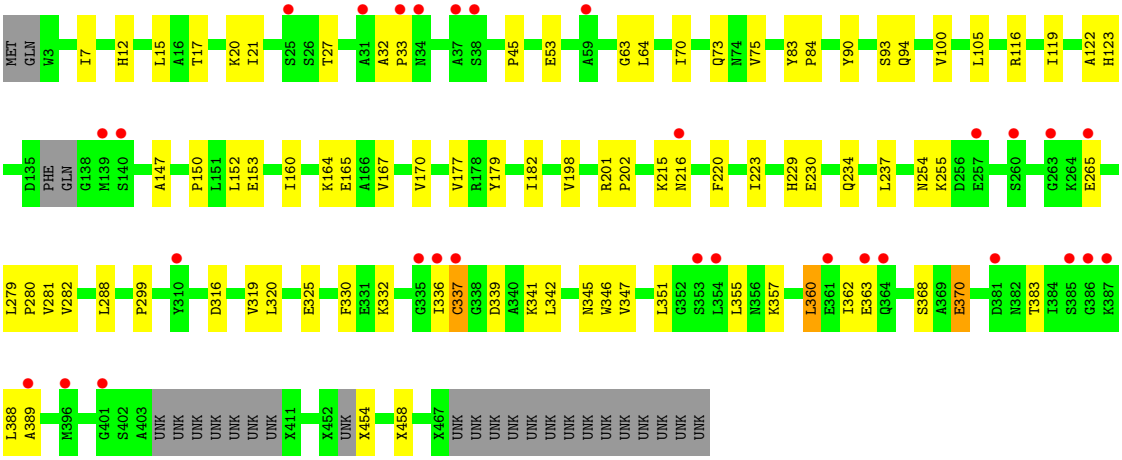
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain E:



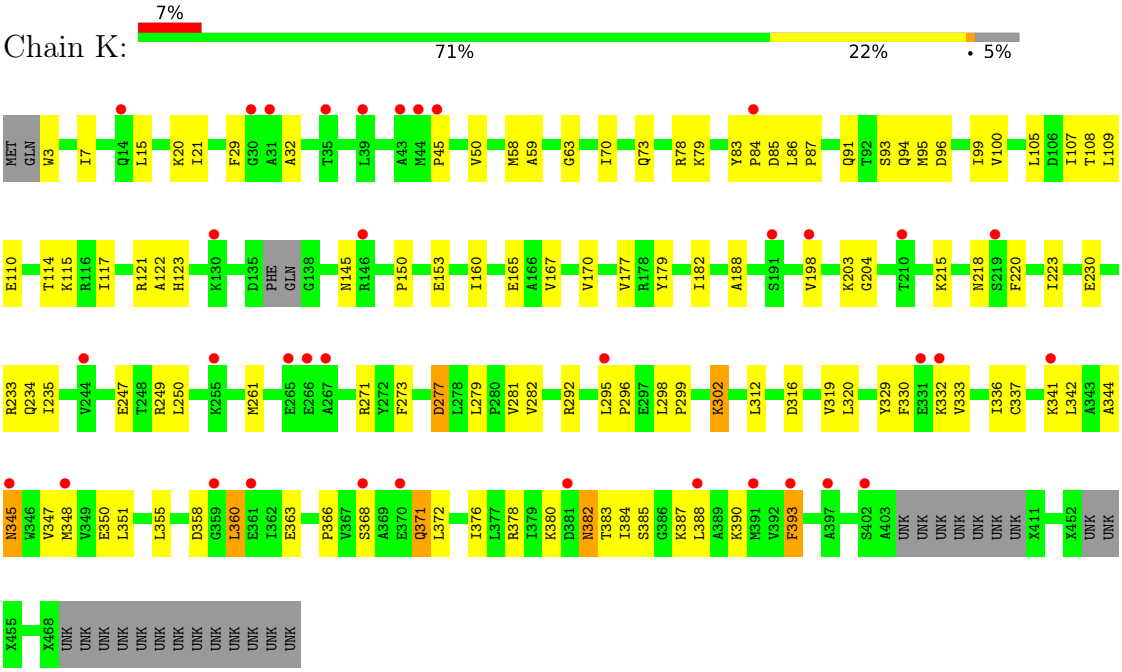
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain H:



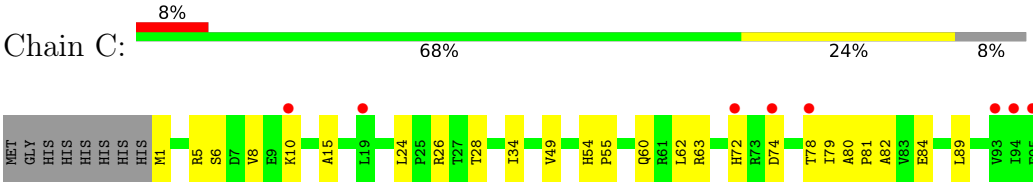
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain K:



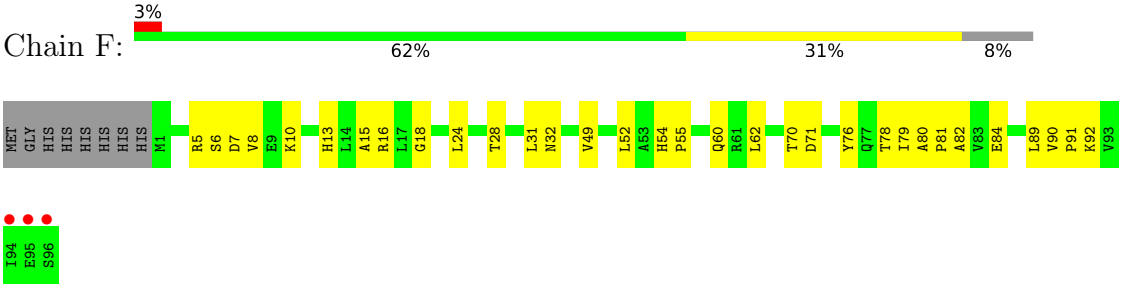
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain C:



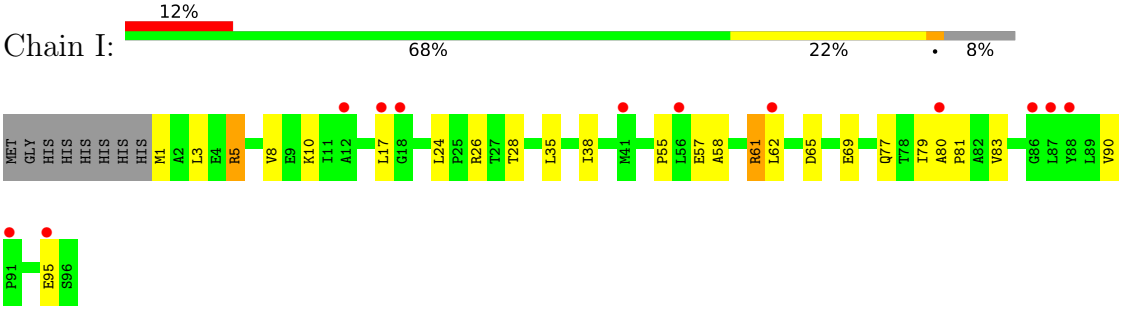
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain F:



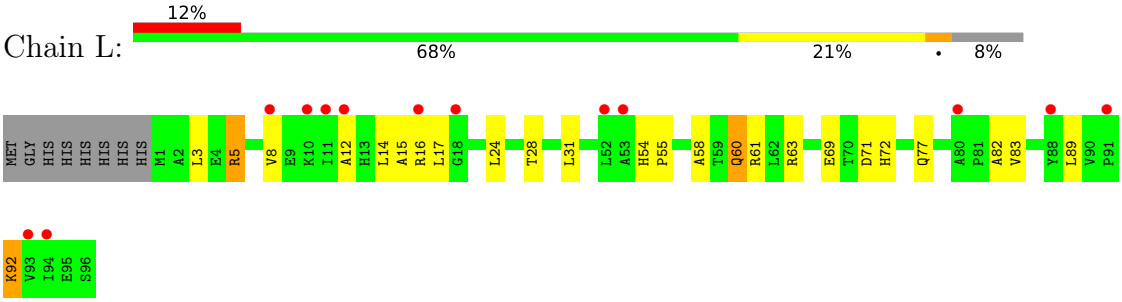
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain I:



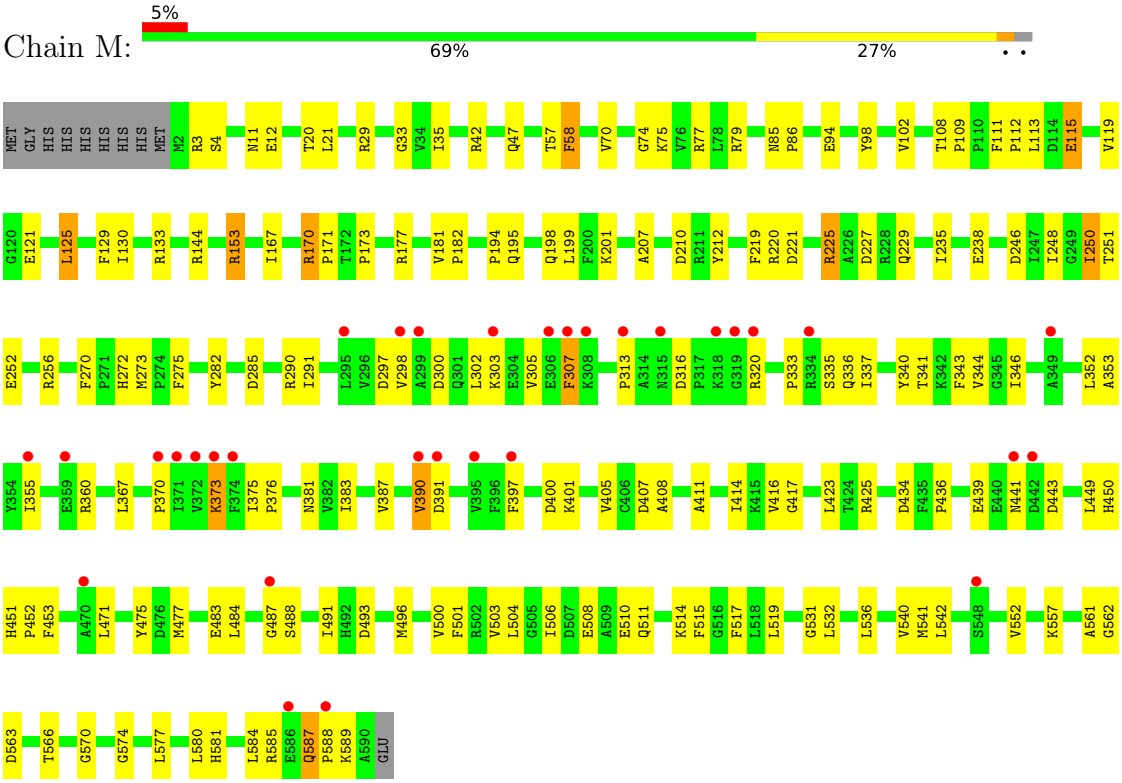
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain L:



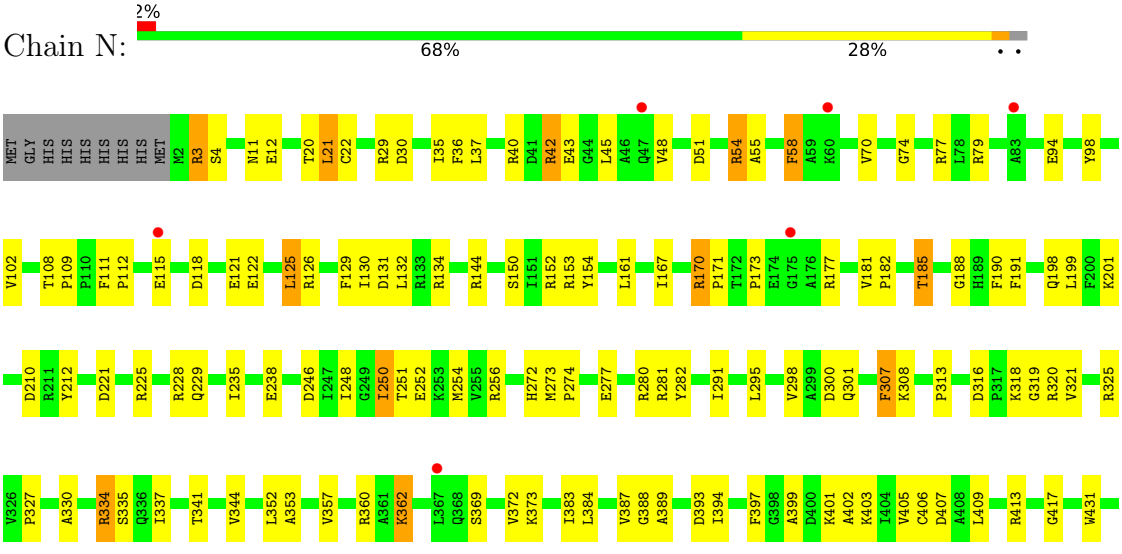
• Molecule 4: Aspartate--tRNA(Asp/Asn) ligase

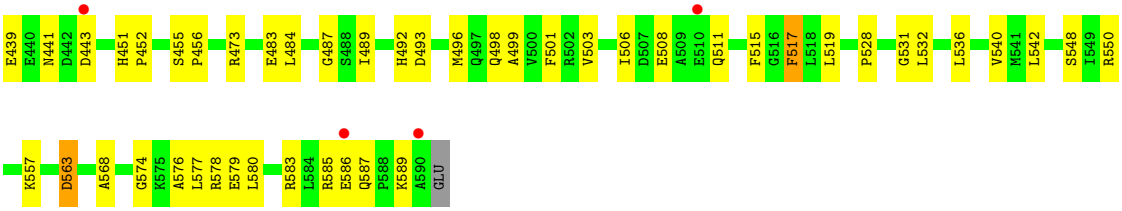
Chain M:



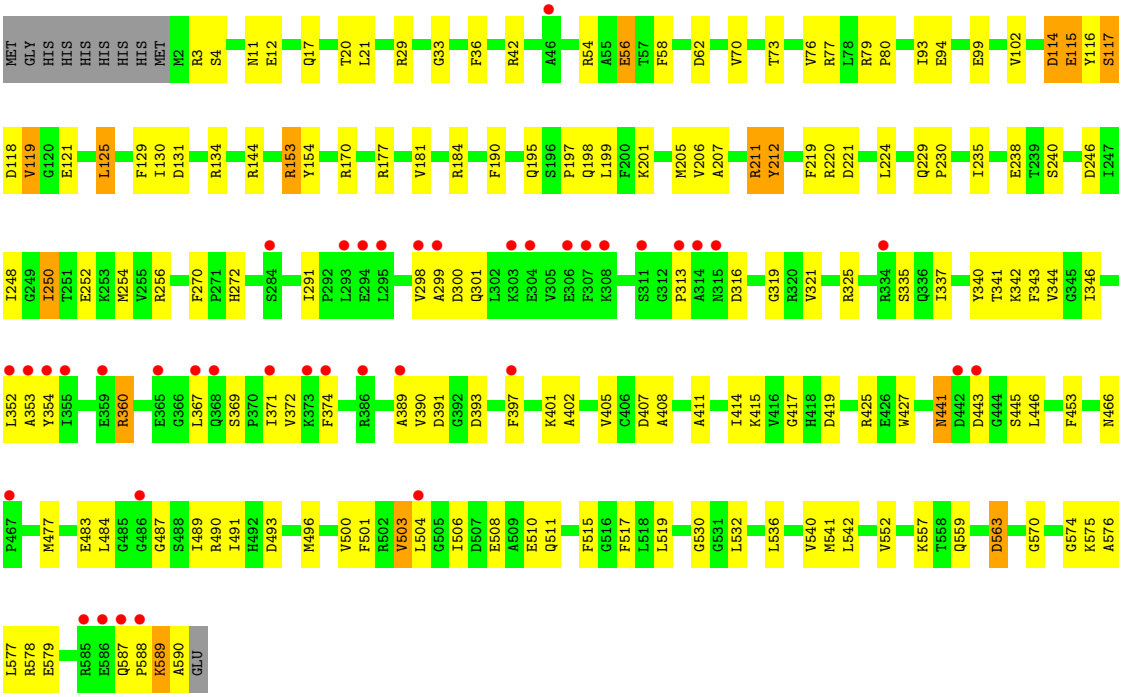
• Molecule 4: Aspartate--tRNA(Asp/Asn) ligase

Chain N:

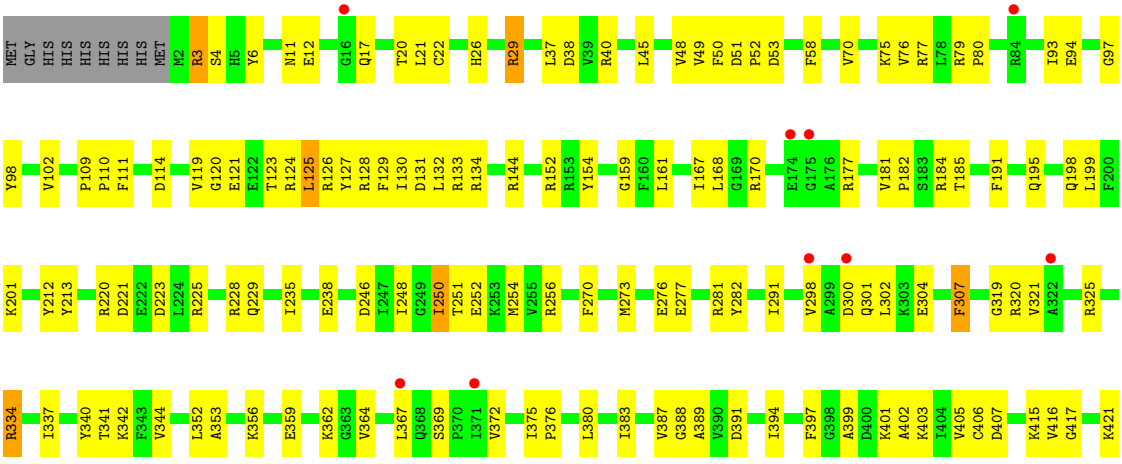


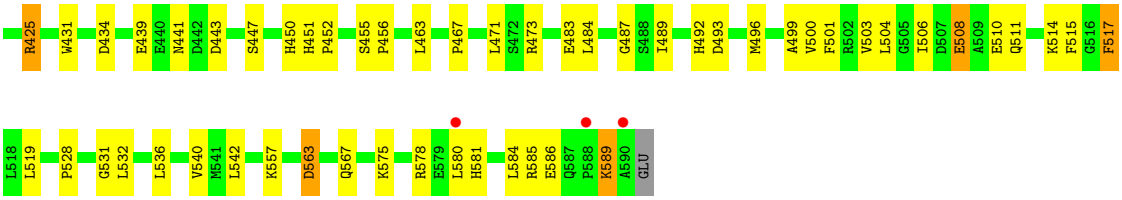


• Molecule 4: Aspartate--tRNA(Asp/Asn) ligase

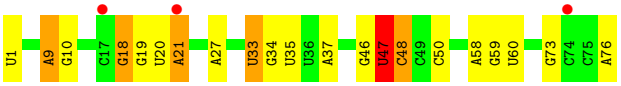


• Molecule 4: Aspartate--tRNA(Asp/Asn) ligase

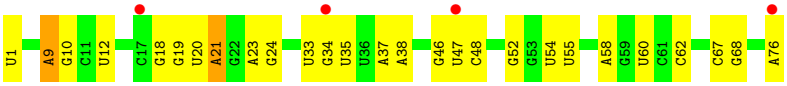




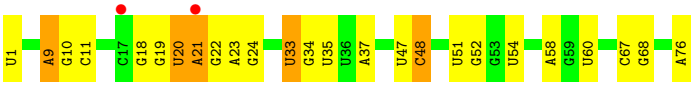
• Molecule 5: 76mer-tRNA



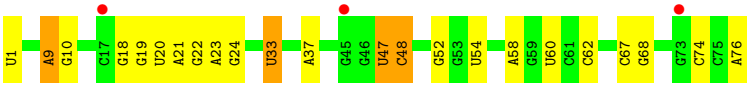
• Molecule 5: 76mer-tRNA



• Molecule 5: 76mer-tRNA



• Molecule 5: 76mer-tRNA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.14Å 185.68Å 290.36Å 90.00° 92.98° 90.00°	Depositor
Resolution (Å)	46.77 – 3.71 48.12 – 3.70	Depositor EDS
% Data completeness (in resolution range)	92.1 (46.77-3.71) 79.8 (48.12-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.292 , 0.329 0.295 , 0.327	Depositor DCC
R_{free} test set	4823 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	80.5	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	56045	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4505e-03.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.21	0/3711	0.40	0/5044
1	D	0.21	0/3711	0.41	0/5044
1	G	0.22	0/3711	0.45	1/5044 (0.0%)
1	J	0.21	0/3711	0.44	0/5044
2	B	0.21	0/3137	0.42	0/4233
2	E	0.21	0/3137	0.42	0/4233
2	H	0.21	0/3137	0.42	0/4233
2	K	0.21	0/3137	0.42	0/4233
3	C	0.21	0/748	0.44	0/1020
3	F	0.21	0/748	0.45	0/1020
3	I	0.20	0/748	0.46	0/1020
3	L	0.20	0/748	0.45	0/1020
4	M	0.25	0/4743	0.55	1/6410 (0.0%)
4	N	0.25	0/4743	0.54	1/6410 (0.0%)
4	O	0.25	0/4743	0.54	1/6410 (0.0%)
4	P	0.25	0/4743	0.54	1/6410 (0.0%)
5	Q	0.28	1/1812 (0.1%)	0.69	1/2821 (0.0%)
5	R	0.28	1/1812 (0.1%)	0.67	0/2821
5	S	0.29	1/1812 (0.1%)	0.69	0/2821
5	T	0.28	1/1812 (0.1%)	0.68	0/2821
All	All	0.24	4/56604 (0.0%)	0.51	6/78112 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	O	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	1	U	OP3-P	-10.66	1.48	1.61
5	Q	1	U	OP3-P	-10.60	1.48	1.61
5	R	1	U	OP3-P	-10.58	1.48	1.61
5	T	1	U	OP3-P	-10.53	1.48	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	250	ILE	CG1-CB-CG2	-6.66	96.76	111.40
4	M	250	ILE	CG1-CB-CG2	-6.63	96.82	111.40
5	Q	47	U	P-O3'-C3'	6.58	127.59	119.70
4	N	250	ILE	CG1-CB-CG2	-6.47	97.16	111.40
4	P	250	ILE	CG1-CB-CG2	-6.41	97.29	111.40
1	G	120	LEU	CA-CB-CG	5.56	128.09	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	O	114	ASP	Peptide
4	O	117	SER	Peptide

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	3639	0	3612	67	0
1	D	3639	0	3612	75	0
1	G	3639	0	3612	98	1
1	J	3639	0	3612	73	1
2	B	3372	0	3129	55	0
2	E	3367	0	3128	61	0
2	H	3367	0	3129	54	0
2	K	3367	0	3128	72	0
3	C	738	0	741	17	0
3	F	738	0	741	24	0
3	I	738	0	741	17	0
3	L	738	0	741	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	4644	0	4618	115	1
4	N	4644	0	4618	131	0
4	O	4644	0	4618	111	1
4	P	4644	0	4618	126	0
5	Q	1622	0	819	12	0
5	R	1622	0	819	14	0
5	S	1622	0	819	14	0
5	T	1622	0	819	10	0
All	All	56045	0	51674	1052	2

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 10.

All (1052) 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)
4:M:585:ARG:HH12	4:M:589:LYS:HB2	1.41	0.84
4:M:584:LEU:HD13	4:N:188:GLY:HA2	1.62	0.80
4:P:79:ARG:NH2	4:P:93:ILE:O	2.13	0.80
1:D:141:ASN:HD22	1:D:149:PRO:HA	1.50	0.77
1:G:178:ARG:NH1	1:G:426:THR:OG1	2.17	0.77
4:M:229:GLN:NE2	4:M:557:LYS:O	2.18	0.76
4:O:313:PRO:HA	4:O:316:ASP:HB2	1.67	0.76
1:G:172:ASP:OD2	1:G:178:ARG:NH2	2.18	0.76
4:P:334:ARG:HH11	4:P:334:ARG:H	1.34	0.76
1:G:93:MET:HG3	1:G:329:TYR:HB3	1.68	0.75
4:N:229:GLN:NE2	4:N:557:LYS:O	2.20	0.74
1:G:97:PHE:HA	3:I:79:ILE:HD11	1.68	0.74
4:N:403:LYS:NZ	4:N:407:ASP:OD2	2.18	0.74
4:O:79:ARG:NH2	4:O:93:ILE:O	2.14	0.74
2:B:4:GLU:HG3	2:B:201:ARG:HG3	1.69	0.73
4:N:3:ARG:HD3	4:N:22:CYS:H	1.50	0.73
1:J:304:ILE:HG13	1:J:305:PRO:HD3	1.71	0.73
1:J:325:VAL:HG13	1:J:326:ARG:HG3	1.70	0.73
3:I:3:LEU:HD11	3:I:35:LEU:HD21	1.71	0.73
2:H:75:VAL:HG22	2:H:280:PRO:HB3	1.70	0.73
4:M:333:PRO:HG2	4:M:336:GLN:HG2	1.70	0.72
1:A:143:TRP:HZ3	1:A:161:ALA:HB1	1.54	0.72
1:G:325:VAL:HG13	1:G:326:ARG:HG3	1.71	0.72
4:O:489:ILE:HD13	4:O:530:GLY:HA3	1.71	0.72
1:J:77:LYS:HG3	1:J:122:MET:HG3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:229:GLN:NE2	4:O:557:LYS:O	2.23	0.71
1:G:122:MET:SD	1:G:123:ASP:N	2.61	0.71
2:B:75:VAL:HG22	2:B:280:PRO:HB3	1.71	0.71
2:K:279:LEU:HD22	3:L:58:ALA:HB3	1.72	0.71
1:A:325:VAL:HG13	1:A:326:ARG:HG3	1.72	0.71
2:K:21:ILE:HB	2:K:150:PRO:HB3	1.73	0.71
4:P:229:GLN:NE2	4:P:557:LYS:O	2.23	0.71
1:D:325:VAL:HG13	1:D:326:ARG:HG3	1.71	0.70
2:E:4:GLU:HG3	2:E:201:ARG:HG3	1.73	0.70
2:B:201:ARG:HB3	2:B:208:PHE:HB3	1.72	0.70
3:C:78:THR:HG23	3:C:79:ILE:HG13	1.73	0.70
1:D:160:VAL:HB	1:D:186:LEU:HD21	1.73	0.70
1:J:51:ILE:HG12	1:J:55:LYS:HE2	1.74	0.70
4:P:201:LYS:HE2	4:P:238:GLU:HB2	1.74	0.70
4:P:403:LYS:NZ	4:P:407:ASP:OD2	2.22	0.70
1:D:184:THR:HG23	1:D:186:LEU:HD13	1.72	0.70
1:D:32:ILE:HD13	1:D:164:LEU:HD22	1.74	0.70
3:C:82:ALA:HB1	3:C:89:LEU:HB2	1.72	0.70
1:D:217:THR:HA	1:D:471:GLN:HE22	1.57	0.70
4:P:493:ASP:HB3	4:P:496:MET:HB3	1.74	0.70
1:G:77:LYS:HA	1:G:120:LEU:HB3	1.74	0.70
1:D:120:LEU:HD13	1:D:156:SER:HA	1.74	0.69
1:J:35:LEU:HD23	1:J:163:ARG:HH12	1.57	0.69
4:M:235:ILE:HD11	4:M:536:LEU:HD13	1.72	0.69
4:O:589:LYS:HG3	4:O:590:ALA:H	1.57	0.69
4:N:122:GLU:HG2	4:N:126:ARG:HH12	1.57	0.69
4:O:235:ILE:HD11	4:O:536:LEU:HD13	1.73	0.69
2:K:29:PHE:HE2	2:K:32:ALA:HB3	1.58	0.69
4:M:302:LEU:HD23	4:M:305:VAL:HG21	1.75	0.69
4:O:211:ARG:NH2	4:P:6:TYR:OH	2.26	0.69
2:E:75:VAL:HG22	2:E:280:PRO:HB3	1.75	0.68
1:D:157:ALA:HB1	1:D:184:THR:HG21	1.75	0.68
4:M:587:GLN:HG2	4:M:588:PRO:HD3	1.75	0.68
4:N:235:ILE:HD11	4:N:536:LEU:HD13	1.76	0.68
4:O:587:GLN:HG2	4:O:588:PRO:HD3	1.74	0.68
2:K:78:ARG:NH2	2:K:277:ASP:OD2	2.27	0.68
2:E:381:ASP:OD1	2:E:382:ASN:N	2.27	0.67
4:P:37:LEU:HB2	4:P:48:VAL:HG13	1.76	0.67
1:G:189:ILE:HG12	1:G:437:LEU:HD23	1.77	0.67
1:G:195:ARG:HH21	1:G:225:LEU:HD11	1.60	0.67
1:G:440:PRO:HA	1:G:450:GLY:HA2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:387:LYS:HD2	2:E:455:UNK:H2	1.60	0.67
4:N:369:SER:HB3	4:N:372:VAL:HG23	1.76	0.67
5:Q:47:U:O2'	5:Q:48:C:OP1	2.09	0.67
1:A:274:ILE:HD12	1:A:449:VAL:HG21	1.77	0.66
4:N:37:LEU:HB2	4:N:48:VAL:HG13	1.75	0.66
4:M:181:VAL:HG22	4:N:181:VAL:HG22	1.78	0.66
4:N:325:ARG:NH1	4:N:388:GLY:O	2.28	0.66
4:P:29:ARG:NH2	4:P:38:ASP:OD2	2.27	0.66
3:I:5:ARG:HB2	3:I:24:LEU:HD21	1.77	0.66
2:E:73:GLN:HG2	2:E:282:VAL:HG22	1.77	0.66
4:P:353:ALA:HB3	4:P:397:PHE:HB2	1.77	0.66
1:A:147:ARG:HA	1:A:408:LYS:HA	1.77	0.66
4:N:320:ARG:NH2	4:N:406:CYS:SG	2.69	0.65
4:O:181:VAL:HG22	4:P:181:VAL:HG22	1.79	0.65
1:J:270:LEU:HB2	1:J:274:ILE:HD11	1.78	0.65
4:N:77:ARG:HG2	4:N:94:GLU:HG3	1.77	0.65
4:N:493:ASP:HB3	4:N:496:MET:HB3	1.76	0.65
4:P:447:SER:HA	4:P:504:LEU:HD11	1.78	0.65
1:D:22:GLU:OE2	1:D:55:LYS:NZ	2.23	0.65
2:K:167:VAL:HG13	2:K:220:PHE:HB3	1.78	0.65
4:P:273:MET:HE2	4:P:277:GLU:HG2	1.78	0.65
2:B:7:ILE:HG13	2:B:160:ILE:HG23	1.79	0.65
4:N:277:GLU:OE2	4:N:281:ARG:NH2	2.29	0.65
2:H:7:ILE:HG13	2:H:160:ILE:HG23	1.77	0.65
4:O:54:ARG:NH1	4:O:99:GLU:OE2	2.29	0.65
1:J:178:ARG:HG2	1:J:438:SER:HB2	1.78	0.65
2:E:140:SER:HB2	3:F:92:LYS:HB2	1.78	0.64
2:K:355:LEU:HA	2:K:360:LEU:HD11	1.79	0.64
2:E:345:ASN:HD21	5:T:54:U:H5"	1.62	0.64
4:N:77:ARG:NH2	5:R:34:G:O6	2.31	0.64
4:O:42:ARG:HH21	4:P:161:LEU:HD13	1.62	0.64
4:N:170:ARG:HG3	4:N:171:PRO:HD2	1.79	0.64
4:P:487:GLY:HA3	4:P:532:LEU:HA	1.80	0.64
5:R:58:A:O2'	5:R:60:U:OP2	2.14	0.64
1:A:351:SER:O	1:A:355:ASN:ND2	2.23	0.64
1:A:5:LEU:O	1:A:216:ARG:NH1	2.31	0.63
4:M:210:ASP:OD2	4:N:3:ARG:NH2	2.31	0.63
5:Q:9:A:O2'	5:Q:10:G:N7	2.31	0.63
4:P:291:ILE:HD13	4:P:417:GLY:HA3	1.78	0.63
2:H:229:HIS:HB3	4:O:588:PRO:HG3	1.79	0.63
1:A:258:ARG:NH1	1:A:395:ASP:OD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:229:GLN:HE22	4:N:557:LYS:H	1.46	0.63
4:N:144:ARG:HG3	4:N:540:VAL:HG21	1.81	0.63
4:O:493:ASP:HB3	4:O:496:MET:HB3	1.81	0.63
1:A:141:ASN:HD22	1:A:149:PRO:HA	1.64	0.62
2:K:7:ILE:HG13	2:K:160:ILE:HG23	1.79	0.62
4:M:177:ARG:HB2	4:M:221:ASP:HB3	1.80	0.62
4:O:201:LYS:HE2	4:O:238:GLU:HB2	1.79	0.62
4:N:499:ALA:O	4:N:503:VAL:HG13	1.98	0.62
1:D:439:MET:HE2	1:D:440:PRO:HD2	1.82	0.62
4:M:508:GLU:OE2	4:M:511:GLN:NE2	2.32	0.62
1:D:178:ARG:NH2	1:D:430:ASN:OD1	2.32	0.62
1:A:32:ILE:HD13	1:A:164:LEU:HD22	1.82	0.62
4:O:390:VAL:HG22	4:O:391:ASP:H	1.64	0.62
5:R:9:A:O2'	5:R:10:G:N7	2.32	0.62
2:H:100:VAL:HB	2:H:122:ALA:HB3	1.81	0.62
1:A:157:ALA:HB1	1:A:184:THR:HG21	1.80	0.62
2:B:305:ARG:NH2	2:B:331:GLU:OE1	2.31	0.62
2:E:12:HIS:HB2	2:E:193:ARG:HG3	1.82	0.62
1:G:148:VAL:HG22	1:G:150:GLY:H	1.63	0.62
3:I:35:LEU:HA	3:I:38:ILE:HG12	1.82	0.62
4:O:574:GLY:HA2	4:O:577:LEU:HD12	1.82	0.62
4:O:77:ARG:HH21	5:S:34:G:H1	1.45	0.62
2:E:127:ASP:OD2	2:E:193:ARG:NH2	2.33	0.61
1:G:61:ARG:HG3	1:G:70:LEU:HB3	1.82	0.61
1:J:326:ARG:NH1	2:K:87:PRO:O	2.33	0.61
4:M:561:ALA:HB3	4:N:185:THR:HG21	1.82	0.61
4:N:291:ILE:HD13	4:N:417:GLY:HA3	1.82	0.61
4:O:184:ARG:NH1	4:P:221:ASP:OD1	2.33	0.61
1:D:304:ILE:HD11	1:D:424:ILE:HG23	1.82	0.61
2:E:7:ILE:HG13	2:E:160:ILE:HG23	1.82	0.61
1:G:32:ILE:HD12	1:G:42:PHE:HE2	1.64	0.61
2:H:73:GLN:HG2	2:H:282:VAL:HG22	1.81	0.61
4:O:590:ALA:O	4:P:578:ARG:NH1	2.34	0.61
4:P:131:ASP:OD1	4:P:134:ARG:NH1	2.33	0.61
4:N:357:VAL:HG11	4:N:384:LEU:HD21	1.82	0.61
4:O:177:ARG:NH1	4:O:221:ASP:O	2.34	0.61
1:A:346:ALA:C	1:A:348:GLY:HA3	2.21	0.61
2:B:44:MET:HG3	2:B:45:PRO:HD2	1.83	0.61
2:K:32:ALA:O	2:K:145:ASN:ND2	2.34	0.61
4:M:574:GLY:HA2	4:M:577:LEU:HD12	1.83	0.61
4:O:170:ARG:HH21	4:P:567:GLN:HB3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:249:ARG:NH1	2:E:258:THR:O	2.34	0.61
1:J:338:GLU:HG3	3:L:16:ARG:HH21	1.66	0.61
4:O:325:ARG:HH11	4:O:389:ALA:HA	1.65	0.61
4:P:325:ARG:NH1	4:P:388:GLY:O	2.33	0.61
2:H:17:THR:O	2:H:27:THR:OG1	2.10	0.60
4:M:487:GLY:HA3	4:M:532:LEU:HA	1.83	0.60
4:O:144:ARG:HG3	4:O:540:VAL:HG21	1.81	0.60
2:E:70:ILE:HD11	2:E:288:LEU:HD11	1.83	0.60
4:M:3:ARG:NH2	4:N:210:ASP:OD2	2.29	0.60
3:F:78:THR:HG23	3:F:79:ILE:HG13	1.83	0.60
4:M:320:ARG:HG3	4:M:405:VAL:HG11	1.84	0.60
4:N:353:ALA:HB3	4:N:397:PHE:HB2	1.83	0.60
3:C:5:ARG:HD2	3:C:24:LEU:HD13	1.82	0.60
2:H:21:ILE:HB	2:H:150:PRO:HB3	1.82	0.60
2:K:188:ALA:O	5:Q:73:G:O2'	2.18	0.60
4:O:369:SER:HB3	4:O:372:VAL:HG23	1.83	0.60
3:F:5:ARG:HB2	3:F:24:LEU:HD21	1.82	0.60
2:K:73:GLN:HG2	2:K:282:VAL:HG22	1.83	0.60
2:K:250:LEU:HD23	2:K:261:MET:HB2	1.84	0.60
4:O:195:GLN:OE1	4:O:220:ARG:HG3	2.01	0.60
5:S:58:A:O2'	5:S:60:U:OP2	2.20	0.60
4:N:280:ARG:HH21	4:N:281:ARG:HE	1.50	0.60
4:O:117:SER:HB3	4:O:119:VAL:H	1.67	0.60
4:P:514:LYS:HG3	4:P:515:PHE:CD2	2.36	0.60
4:P:499:ALA:O	4:P:503:VAL:HG13	2.01	0.60
3:F:84:GLU:HG3	3:F:89:LEU:HD11	1.83	0.59
4:M:219:PHE:HZ	4:N:167:ILE:HD12	1.67	0.59
2:K:378:ARG:O	2:K:382:ASN:ND2	2.34	0.59
4:P:344:VAL:HG21	4:P:352:LEU:HB2	1.84	0.59
5:Q:58:A:O2'	5:Q:60:U:OP2	2.19	0.59
2:H:355:LEU:HA	2:H:360:LEU:HD11	1.84	0.59
4:N:574:GLY:HA2	4:N:577:LEU:HD12	1.84	0.59
4:P:372:VAL:HG13	4:P:380:LEU:HD21	1.84	0.59
2:E:146:ARG:NH2	2:E:190:GLY:O	2.36	0.59
1:G:28:LEU:O	1:G:32:ILE:HG12	2.03	0.59
2:H:167:VAL:HG13	2:H:220:PHE:HB3	1.83	0.59
2:K:360:LEU:HD12	2:K:366:PRO:HG2	1.82	0.59
2:E:197:ASN:HB3	2:E:211:ARG:HD3	1.85	0.59
2:H:53:GLU:HG3	3:I:62:LEU:HD23	1.85	0.59
4:N:506:ILE:HD12	4:N:506:ILE:O	2.03	0.59
4:P:229:GLN:HE22	4:P:557:LYS:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:195:GLN:OE1	4:M:220:ARG:HG3	2.03	0.58
1:G:160:VAL:HB	1:G:186:LEU:HD21	1.84	0.58
1:A:148:VAL:HG22	1:A:150:GLY:H	1.67	0.58
2:B:225:LYS:O	2:B:229:HIS:ND1	2.35	0.58
1:D:441:ALA:HB2	1:D:451:VAL:HG23	1.85	0.58
1:J:141:ASN:HD22	1:J:149:PRO:HA	1.67	0.58
2:B:21:ILE:HB	2:B:150:PRO:HB3	1.85	0.58
4:P:235:ILE:HD11	4:P:536:LEU:HD13	1.85	0.58
1:G:93:MET:HB2	1:G:348:GLY:HA2	1.85	0.58
2:K:281:VAL:HG23	3:L:60:GLN:HG2	1.86	0.58
2:B:387:LYS:HG3	2:B:454:UNK:HA	1.85	0.58
2:E:398:ASN:OD1	2:E:399:GLY:N	2.37	0.58
1:J:28:LEU:O	1:J:32:ILE:HG12	2.04	0.58
1:J:44:SER:HB2	1:J:86:ARG:HH21	1.68	0.58
1:G:321:ARG:NH2	2:H:90:TYR:OH	2.37	0.58
4:P:152:ARG:NH2	4:P:213:TYR:OH	2.37	0.58
3:F:8:VAL:HG21	3:F:28:THR:HG22	1.85	0.58
4:P:455:SER:HB3	4:P:489:ILE:HG23	1.86	0.58
4:M:407:ASP:OD1	4:M:408:ALA:N	2.36	0.57
4:O:201:LYS:HG2	4:O:212:TYR:HE2	1.69	0.57
3:F:82:ALA:HB1	3:F:89:LEU:HB2	1.86	0.57
1:J:345:ARG:NH1	3:L:15:ALA:O	2.37	0.57
1:J:398:LEU:HG	1:J:453:LEU:HB3	1.87	0.57
1:J:236:SER:O	3:L:61:ARG:NE	2.29	0.57
2:K:342:LEU:HD23	2:K:380:LYS:HE3	1.85	0.57
4:P:11:ASN:OD1	4:P:12:GLU:N	2.34	0.57
1:D:361:THR:HG23	2:E:271:ARG:HH11	1.68	0.57
3:I:8:VAL:HG21	3:I:28:THR:HG22	1.86	0.57
1:D:104:THR:HG21	1:D:197:SER:HB2	1.87	0.57
4:M:42:ARG:HH21	4:N:161:LEU:HB2	1.70	0.57
4:M:434:ASP:HB3	4:M:471:LEU:HD23	1.86	0.57
1:A:198:ARG:NH2	1:A:206:SER:O	2.38	0.57
1:G:345:ARG:HB3	3:I:17:LEU:HD23	1.85	0.57
1:J:336:ASN:H	1:J:339:ASP:HB3	1.69	0.57
4:O:344:VAL:HG21	4:O:352:LEU:HB2	1.86	0.57
1:A:7:LEU:HD23	1:A:10:ILE:HD12	1.87	0.57
1:A:178:ARG:NH2	1:A:430:ASN:OD1	2.38	0.57
4:O:360:ARG:NH2	4:O:389:ALA:O	2.37	0.57
4:O:407:ASP:OD1	4:O:408:ALA:N	2.37	0.57
4:P:79:ARG:HG3	4:P:80:PRO:HD2	1.87	0.57
4:P:506:ILE:HD12	4:P:506:ILE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:21:ILE:HB	2:E:150:PRO:HB3	1.86	0.57
5:S:9:A:O2'	5:S:10:G:N7	2.36	0.57
2:E:53:GLU:HG3	3:F:62:LEU:HD23	1.86	0.56
1:D:7:LEU:HD23	1:D:10:ILE:HD12	1.87	0.56
1:G:349:PHE:O	1:G:354:LYS:NZ	2.36	0.56
4:O:576:ALA:HA	4:O:579:GLU:HG2	1.87	0.56
2:B:53:GLU:HG3	3:C:62:LEU:HD23	1.88	0.56
1:A:178:ARG:HH12	1:A:429:ALA:HB3	1.70	0.56
1:D:274:ILE:HD12	1:D:449:VAL:HG11	1.86	0.56
1:D:351:SER:O	1:D:355:ASN:ND2	2.25	0.56
5:T:58:A:O2'	5:T:60:U:OP2	2.22	0.56
4:M:77:ARG:HH21	5:Q:34:G:H1	1.52	0.56
4:N:334:ARG:HD2	4:N:335:SER:N	2.20	0.56
4:O:219:PHE:HZ	4:P:167:ILE:HD12	1.71	0.56
2:H:7:ILE:HG22	2:H:198:VAL:HG13	1.87	0.56
4:N:273:MET:HE2	4:N:277:GLU:HG2	1.88	0.56
4:M:275:PHE:HE1	4:M:285:ASP:HB3	1.71	0.56
4:M:493:ASP:HB3	4:M:496:MET:HB3	1.86	0.56
4:P:121:GLU:O	4:P:125:LEU:HD13	2.06	0.56
4:P:367:LEU:HD12	4:P:380:LEU:HD23	1.86	0.56
4:O:4:SER:HB3	4:O:20:THR:H	1.69	0.56
4:P:144:ARG:HG3	4:P:540:VAL:HG21	1.88	0.56
4:P:575:LYS:O	4:P:578:ARG:HG2	2.05	0.56
1:G:178:ARG:HH11	1:G:178:ARG:HB2	1.70	0.56
1:J:354:LYS:HG3	3:L:17:LEU:HD23	1.88	0.56
2:K:123:HIS:NE2	2:K:153:GLU:OE1	2.38	0.56
4:M:4:SER:HB3	4:M:20:THR:H	1.70	0.56
4:N:330:ALA:HA	4:N:394:ILE:HG13	1.88	0.56
1:A:455:ALA:HB2	1:A:463:LEU:HD13	1.88	0.55
2:E:344:ALA:O	2:E:348:MET:HG3	2.05	0.55
1:G:175:GLY:HA2	1:G:178:ARG:HH12	1.71	0.55
2:K:107:ILE:HG13	2:K:117:ILE:HD12	1.88	0.55
4:M:225:ARG:HD2	4:M:227:ASP:H	1.71	0.55
4:P:320:ARG:HG3	4:P:405:VAL:HG11	1.87	0.55
4:N:79:ARG:NH2	5:R:35:U:O4	2.37	0.55
4:P:124:ARG:HH21	4:P:128:ARG:HH12	1.52	0.55
1:D:178:ARG:HH12	1:D:429:ALA:HB3	1.70	0.55
1:A:347:GLU:N	1:A:348:GLY:HA3	2.22	0.55
4:P:184:ARG:O	4:P:581:HIS:NE2	2.37	0.55
4:P:356:LYS:NZ	4:P:394:ILE:HD11	2.22	0.55
5:T:9:A:O2'	5:T:10:G:N7	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:291:ILE:O	4:N:413:ARG:NH2	2.40	0.55
4:N:576:ALA:HA	4:N:579:GLU:HG2	1.87	0.55
1:A:69:LEU:HD21	1:A:223:LEU:HB3	1.88	0.54
1:G:3:HIS:HB2	1:G:163:ARG:HG3	1.87	0.54
4:P:195:GLN:OE1	4:P:220:ARG:HG3	2.07	0.54
4:N:4:SER:HB3	4:N:20:THR:H	1.73	0.54
4:O:17:GLN:O	4:O:76:VAL:HG12	2.07	0.54
2:H:63:GLY:HA3	2:H:70:ILE:HD11	1.89	0.54
1:A:258:ARG:NH1	1:A:393:GLU:O	2.41	0.54
3:C:84:GLU:HB2	3:C:89:LEU:HD21	1.90	0.54
2:E:177:VAL:HG13	2:E:182:ILE:HB	1.89	0.54
1:G:141:ASN:HD21	1:G:143:TRP:HB2	1.72	0.54
1:G:265:TYR:HD2	1:G:400:PRO:HD2	1.72	0.54
2:H:230:GLU:HG3	2:H:234:GLN:HE21	1.71	0.54
2:K:382:ASN:HD22	2:K:383:THR:HG23	1.71	0.54
4:N:131:ASP:OD1	4:N:134:ARG:NH1	2.40	0.54
1:D:278:VAL:HG22	1:D:451:VAL:HG22	1.88	0.54
3:F:71:ASP:O	3:F:76:TYR:OH	2.25	0.54
1:G:144:SER:OG	1:G:147:ARG:NE	2.40	0.54
4:N:121:GLU:O	4:N:125:LEU:HD13	2.08	0.54
4:O:79:ARG:NE	4:O:94:GLU:HG3	2.21	0.54
1:A:28:LEU:O	1:A:32:ILE:HG12	2.08	0.54
4:M:11:ASN:OD1	4:M:12:GLU:N	2.37	0.54
4:M:291:ILE:HD13	4:M:417:GLY:HA3	1.89	0.54
4:O:508:GLU:HA	4:O:511:GLN:HB2	1.89	0.54
1:A:185:ASN:HB2	1:A:448:PRO:HB3	1.89	0.54
3:L:8:VAL:HG21	3:L:28:THR:HG22	1.89	0.54
4:O:319:GLY:HA2	4:O:402:ALA:N	2.23	0.54
4:M:344:VAL:HG21	4:M:352:LEU:HB2	1.89	0.54
4:P:50:PHE:CE2	4:P:97:GLY:HA3	2.43	0.54
2:K:378:ARG:HG3	2:K:382:ASN:HD21	1.73	0.54
4:P:177:ARG:HB2	4:P:221:ASP:HB3	1.90	0.54
4:M:451:HIS:HD2	4:M:453:PHE:HB2	1.73	0.53
2:B:73:GLN:HG2	2:B:282:VAL:HG22	1.89	0.53
1:D:455:ALA:HB2	1:D:463:LEU:HD13	1.90	0.53
2:H:325:GLU:HG2	2:H:362:ILE:HG22	1.90	0.53
4:N:401:LYS:O	4:N:405:VAL:HG12	2.08	0.53
2:H:345:ASN:HD21	5:S:54:U:H5”	1.72	0.53
4:N:252:GLU:HG2	4:N:256:ARG:HE	1.74	0.53
1:D:254:LEU:HD13	1:D:288:LEU:HB3	1.90	0.53
1:D:258:ARG:HB2	1:D:395:ASP:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:585:ARG:HH22	4:N:578:ARG:HG2	1.72	0.53
2:E:79:LYS:HB3	2:E:91:GLN:HB3	1.90	0.53
4:P:456:PRO:O	4:P:473:ARG:NH1	2.42	0.53
2:B:236:GLU:OE1	4:N:585:ARG:HD2	2.07	0.53
1:D:143:TRP:CH2	1:D:479:ARG:HB3	2.43	0.53
1:G:77:LYS:NZ	1:G:152:SER:O	2.41	0.53
2:H:12:HIS:NE2	2:H:153:GLU:OE2	2.42	0.53
4:M:121:GLU:O	4:M:125:LEU:HD13	2.09	0.53
4:O:197:PRO:O	4:O:201:LYS:HG3	2.09	0.53
4:N:557:LYS:HG2	4:N:563:ASP:HB3	1.89	0.53
1:G:172:ASP:HA	1:G:176:SER:HB3	1.90	0.53
4:M:144:ARG:HG3	4:M:540:VAL:HG21	1.89	0.53
4:O:121:GLU:O	4:O:125:LEU:HD13	2.09	0.53
4:M:70:VAL:HG12	4:M:102:VAL:HA	1.89	0.53
1:D:245:ASP:OD1	1:D:245:ASP:N	2.39	0.52
4:P:198:GLN:O	4:P:201:LYS:HG2	2.09	0.52
4:P:199:LEU:HD21	4:P:517:PHE:HE2	1.74	0.52
2:K:79:LYS:HB3	2:K:91:GLN:HB3	1.91	0.52
1:G:381:ARG:NH2	3:I:57:GLU:OE2	2.40	0.52
1:J:73:PRO:HA	1:J:115:VAL:HG23	1.92	0.52
4:N:199:LEU:HD21	4:N:517:PHE:HE2	1.73	0.52
4:P:198:GLN:HG3	4:P:199:LEU:H	1.75	0.52
2:H:216:ASN:O	2:H:216:ASN:ND2	2.42	0.52
2:H:341:LYS:O	2:H:345:ASN:HB2	2.09	0.52
4:M:484:LEU:HD21	4:M:542:LEU:HD12	1.91	0.52
4:P:508:GLU:HA	4:P:511:GLN:HB2	1.89	0.52
4:P:252:GLU:HG2	4:P:256:ARG:HE	1.73	0.52
4:P:401:LYS:O	4:P:405:VAL:HG12	2.09	0.52
5:Q:47:U:O2'	5:Q:50:C:OP1	2.27	0.52
1:J:441:ALA:HB2	1:J:451:VAL:HG13	1.92	0.52
1:D:382:LEU:HD12	3:F:49:VAL:HG21	1.92	0.52
1:G:162:ALA:O	1:G:163:ARG:HG2	2.08	0.52
2:K:100:VAL:HB	2:K:122:ALA:HB3	1.90	0.52
4:N:77:ARG:NE	4:N:94:GLU:OE2	2.40	0.52
1:D:31:ARG:HH11	1:D:163:ARG:HD2	1.74	0.52
1:D:82:THR:HG22	1:D:106:VAL:HG11	1.92	0.52
1:G:437:LEU:HD12	1:G:453:LEU:HD11	1.91	0.52
2:H:281:VAL:HG13	3:I:61:ARG:HH21	1.75	0.52
2:K:94:GLN:O	2:K:121:ARG:NH2	2.43	0.52
4:O:341:THR:HG22	4:O:352:LEU:HB3	1.92	0.52
1:A:330:ARG:NH1	3:C:89:LEU:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:274:ILE:HG23	1:G:449:VAL:HG11	1.92	0.52
2:K:108:THR:HA	2:K:114:THR:HG23	1.91	0.52
1:J:198:ARG:HH12	1:J:203:ALA:HB2	1.73	0.51
4:O:79:ARG:HG3	4:O:80:PRO:HD2	1.91	0.51
4:P:441:ASN:O	4:P:443:ASP:N	2.43	0.51
3:I:77:GLN:HG3	3:I:83:VAL:HG11	1.91	0.51
1:J:331:CYS:HB3	1:J:343:ARG:HE	1.75	0.51
2:E:232:GLN:OE1	4:P:585:ARG:NH1	2.42	0.51
1:G:41:SER:O	1:G:120:LEU:HD22	2.11	0.51
1:G:325:VAL:HG23	3:I:90:VAL:HG21	1.92	0.51
1:J:204:TYR:OH	1:J:356:ARG:NH1	2.36	0.51
4:N:456:PRO:O	4:N:473:ARG:NH1	2.43	0.51
1:J:7:LEU:HA	1:J:10:ILE:HG22	1.92	0.51
4:P:111:PHE:HB2	4:P:119:VAL:HG21	1.92	0.51
4:P:220:ARG:HH22	4:P:228:ARG:HD3	1.76	0.51
1:A:403:PRO:HD3	1:A:425:TYR:CE1	2.46	0.51
1:G:441:ALA:HB2	1:G:451:VAL:HG23	1.92	0.51
4:M:170:ARG:HG2	4:M:171:PRO:HD2	1.92	0.51
4:M:514:LYS:HG3	4:M:515:PHE:CE2	2.46	0.51
3:C:8:VAL:HG21	3:C:28:THR:HG22	1.92	0.51
1:G:330:ARG:NH1	1:G:331:CYS:O	2.43	0.51
4:N:198:GLN:O	4:N:201:LYS:HG2	2.11	0.51
4:N:501:PHE:CD1	4:N:506:ILE:HD11	2.45	0.51
4:O:487:GLY:HA3	4:O:532:LEU:HA	1.92	0.51
5:T:23:A:H2'	5:T:24:G:C8	2.46	0.51
4:M:570:GLY:HA3	4:N:170:ARG:HH11	1.75	0.51
4:O:453:PHE:O	4:O:491:ILE:HG12	2.10	0.51
4:M:370:PRO:HA	4:M:373:LYS:HE2	1.92	0.51
4:P:182:PRO:HB2	4:P:580:LEU:HG	1.92	0.51
1:G:79:LEU:HD22	1:G:171:THR:HG21	1.92	0.51
2:H:170:VAL:HG21	2:H:223:ILE:HD13	1.93	0.51
4:P:369:SER:HB3	4:P:372:VAL:HG23	1.93	0.51
2:B:177:VAL:HG11	2:B:183:CYS:HB3	1.93	0.51
1:J:3:HIS:HB2	1:J:163:ARG:HG3	1.93	0.51
4:O:575:LYS:O	4:O:578:ARG:HG2	2.10	0.51
1:A:307:TYR:CD1	1:A:427:ILE:HD11	2.45	0.50
4:M:297:ASP:OD1	4:M:320:ARG:NH1	2.43	0.50
4:O:201:LYS:HG2	4:O:212:TYR:CE2	2.46	0.50
1:D:274:ILE:HG23	1:D:449:VAL:HG11	1.92	0.50
2:K:50:VAL:O	3:L:63:ARG:NH1	2.44	0.50
2:K:105:LEU:HD22	2:K:107:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:343:PHE:O	4:O:346:ILE:HG22	2.11	0.50
2:B:167:VAL:HG13	2:B:220:PHE:HB3	1.94	0.50
2:H:237:LEU:HD11	4:O:590:ALA:HB2	1.94	0.50
2:K:230:GLU:HG3	2:K:234:GLN:HE21	1.76	0.50
4:N:252:GLU:OE2	4:N:256:ARG:NH2	2.44	0.50
4:N:487:GLY:HA3	4:N:532:LEU:HA	1.94	0.50
5:T:52:G:H1	5:T:62:C:H42	1.58	0.50
2:E:316:ASP:OD1	2:E:316:ASP:N	2.39	0.50
1:J:354:LYS:HE2	3:L:17:LEU:HG	1.92	0.50
4:M:198:GLN:O	4:M:201:LYS:HG2	2.11	0.50
4:M:584:LEU:HD21	4:N:190:PHE:CZ	2.46	0.50
4:N:30:ASP:O	5:R:38:A:N6	2.43	0.50
4:N:70:VAL:HG12	4:N:102:VAL:HA	1.93	0.50
4:N:182:PRO:HB2	4:N:580:LEU:HG	1.92	0.50
4:N:574:GLY:O	4:N:578:ARG:HG3	2.11	0.50
1:D:2:LEU:HD13	1:D:24:LEU:HG	1.93	0.50
1:D:403:PRO:HB3	1:D:425:TYR:HE2	1.75	0.50
2:E:15:LEU:HB3	2:E:58:MET:HE1	1.94	0.50
4:M:500:VAL:HA	4:M:503:VAL:HG12	1.94	0.50
4:M:557:LYS:HB3	4:M:562:GLY:H	1.75	0.50
4:P:421:LYS:HE2	4:P:425:ARG:NH1	2.26	0.50
2:B:32:ALA:O	2:B:145:ASN:ND2	2.43	0.50
2:B:341:LYS:O	2:B:345:ASN:HB2	2.12	0.50
1:J:368:TYR:HB3	1:J:372:TYR:HD2	1.77	0.50
4:P:4:SER:HB3	4:P:20:THR:H	1.76	0.50
5:R:21:A:H2'	5:R:46:G:H1	1.76	0.50
4:M:514:LYS:HG3	4:M:515:PHE:CD2	2.46	0.50
4:O:117:SER:CB	4:O:119:VAL:H	2.24	0.50
4:P:302:LEU:HD21	4:P:375:ILE:HD12	1.93	0.50
1:A:143:TRP:CZ3	1:A:161:ALA:HB1	2.40	0.50
4:P:79:ARG:NE	4:P:94:GLU:HG3	2.27	0.50
2:E:347:VAL:HG13	2:E:351:LEU:HD12	1.92	0.49
4:O:11:ASN:OD1	4:O:12:GLU:N	2.38	0.49
1:G:147:ARG:HD3	1:G:147:ARG:N	2.27	0.49
1:J:278:VAL:HG22	1:J:451:VAL:HG12	1.94	0.49
2:K:360:LEU:H	2:K:360:LEU:HD22	1.77	0.49
4:O:411:ALA:O	4:O:414:ILE:HG13	2.13	0.49
4:P:29:ARG:HH11	4:P:29:ARG:HB2	1.77	0.49
1:A:427:ILE:HG13	1:A:431:LEU:HD13	1.95	0.49
2:H:360:LEU:HD13	2:H:360:LEU:H	1.78	0.49
4:M:589:LYS:HB3	4:N:578:ARG:HG2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:198:GLN:HG3	4:O:199:LEU:H	1.76	0.49
4:P:17:GLN:O	4:P:76:VAL:HG12	2.12	0.49
1:D:380:ARG:HG2	3:F:52:LEU:HD23	1.94	0.49
3:F:84:GLU:HB2	3:F:89:LEU:HD21	1.93	0.49
4:O:360:ARG:HH12	4:O:390:VAL:HG23	1.78	0.49
2:B:69:ARG:NH1	2:B:70:ILE:O	2.46	0.49
1:D:297:LEU:HB3	1:D:300:MET:HB2	1.95	0.49
1:D:307:TYR:CD1	1:D:427:ILE:HD11	2.48	0.49
1:J:26:ARG:HG3	1:J:27:THR:N	2.28	0.49
4:N:441:ASN:O	4:N:443:ASP:N	2.44	0.49
4:O:119:VAL:HG23	5:S:11:C:O2'	2.11	0.49
4:P:75:LYS:HB2	4:P:98:TYR:HE2	1.78	0.49
4:P:484:LEU:HD21	4:P:542:LEU:HD12	1.94	0.49
2:B:297:GLU:HG2	2:B:324:ARG:HH12	1.78	0.49
1:G:75:ALA:H	1:G:165:LEU:HD21	1.78	0.49
1:J:104:THR:HG23	1:J:199:TRP:HE3	1.78	0.49
2:K:247:GLU:OE2	2:K:249:ARG:NH2	2.45	0.49
4:M:307:PHE:HD1	4:M:307:PHE:O	1.96	0.49
4:N:325:ARG:HH21	4:N:327:PRO:HB3	1.78	0.49
4:O:501:PHE:CD1	4:O:506:ILE:HD11	2.47	0.49
1:A:368:TYR:HB3	1:A:372:TYR:HD2	1.78	0.49
2:B:281:VAL:HA	3:C:60:GLN:HB3	1.95	0.49
1:D:358:MET:HG2	3:F:31:LEU:HD21	1.95	0.49
2:E:383:THR:HB	2:E:388:LEU:HD13	1.95	0.49
1:A:48:ASP:N	1:A:48:ASP:OD1	2.46	0.49
4:M:182:PRO:HB2	4:M:580:LEU:HG	1.93	0.49
4:N:325:ARG:HD2	4:N:389:ALA:HA	1.94	0.49
4:P:501:PHE:CD1	4:P:506:ILE:HD11	2.47	0.49
1:G:69:LEU:HD23	1:G:69:LEU:H	1.78	0.49
1:G:143:TRP:NE1	1:G:483:GLY:O	2.46	0.49
1:D:130:SER:HB3	1:D:407:TRP:HH2	1.78	0.48
1:G:262:PRO:HB3	1:G:297:LEU:HD13	1.95	0.48
4:M:373:LYS:H	4:M:373:LYS:HD2	1.77	0.48
4:N:11:ASN:OD1	4:N:12:GLU:N	2.41	0.48
2:E:167:VAL:HG13	2:E:220:PHE:HB3	1.94	0.48
2:B:4:GLU:HB2	2:B:161:ARG:HH21	1.79	0.48
3:F:13:HIS:O	3:F:16:ARG:NH1	2.46	0.48
2:K:329:TYR:OH	2:K:372:LEU:HD13	2.14	0.48
4:M:198:GLN:HG3	4:M:199:LEU:H	1.77	0.48
4:P:307:PHE:O	4:P:307:PHE:HD1	1.95	0.48
2:K:271:ARG:HD2	3:L:14:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:248:ILE:HD12	4:M:272:HIS:NE2	2.28	0.48
4:P:248:ILE:HG23	4:P:431:TRP:CE2	2.49	0.48
1:A:331:CYS:SG	1:A:343:ARG:NE	2.64	0.48
1:D:143:TRP:CD1	1:D:448:PRO:HG3	2.48	0.48
2:K:333:VAL:HG13	2:K:376:ILE:HG21	1.95	0.48
4:N:198:GLN:HG3	4:N:199:LEU:H	1.79	0.48
4:N:251:THR:OG1	4:N:532:LEU:HD21	2.13	0.48
1:D:163:ARG:HH21	1:D:483:GLY:HA2	1.77	0.48
1:D:368:TYR:HB3	1:D:372:TYR:HD2	1.78	0.48
4:M:585:ARG:HD3	4:N:583:ARG:HB3	1.94	0.48
2:B:117:ILE:HG21	2:B:169:TYR:CD1	2.49	0.48
4:M:252:GLU:HG2	4:M:256:ARG:HE	1.79	0.48
4:M:355:ILE:HD11	4:M:367:LEU:HD23	1.95	0.48
4:N:321:VAL:HG13	4:N:399:ALA:HB2	1.94	0.48
1:A:441:ALA:HB2	1:A:451:VAL:HG23	1.94	0.48
1:D:28:LEU:O	1:D:32:ILE:HG12	2.13	0.48
1:G:236:SER:HB3	3:I:61:ARG:HD2	1.95	0.48
1:G:320:SER:HA	1:G:345:ARG:HH21	1.77	0.48
1:G:437:LEU:HD11	1:G:439:MET:HG3	1.95	0.48
1:J:304:ILE:HG13	1:J:305:PRO:CD	2.43	0.48
4:N:280:ARG:NH2	4:N:281:ARG:HE	2.12	0.48
4:N:484:LEU:HD21	4:N:542:LEU:HD12	1.95	0.48
4:O:129:PHE:CD1	4:O:130:ILE:HG23	2.49	0.48
1:A:74:ILE:HG12	1:A:114:ALA:HB1	1.95	0.48
3:F:71:ASP:HB2	3:F:76:TYR:CE1	2.49	0.48
4:O:70:VAL:HG12	4:O:102:VAL:HA	1.95	0.48
4:O:252:GLU:OE2	4:O:256:ARG:NH2	2.47	0.48
1:A:304:ILE:HD11	1:A:424:ILE:HG23	1.95	0.48
4:O:77:ARG:NH2	5:S:34:G:H1	2.12	0.48
4:O:484:LEU:HD21	4:O:542:LEU:HD12	1.96	0.48
2:B:249:ARG:HD2	2:B:258:THR:HG22	1.96	0.47
2:K:179:TYR:CZ	2:K:299:PRO:HB3	2.49	0.47
4:M:153:ARG:HH22	4:N:152:ARG:HB3	1.78	0.47
4:N:515:PHE:O	4:N:519:LEU:HG	2.13	0.47
4:O:224:LEU:HD21	4:O:230:PRO:HD3	1.96	0.47
2:E:347:VAL:O	2:E:351:LEU:HB2	2.14	0.47
4:M:112:PRO:HD2	4:M:119:VAL:HG21	1.96	0.47
4:P:557:LYS:HG2	4:P:563:ASP:HB3	1.96	0.47
2:E:42:LEU:HD12	2:E:144:LEU:HD22	1.95	0.47
1:G:187:THR:HG22	1:G:439:MET:HG2	1.94	0.47
2:H:316:ASP:HA	2:H:319:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:5:ARG:HB2	3:L:24:LEU:HD21	1.96	0.47
4:O:401:LYS:O	4:O:405:VAL:HG12	2.13	0.47
1:J:7:LEU:HD22	1:J:72:ALA:HB1	1.97	0.47
4:N:181:VAL:HB	4:N:191:PHE:HB2	1.96	0.47
4:N:229:GLN:HE22	4:N:557:LYS:N	2.12	0.47
4:O:114:ASP:HA	4:O:115:GLU:HA	1.57	0.47
4:P:3:ARG:CD	4:P:22:CYS:H	2.26	0.47
1:A:120:LEU:HD13	1:A:156:SER:HA	1.97	0.47
1:D:179:GLN:HB3	1:D:180:PRO:HD3	1.96	0.47
1:G:172:ASP:HB2	1:G:177:ILE:HD12	1.97	0.47
2:H:339:ASP:HB3	2:H:342:LEU:HG	1.97	0.47
4:M:515:PHE:O	4:M:519:LEU:HG	2.14	0.47
4:N:508:GLU:HA	4:N:511:GLN:HB2	1.94	0.47
5:S:23:A:H2'	5:S:24:G:C8	2.50	0.47
1:D:346:ALA:HB2	3:F:18:GLY:HA3	1.96	0.47
4:N:129:PHE:CD1	4:N:130:ILE:HG23	2.50	0.47
4:N:225:ARG:HB2	4:N:228:ARG:HD2	1.97	0.47
4:N:357:VAL:HG22	4:N:393:ASP:O	2.14	0.47
4:O:42:ARG:NH2	4:P:161:LEU:HD13	2.29	0.47
4:P:340:TYR:CZ	4:P:416:VAL:HG22	2.49	0.47
5:T:67:C:H2'	5:T:68:G:C8	2.50	0.47
2:B:117:ILE:HD11	2:B:160:ILE:HA	1.95	0.47
1:D:427:ILE:HG13	1:D:431:LEU:HD13	1.97	0.47
2:E:383:THR:HG21	2:E:388:LEU:HD22	1.97	0.47
1:G:32:ILE:HD13	1:G:164:LEU:HD23	1.97	0.47
1:G:427:ILE:HG13	1:G:431:LEU:HD13	1.97	0.47
2:H:105:LEU:HB2	2:H:119:ILE:HD11	1.97	0.47
1:J:178:ARG:NE	1:J:190:LYS:HD3	2.30	0.47
4:M:401:LYS:O	4:M:405:VAL:HG12	2.14	0.47
4:N:344:VAL:HG21	4:N:352:LEU:HB2	1.97	0.47
2:E:230:GLU:HG3	2:E:234:GLN:HE21	1.79	0.47
2:K:368:SER:H	2:K:371:GLN:HE21	1.62	0.47
4:M:337:ILE:O	4:M:341:THR:HG23	2.15	0.47
4:O:246:ASP:O	4:O:250:ILE:HD13	2.15	0.47
4:O:557:LYS:HG2	4:O:563:ASP:HB3	1.97	0.47
4:P:321:VAL:HG13	4:P:399:ALA:HB2	1.95	0.47
1:J:77:LYS:HG2	1:J:79:LEU:H	1.80	0.47
2:E:93:SER:OG	2:E:94:GLN:N	2.46	0.47
1:G:26:ARG:HG3	1:G:27:THR:N	2.30	0.47
2:H:254:ASN:OD1	2:H:255:LYS:N	2.48	0.47
3:L:82:ALA:HB1	3:L:89:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:VAL:HG21	1:A:400:PRO:HB3	1.97	0.46
2:B:374:GLY:O	2:B:378:ARG:HG2	2.14	0.46
1:D:345:ARG:NH1	3:F:15:ALA:O	2.48	0.46
2:H:177:VAL:HG13	2:H:182:ILE:HB	1.96	0.46
3:L:77:GLN:HG2	3:L:83:VAL:HG21	1.96	0.46
4:M:400:ASP:OD1	4:M:401:LYS:N	2.39	0.46
4:M:411:ALA:HA	4:M:414:ILE:HG22	1.96	0.46
4:M:506:ILE:HD12	4:M:506:ILE:O	2.15	0.46
4:M:510:GLU:O	4:M:514:LYS:HG2	2.15	0.46
4:N:201:LYS:HE3	4:N:238:GLU:OE1	2.15	0.46
4:N:273:MET:HE1	4:N:282:TYR:CE2	2.50	0.46
4:N:548:SER:OG	4:N:550:ARG:HG2	2.14	0.46
4:O:131:ASP:OD1	4:O:134:ARG:NH1	2.48	0.46
5:T:67:C:H2'	5:T:68:G:H8	1.81	0.46
1:G:254:LEU:HD21	1:G:466:VAL:HG23	1.97	0.46
4:M:113:LEU:HD21	4:M:133:ARG:CB	2.45	0.46
4:M:453:PHE:O	4:M:491:ILE:HG12	2.14	0.46
4:O:353:ALA:HB1	4:O:371:ILE:HD13	1.96	0.46
5:Q:21:A:H2'	5:Q:46:G:H22	1.80	0.46
5:S:21:A:OP1	5:S:48:C:N4	2.48	0.46
1:A:127:MET:SD	1:A:353:VAL:HA	2.55	0.46
1:J:152:SER:H	1:J:176:SER:HB3	1.80	0.46
1:J:241:GLN:HA	1:J:242:PRO:HD3	1.79	0.46
4:O:506:ILE:O	4:O:506:ILE:HD12	2.15	0.46
4:P:251:THR:OG1	4:P:532:LEU:HD21	2.15	0.46
1:A:172:ASP:HA	1:A:176:SER:HB2	1.97	0.46
1:D:189:ILE:HD11	1:D:460:GLU:HB3	1.98	0.46
2:K:3:TRP:CZ2	2:K:235:ILE:HG23	2.50	0.46
1:A:202:ILE:HG12	2:B:45:PRO:HB2	1.98	0.46
2:B:170:VAL:HG21	2:B:223:ILE:HD13	1.97	0.46
2:E:394:GLU:O	2:E:398:ASN:ND2	2.49	0.46
2:K:78:ARG:HD2	2:K:273:PHE:CZ	2.51	0.46
2:K:347:VAL:HA	2:K:351:LEU:HD21	1.97	0.46
4:N:246:ASP:O	4:N:250:ILE:HD13	2.16	0.46
4:P:246:ASP:O	4:P:250:ILE:HD13	2.16	0.46
4:P:451:HIS:CG	4:P:452:PRO:HD2	2.51	0.46
1:G:25:THR:HA	1:G:28:LEU:HG	1.97	0.46
1:G:141:ASN:ND2	1:G:143:TRP:HB2	2.29	0.46
1:G:307:TYR:CD1	1:G:427:ILE:HD11	2.50	0.46
2:H:93:SER:OG	2:H:94:GLN:N	2.48	0.46
2:H:279:LEU:HD22	3:I:58:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:29:ARG:HD2	5:Q:35:U:O2'	2.15	0.46
4:M:270:PHE:HE2	4:M:477:MET:HE3	1.81	0.46
4:M:390:VAL:HG12	4:M:391:ASP:H	1.80	0.46
4:O:299:ALA:HB2	4:O:321:VAL:HG13	1.98	0.46
4:P:510:GLU:O	4:P:514:LYS:HG2	2.15	0.46
2:H:383:THR:HG21	2:H:388:LEU:HD22	1.97	0.46
4:M:238:GLU:OE1	4:M:531:GLY:HA3	2.16	0.46
4:O:500:VAL:HA	4:O:503:VAL:HG12	1.98	0.46
4:P:341:THR:HG22	4:P:352:LEU:HB3	1.97	0.46
3:L:71:ASP:OD2	3:L:72:HIS:N	2.49	0.46
4:P:375:ILE:HG23	4:P:380:LEU:HD11	1.97	0.46
1:D:130:SER:HB3	1:D:407:TRP:CH2	2.49	0.46
2:E:179:TYR:CZ	2:E:299:PRO:HB3	2.50	0.46
1:G:120:LEU:HD11	1:G:156:SER:N	2.30	0.46
1:J:349:PHE:CG	1:J:350:GLY:N	2.84	0.46
1:J:440:PRO:HA	1:J:450:GLY:HA2	1.98	0.46
1:J:460:GLU:O	1:J:463:LEU:HG	2.15	0.46
2:K:170:VAL:HG21	2:K:223:ILE:HD13	1.97	0.46
4:M:246:ASP:O	4:M:250:ILE:HD13	2.16	0.46
4:N:248:ILE:HG23	4:N:431:TRP:CE2	2.51	0.46
4:P:376:PRO:O	4:P:380:LEU:HD13	2.16	0.46
1:A:361:THR:HG23	2:B:271:ARG:HH11	1.81	0.46
2:B:230:GLU:HG3	2:B:234:GLN:HE21	1.80	0.46
1:D:71:GLY:N	1:D:113:GLY:O	2.48	0.46
1:D:321:ARG:HB3	2:E:88:LYS:HA	1.98	0.46
4:M:353:ALA:HB3	4:M:397:PHE:HB2	1.98	0.46
4:N:307:PHE:HD1	4:N:308:LYS:N	2.13	0.46
4:N:318:LYS:HD2	4:N:318:LYS:HA	1.60	0.46
4:N:362:LYS:HD2	4:N:362:LYS:HA	1.46	0.46
4:N:369:SER:HB3	4:N:372:VAL:CG2	2.45	0.46
4:P:320:ARG:NH2	4:P:406:CYS:SG	2.89	0.46
1:A:82:THR:HG22	1:A:106:VAL:HG11	1.98	0.45
1:A:271:ASP:OD1	1:A:274:ILE:HG12	2.15	0.45
1:J:122:MET:SD	1:J:153:SER:HA	2.56	0.45
1:J:163:ARG:HG2	1:J:163:ARG:O	2.16	0.45
2:B:347:VAL:HA	2:B:351:LEU:HD21	1.96	0.45
1:D:143:TRP:CZ2	1:D:479:ARG:HB3	2.51	0.45
1:G:69:LEU:HB3	1:G:223:LEU:HD11	1.97	0.45
4:N:319:GLY:HA2	4:N:402:ALA:N	2.31	0.45
4:P:109:PRO:HA	4:P:110:PRO:HD2	1.81	0.45
2:E:12:HIS:NE2	2:E:153:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:265:TYR:CD2	1:J:399:GLY:HA3	2.50	0.45
1:J:330:ARG:NH1	1:J:331:CYS:O	2.50	0.45
2:K:85:ASP:OD1	2:K:86:LEU:N	2.50	0.45
4:M:566:THR:O	4:N:170:ARG:HD3	2.15	0.45
4:N:451:HIS:CG	4:N:452:PRO:HD2	2.51	0.45
4:O:153:ARG:HA	4:O:153:ARG:HD3	1.59	0.45
4:O:441:ASN:O	4:O:443:ASP:N	2.48	0.45
5:S:20:U:H2'	5:S:21:A:H5"	1.98	0.45
3:C:5:ARG:HH11	3:C:24:LEU:HD13	1.82	0.45
3:F:80:ALA:HA	3:F:81:PRO:HD3	1.86	0.45
1:G:216:ARG:NH2	1:G:477:HIS:O	2.50	0.45
2:H:347:VAL:HA	2:H:351:LEU:HD21	1.99	0.45
4:M:35:ILE:HG13	4:M:58:PHE:CZ	2.52	0.45
4:M:341:THR:HG22	4:M:352:LEU:HB3	1.97	0.45
4:M:343:PHE:O	4:M:346:ILE:HG12	2.16	0.45
3:F:6:SER:O	3:F:10:LYS:HG2	2.17	0.45
4:N:229:GLN:NE2	4:N:557:LYS:H	2.14	0.45
2:B:252:ASP:HA	2:B:253:PRO:HD3	1.86	0.45
1:J:259:ILE:HG23	1:J:398:LEU:HD13	1.99	0.45
4:O:206:VAL:HG13	4:P:133:ARG:HH21	1.81	0.45
4:P:129:PHE:CD1	4:P:130:ILE:HG23	2.52	0.45
1:A:160:VAL:HB	1:A:186:LEU:HD11	1.99	0.45
2:B:344:ALA:O	2:B:348:MET:HG3	2.17	0.45
1:J:42:PHE:HA	1:J:120:LEU:HA	1.98	0.45
1:J:189:ILE:HB	1:J:437:LEU:HD13	1.99	0.45
2:K:109:LEU:HD21	2:K:165:GLU:HA	1.99	0.45
2:K:177:VAL:HG13	2:K:182:ILE:HB	1.99	0.45
4:O:371:ILE:HG23	4:O:374:PHE:CE2	2.52	0.45
4:O:466:ASN:OD1	4:O:466:ASN:N	2.48	0.45
4:P:514:LYS:HG3	4:P:515:PHE:CE2	2.51	0.45
1:A:354:LYS:HE2	1:A:354:LYS:HB3	1.72	0.45
2:B:355:LEU:O	2:B:359:GLY:HA2	2.16	0.45
1:G:412:LYS:HD2	1:G:418:SER:HB3	1.98	0.45
1:J:179:GLN:HB3	1:J:180:PRO:HD3	1.98	0.45
4:M:74:GLY:HA2	4:M:98:TYR:HD2	1.82	0.45
4:N:35:ILE:HG13	4:N:58:PHE:CZ	2.52	0.45
4:O:367:LEU:O	4:O:372:VAL:HG21	2.17	0.45
4:O:589:LYS:CB	4:P:578:ARG:HB2	2.47	0.45
1:A:179:GLN:HB3	1:A:180:PRO:HD3	1.99	0.45
1:A:270:LEU:HD11	1:A:274:ILE:HB	1.97	0.45
1:G:278:VAL:HG22	1:G:451:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:351:SER:O	1:G:355:ASN:ND2	2.31	0.45
2:K:341:LYS:O	2:K:345:ASN:HB2	2.17	0.45
4:N:29:ARG:HD2	5:R:35:U:O2'	2.16	0.45
4:N:313:PRO:HA	4:N:316:ASP:HB3	1.99	0.45
4:N:320:ARG:HG3	4:N:405:VAL:HG11	1.99	0.45
4:P:70:VAL:HG12	4:P:102:VAL:HA	1.97	0.45
2:B:332:LYS:HD3	2:B:369:ALA:HB3	1.99	0.44
3:C:6:SER:O	3:C:10:LYS:HG2	2.17	0.44
2:K:63:GLY:HA3	2:K:70:ILE:HD11	1.99	0.44
4:N:40:ARG:HB2	4:N:45:LEU:HD23	1.99	0.44
4:O:190:PHE:CZ	4:P:584:LEU:HD21	2.52	0.44
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.82	0.44
1:A:345:ARG:NH1	3:C:15:ALA:O	2.50	0.44
2:B:104:HIS:CE1	2:B:116:ARG:HH21	2.35	0.44
2:B:231:ILE:HG21	4:N:589:LYS:NZ	2.32	0.44
1:D:34:GLN:OE1	1:D:35:LEU:HD12	2.17	0.44
2:H:179:TYR:CZ	2:H:299:PRO:HB3	2.52	0.44
2:K:94:GLN:HB2	2:K:123:HIS:HB2	1.98	0.44
3:L:12:ALA:HA	3:L:17:LEU:HD13	1.99	0.44
4:N:238:GLU:OE1	4:N:531:GLY:HA3	2.17	0.44
1:A:447:LEU:HA	1:A:448:PRO:HD3	1.78	0.44
1:D:339:ASP:O	1:D:343:ARG:HB2	2.17	0.44
1:G:179:GLN:HB3	1:G:180:PRO:HD3	1.99	0.44
2:K:350:GLU:HB3	2:K:393:PHE:CE2	2.53	0.44
2:K:378:ARG:HA	2:K:382:ASN:OD1	2.18	0.44
4:M:47:GLN:NE2	4:M:94:GLU:OE1	2.50	0.44
4:M:75:LYS:HB2	4:M:98:TYR:HE2	1.83	0.44
4:M:501:PHE:CD1	4:M:506:ILE:HD11	2.53	0.44
4:M:504:LEU:HD12	4:M:506:ILE:HG12	1.99	0.44
4:P:340:TYR:HE1	4:P:415:LYS:HZ2	1.66	0.44
5:S:67:C:H2'	5:S:68:G:H8	1.81	0.44
2:B:50:VAL:O	3:C:63:ARG:NH1	2.51	0.44
2:B:119:ILE:HA	2:B:156:SER:HA	1.98	0.44
1:D:77:LYS:HD3	1:D:171:THR:HG23	1.99	0.44
2:H:32:ALA:HA	2:H:33:PRO:HD3	1.82	0.44
1:J:368:TYR:HB3	1:J:372:TYR:CD2	2.53	0.44
4:P:3:ARG:HD3	4:P:22:CYS:H	1.81	0.44
5:R:23:A:H2'	5:R:24:G:C8	2.53	0.44
1:D:74:ILE:HG12	1:D:114:ALA:HB1	1.99	0.44
1:G:383:ILE:HA	1:G:386:ASP:OD2	2.17	0.44
4:O:154:TYR:CE1	4:O:254:MET:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:434:ASP:HB3	4:P:471:LEU:HD13	1.99	0.44
1:A:359:VAL:HG11	3:C:34:ILE:HG21	2.00	0.44
2:B:360:LEU:HD12	2:B:366:PRO:HG3	1.99	0.44
2:H:15:LEU:HD21	2:H:152:LEU:HB2	2.00	0.44
2:K:115:LYS:HD3	2:K:115:LYS:HA	1.80	0.44
4:M:170:ARG:HB2	4:N:568:ALA:HB2	1.99	0.44
4:N:118:ASP:HB3	5:R:12:U:H4'	1.98	0.44
4:O:29:ARG:HD2	5:S:35:U:O2'	2.17	0.44
2:B:130:LYS:HD2	2:B:146:ARG:HH11	1.83	0.44
4:N:150:SER:N	4:N:153:ARG:HH21	2.16	0.44
4:O:291:ILE:HD13	4:O:417:GLY:HA3	2.00	0.44
4:O:515:PHE:O	4:O:519:LEU:HG	2.18	0.44
1:D:323:ASP:OD1	1:D:325:VAL:HG12	2.18	0.44
2:E:117:ILE:HG21	2:E:169:TYR:CD1	2.52	0.44
2:H:229:HIS:CB	4:O:588:PRO:HG3	2.48	0.44
2:K:93:SER:OG	2:K:94:GLN:N	2.49	0.44
4:M:313:PRO:HA	4:M:316:ASP:CG	2.38	0.44
4:N:118:ASP:O	5:R:12:U:H5'	2.17	0.44
5:S:51:U:H2'	5:S:52:G:C8	2.53	0.44
1:G:368:TYR:HB3	1:G:372:TYR:HD2	1.83	0.44
1:J:124:GLU:HG2	1:J:349:PHE:CD1	2.52	0.44
4:M:167:ILE:O	4:M:194:PRO:HD3	2.18	0.44
4:M:581:HIS:HA	4:N:585:ARG:HE	1.83	0.44
4:P:238:GLU:OE1	4:P:531:GLY:HA3	2.18	0.44
4:P:515:PHE:O	4:P:519:LEU:HG	2.18	0.44
2:B:160:ILE:HD11	2:B:165:GLU:C	2.39	0.43
1:D:79:LEU:HD23	1:D:79:LEU:HA	1.83	0.43
1:D:304:ILE:H	1:D:304:ILE:HD12	1.83	0.43
2:E:88:LYS:HD2	2:E:90:TYR:CE1	2.53	0.43
2:E:243:LYS:HB3	2:E:243:LYS:HE2	1.75	0.43
2:E:281:VAL:HA	3:F:60:GLN:HB3	2.00	0.43
1:G:162:ALA:O	1:G:164:LEU:HD12	2.18	0.43
1:G:293:LYS:HD3	1:G:294:ASP:H	1.83	0.43
2:K:344:ALA:O	2:K:348:MET:HG2	2.18	0.43
4:N:295:LEU:HD21	4:N:409:LEU:HB3	1.99	0.43
4:N:307:PHE:HD1	4:N:308:LYS:H	1.66	0.43
5:Q:48:C:H2'	5:Q:59:G:H4'	2.00	0.43
1:D:327:TYR:CZ	2:E:45:PRO:HD3	2.52	0.43
2:E:341:LYS:O	2:E:345:ASN:HB2	2.17	0.43
1:J:142:PRO:HB2	1:J:143:TRP:CE3	2.53	0.43
4:M:251:THR:OG1	4:M:532:LEU:HD21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:108:THR:HA	4:N:109:PRO:HD2	1.86	0.43
4:N:111:PHE:HA	4:N:112:PRO:HD3	1.67	0.43
4:O:589:LYS:HB3	4:P:578:ARG:HB2	2.00	0.43
4:P:120:GLY:O	4:P:123:THR:OG1	2.34	0.43
5:S:67:C:H2'	5:S:68:G:C8	2.53	0.43
2:E:363:GLU:OE2	2:E:363:GLU:N	2.51	0.43
1:J:72:ALA:HA	1:J:73:PRO:HD3	1.83	0.43
4:M:303:LYS:H	4:M:303:LYS:HG2	1.62	0.43
4:M:375:ILE:HA	4:M:376:PRO:HD2	1.82	0.43
4:M:541:MET:HA	4:M:552:VAL:HG11	2.00	0.43
4:O:300:ASP:OD1	4:O:301:GLN:HG3	2.18	0.43
1:A:144:SER:OG	1:A:146:ASP:OD1	2.36	0.43
3:C:54:HIS:HA	3:C:55:PRO:HD3	1.90	0.43
1:G:163:ARG:HD2	1:G:480:THR:HB	1.99	0.43
1:J:82:THR:OG1	1:J:85:VAL:HB	2.19	0.43
2:K:20:LYS:O	3:L:63:ARG:NH2	2.41	0.43
4:N:54:ARG:HD2	4:N:54:ARG:HA	1.70	0.43
4:N:154:TYR:CE1	4:N:254:MET:HB2	2.53	0.43
4:O:445:SER:OG	4:O:446:LEU:N	2.52	0.43
1:A:141:ASN:HA	1:A:142:PRO:HD3	1.92	0.43
1:G:327:TYR:CZ	2:H:45:PRO:HD3	2.54	0.43
2:H:83:TYR:CG	2:H:84:PRO:HD2	2.54	0.43
2:B:98:PRO:HB3	2:B:121:ARG:HH21	1.82	0.43
2:E:254:ASN:OD1	2:E:255:LYS:N	2.52	0.43
3:F:54:HIS:HA	3:F:55:PRO:HD3	1.88	0.43
2:K:59:ALA:HB1	2:K:99:ILE:HG21	2.00	0.43
2:K:299:PRO:HA	2:K:302:LYS:HG2	1.99	0.43
2:K:316:ASP:HA	2:K:319:VAL:HG22	2.00	0.43
4:O:589:LYS:HG3	4:O:590:ALA:N	2.29	0.43
1:A:313:ALA:O	1:A:316:SER:OG	2.20	0.43
1:D:185:ASN:HB2	1:D:448:PRO:HB3	2.01	0.43
2:E:99:ILE:HG22	2:E:100:VAL:HG12	2.00	0.43
2:E:346:TRP:O	2:E:350:GLU:HB2	2.19	0.43
2:H:123:HIS:NE2	2:H:153:GLU:OE1	2.51	0.43
1:J:121:ASN:OD1	1:J:121:ASN:N	2.51	0.43
4:M:275:PHE:CD2	4:M:436:PRO:HD3	2.53	0.43
4:M:439:GLU:HB2	4:M:449:LEU:HD21	2.01	0.43
4:P:229:GLN:HE22	4:P:557:LYS:N	2.16	0.43
2:B:204:GLY:HA3	2:K:204:GLY:HA3	1.99	0.43
1:G:241:GLN:HA	1:G:242:PRO:HD3	1.83	0.43
1:J:259:ILE:HD13	1:J:285:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:338:GLU:HG2	1:J:342:LYS:HD2	2.01	0.43
1:J:455:ALA:HB1	1:J:459:GLN:OE1	2.18	0.43
4:O:42:ARG:NH1	4:P:159:GLY:O	2.44	0.43
4:O:116:TYR:CE2	4:O:118:ASP:HB2	2.53	0.43
4:O:360:ARG:NH1	4:O:390:VAL:HG23	2.33	0.43
4:P:273:MET:HE1	4:P:282:TYR:CD2	2.53	0.43
5:R:67:C:H2'	5:R:68:G:C8	2.54	0.43
1:G:69:LEU:HD12	1:G:72:ALA:HB3	2.00	0.43
1:G:354:LYS:O	1:G:358:MET:HG2	2.19	0.43
2:H:179:TYR:CE1	2:H:299:PRO:HB3	2.54	0.43
4:O:56:GLU:H	4:O:56:GLU:HG3	1.54	0.43
4:O:270:PHE:HE2	4:O:477:MET:HE3	1.84	0.43
1:G:36:ASP:HB3	1:G:37:PRO:HD3	2.01	0.43
2:H:64:LEU:HD11	2:H:288:LEU:HA	2.01	0.43
2:H:368:SER:HB3	2:H:370:GLU:OE2	2.19	0.43
2:K:233:ARG:HG3	4:M:588:PRO:O	2.18	0.43
4:M:108:THR:HA	4:M:109:PRO:HD2	1.87	0.43
4:O:205:MET:SD	4:O:240:SER:OG	2.72	0.43
4:O:325:ARG:NH1	4:O:393:ASP:OD2	2.52	0.43
2:B:93:SER:OG	2:B:94:GLN:N	2.49	0.42
1:G:179:GLN:NE2	1:G:422:GLU:OE2	2.39	0.42
4:M:129:PHE:CD1	4:M:130:ILE:HG23	2.54	0.42
4:O:248:ILE:HD12	4:O:272:HIS:NE2	2.34	0.42
1:A:368:TYR:HB3	1:A:372:TYR:CD2	2.54	0.42
4:M:451:HIS:CG	4:M:452:PRO:HD2	2.53	0.42
1:A:241:GLN:HA	1:A:242:PRO:HD3	1.72	0.42
1:D:163:ARG:NH2	1:D:483:GLY:HA2	2.34	0.42
1:G:132:GLN:HA	1:G:138:ALA:HB2	2.00	0.42
1:G:336:ASN:OD1	1:G:337:LEU:N	2.49	0.42
2:K:83:TYR:CG	2:K:84:PRO:HD2	2.54	0.42
2:K:312:LEU:HG	2:K:316:ASP:OD1	2.19	0.42
4:M:441:ASN:O	4:M:443:ASP:N	2.49	0.42
4:N:3:ARG:CD	4:N:22:CYS:H	2.28	0.42
2:E:316:ASP:HA	2:E:319:VAL:HG12	2.02	0.42
1:G:78:ASP:OD2	1:G:119:LYS:HE3	2.19	0.42
1:G:252:LYS:HB3	1:G:465:ASN:ND2	2.35	0.42
2:H:20:LYS:NZ	2:H:147:ALA:O	2.48	0.42
2:K:15:LEU:HB3	2:K:58:MET:HE1	2.01	0.42
4:M:340:TYR:CZ	4:M:416:VAL:HG12	2.54	0.42
4:O:29:ARG:HB2	4:O:36:PHE:HB2	2.01	0.42
4:P:492:HIS:ND1	4:P:528:PRO:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:52:G:H1	5:R:62:C:H42	1.67	0.42
2:E:29:PHE:HA	2:E:30:GLY:HA3	1.80	0.42
2:E:119:ILE:HA	2:E:156:SER:HA	2.02	0.42
2:H:336:ILE:O	2:H:337:CYS:HB2	2.20	0.42
1:J:447:LEU:HA	1:J:448:PRO:HD3	1.93	0.42
2:K:384:ILE:HG22	2:K:385:SER:H	1.84	0.42
4:M:57:THR:HG21	4:M:98:TYR:O	2.19	0.42
4:O:369:SER:HB3	4:O:372:VAL:CG2	2.50	0.42
4:O:504:LEU:HD13	4:O:504:LEU:O	2.20	0.42
5:T:47:U:HO2'	5:T:48:C:P	2.42	0.42
1:A:104:THR:HG22	1:A:199:TRP:O	2.20	0.42
1:D:159:ALA:O	1:D:164:LEU:HB2	2.20	0.42
3:I:80:ALA:HA	3:I:81:PRO:HD3	1.89	0.42
1:J:178:ARG:HG3	1:J:190:LYS:NZ	2.34	0.42
2:K:390:LYS:HE3	5:Q:18:G:C6	2.54	0.42
4:M:115:GLU:H	4:M:115:GLU:HG3	1.48	0.42
4:P:277:GLU:O	4:P:281:ARG:HG2	2.20	0.42
2:B:70:ILE:HG23	2:B:99:ILE:O	2.19	0.42
1:D:31:ARG:NH1	1:D:163:ARG:HD2	2.35	0.42
1:D:202:ILE:HG12	2:E:45:PRO:HB2	2.02	0.42
2:E:85:ASP:OD1	2:E:86:LEU:N	2.53	0.42
1:G:189:ILE:HG13	1:G:464:LEU:HD21	2.02	0.42
2:K:58:MET:HE2	2:K:182:ILE:HG23	2.02	0.42
2:K:215:LYS:HB3	2:K:215:LYS:HE2	1.91	0.42
2:B:83:TYR:CG	2:B:84:PRO:HD2	2.55	0.42
2:E:183:CYS:SG	2:E:184:ASP:N	2.93	0.42
1:G:304:ILE:HD11	1:G:424:ILE:HG23	2.00	0.42
2:H:215:LYS:HE2	2:H:215:LYS:HB2	1.91	0.42
2:H:454:UNK:O	2:H:458:UNK:N	2.53	0.42
1:J:351:SER:O	1:J:355:ASN:ND2	2.33	0.42
2:K:298:LEU:O	2:K:302:LYS:HB3	2.20	0.42
4:P:40:ARG:HB2	4:P:45:LEU:HD23	2.02	0.42
2:B:208:PHE:HE1	5:T:33:U:OP2	2.03	0.42
1:G:131:ASN:O	1:G:131:ASN:ND2	2.51	0.42
4:M:207:ALA:HB1	4:N:132:LEU:HB2	2.01	0.42
4:N:337:ILE:O	4:N:341:THR:HG23	2.20	0.42
4:O:367:LEU:HD23	4:O:367:LEU:HA	1.88	0.42
4:P:319:GLY:HA2	4:P:402:ALA:N	2.34	0.42
3:C:80:ALA:HA	3:C:81:PRO:HD3	1.90	0.42
1:D:338:GLU:OE2	1:D:342:LYS:NZ	2.43	0.42
2:E:68:ALA:HB1	2:E:101:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:130:LYS:NZ	5:T:74:C:OP2	2.36	0.42
2:E:139:MET:HA	3:F:91:PRO:HA	2.01	0.42
1:G:279:LEU:O	1:G:282:VAL:HG22	2.19	0.42
1:J:190:LYS:N	1:J:190:LYS:HE2	2.35	0.42
4:M:383:ILE:O	4:M:387:VAL:HG13	2.19	0.42
2:B:345:ASN:HD21	5:R:54:U:H4'	1.83	0.41
1:G:399:GLY:O	1:G:451:VAL:HG13	2.20	0.41
2:H:164:LYS:HE2	2:H:164:LYS:HB2	1.91	0.41
2:K:7:ILE:HD11	2:K:160:ILE:HG12	2.01	0.41
4:M:113:LEU:HD21	4:M:133:ARG:HB2	2.02	0.41
2:B:12:HIS:NE2	2:B:153:GLU:OE2	2.53	0.41
1:D:265:TYR:HD2	1:D:399:GLY:HA3	1.84	0.41
1:D:337:LEU:HD13	3:F:90:VAL:HG11	2.02	0.41
1:G:165:LEU:HA	1:G:166:PRO:HD3	1.87	0.41
4:N:3:ARG:HD3	4:N:21:LEU:HA	2.02	0.41
4:N:55:ALA:HA	4:N:58:PHE:HB2	2.01	0.41
4:N:74:GLY:HA2	4:N:98:TYR:HD2	1.85	0.41
4:P:37:LEU:HD12	4:P:50:PHE:HE1	1.85	0.41
1:D:338:GLU:HG2	1:D:342:LYS:HD2	2.02	0.41
2:E:32:ALA:HA	2:E:33:PRO:HD3	1.87	0.41
1:G:177:ILE:HG23	1:G:214:LEU:HD21	2.02	0.41
1:J:5:LEU:HD11	1:J:24:LEU:HD21	2.01	0.41
4:N:42:ARG:HD2	4:N:43:GLU:OE2	2.21	0.41
4:N:225:ARG:HD3	4:N:225:ARG:HA	1.68	0.41
4:O:319:GLY:HA2	4:O:402:ALA:H	1.83	0.41
4:P:463:LEU:HD21	4:P:500:VAL:HG22	2.03	0.41
1:D:204:TYR:OH	1:D:356:ARG:NH1	2.54	0.41
2:E:252:ASP:HA	2:E:253:PRO:HD3	1.83	0.41
2:E:455:UNK:O	2:E:459:UNK:N	2.53	0.41
3:F:70:THR:OG1	3:F:76:TYR:OH	2.33	0.41
1:G:48:ASP:O	1:G:51:ILE:HG13	2.20	0.41
2:K:363:GLU:OE2	2:K:363:GLU:N	2.52	0.41
3:L:3:LEU:HD22	3:L:31:LEU:HD22	2.03	0.41
3:L:92:LYS:HD2	3:L:92:LYS:HA	1.68	0.41
4:M:313:PRO:HA	4:M:316:ASP:OD2	2.20	0.41
4:P:168:LEU:HB3	4:P:191:PHE:CD1	2.54	0.41
4:P:383:ILE:O	4:P:387:VAL:HG13	2.19	0.41
1:A:61:ARG:HD2	1:A:70:LEU:HD13	2.02	0.41
1:D:444:VAL:HG12	1:D:445:ASP:OD2	2.20	0.41
1:G:3:HIS:CE1	1:G:4:GLN:HG2	2.55	0.41
1:G:323:ASP:OD1	1:G:325:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:398:LEU:HB3	1:G:453:LEU:HB3	2.01	0.41
2:H:357:LYS:HE2	2:H:357:LYS:HB3	1.84	0.41
1:J:71:GLY:N	1:J:113:GLY:O	2.49	0.41
1:J:92:LYS:HB3	1:J:348:GLY:O	2.20	0.41
4:M:79:ARG:HG2	4:M:94:GLU:HG3	2.02	0.41
4:N:273:MET:CE	4:N:277:GLU:HG2	2.50	0.41
4:P:342:LYS:HA	4:P:342:LYS:HD2	1.85	0.41
1:A:336:ASN:OD1	1:A:337:LEU:N	2.49	0.41
1:A:382:LEU:HD12	3:C:49:VAL:HG21	2.03	0.41
1:A:427:ILE:HD12	1:A:430:ASN:HB2	2.03	0.41
1:G:459:GLN:OE1	1:G:462:ARG:NH2	2.40	0.41
2:H:201:ARG:HA	2:H:202:PRO:HD3	1.97	0.41
4:M:504:LEU:O	4:M:504:LEU:HD13	2.21	0.41
4:N:248:ILE:HG21	4:N:272:HIS:NE2	2.36	0.41
4:O:93:ILE:HG22	4:O:94:GLU:N	2.35	0.41
2:B:32:ALA:HA	2:B:33:PRO:HD3	1.76	0.41
1:D:141:ASN:HA	1:D:142:PRO:HD3	1.93	0.41
1:D:447:LEU:HA	1:D:448:PRO:HD3	1.94	0.41
1:G:433:GLY:HA3	3:I:55:PRO:HB3	2.03	0.41
4:N:29:ARG:HB2	4:N:36:PHE:HB2	2.03	0.41
4:O:337:ILE:O	4:O:341:THR:HG23	2.21	0.41
4:O:342:LYS:HA	4:O:342:LYS:HD2	1.82	0.41
4:P:337:ILE:O	4:P:341:THR:HG23	2.21	0.41
4:P:356:LYS:HZ3	4:P:394:ILE:HD11	1.86	0.41
4:P:359:GLU:OE2	4:P:362:LYS:HG3	2.20	0.41
4:P:364:VAL:HG13	4:P:372:VAL:HG12	2.03	0.41
2:B:15:LEU:HD11	2:B:152:LEU:HB2	2.02	0.41
3:C:72:HIS:CE1	3:C:74:ASP:HB2	2.55	0.41
2:E:20:LYS:HE3	2:E:25:SER:HB2	2.03	0.41
2:E:295:LEU:HA	2:E:296:PRO:HD3	1.82	0.41
2:H:160:ILE:HD11	2:H:165:GLU:C	2.41	0.41
2:H:346:TRP:CZ2	2:H:389:ALA:HB1	2.55	0.41
1:J:188:GLY:O	1:J:437:LEU:HD12	2.21	0.41
4:M:85:ASN:HA	4:M:86:PRO:HD3	1.80	0.41
4:N:341:THR:HG22	4:N:352:LEU:HB3	2.02	0.41
4:O:207:ALA:HB1	4:P:132:LEU:HB2	2.02	0.41
4:P:225:ARG:HD2	4:P:225:ARG:HA	1.72	0.41
1:A:36:ASP:N	1:A:37:PRO:HD2	2.36	0.41
1:A:104:THR:HG21	1:A:197:SER:HB3	2.03	0.41
1:A:159:ALA:O	1:A:164:LEU:HB2	2.21	0.41
1:A:412:LYS:HD2	1:A:418:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:ILE:HG22	2:B:100:VAL:HG12	2.02	0.41
2:B:342:LEU:HD23	2:B:380:LYS:NZ	2.35	0.41
1:D:31:ARG:HH11	1:D:163:ARG:HH11	1.67	0.41
1:D:241:GLN:HA	1:D:242:PRO:HD3	1.73	0.41
2:E:83:TYR:CG	2:E:84:PRO:HD2	2.56	0.41
1:G:191:PRO:HG2	1:G:210:GLN:HG3	2.03	0.41
1:G:195:ARG:HH22	1:G:460:GLU:HG3	1.86	0.41
1:G:453:LEU:HD12	1:G:463:LEU:HD22	2.03	0.41
2:H:320:LEU:HD21	2:H:330:PHE:CG	2.56	0.41
1:J:258:ARG:H	1:J:258:ARG:HG2	1.66	0.41
2:K:332:LYS:O	2:K:336:ILE:HG13	2.21	0.41
2:K:371:GLN:H	2:K:371:GLN:HG2	1.53	0.41
4:M:252:GLU:OE2	4:M:256:ARG:NH2	2.54	0.41
4:M:475:TYR:CE2	4:M:488:SER:HA	2.56	0.41
4:M:585:ARG:NH2	4:N:578:ARG:HA	2.36	0.41
4:M:589:LYS:HB3	4:N:578:ARG:CD	2.51	0.41
4:N:273:MET:HA	4:N:274:PRO:HD3	1.94	0.41
4:N:455:SER:HB3	4:N:489:ILE:HG23	2.02	0.41
4:O:541:MET:HA	4:O:552:VAL:HG11	2.02	0.41
4:P:154:TYR:CE1	4:P:254:MET:HB2	2.56	0.41
4:P:325:ARG:HD2	4:P:389:ALA:HA	2.03	0.41
4:P:578:ARG:HE	4:P:578:ARG:HB3	1.49	0.41
5:R:55:U:N3	5:R:58:A:OP2	2.36	0.41
1:A:94:LEU:HD13	1:A:322:PHE:HE2	1.85	0.41
1:D:36:ASP:N	1:D:37:PRO:HD2	2.36	0.41
1:G:5:LEU:HD13	1:G:10:ILE:HG12	2.02	0.41
1:J:284:GLU:O	1:J:287:THR:OG1	2.27	0.41
4:M:33:GLY:HA3	5:Q:33:U:C6	2.56	0.41
4:N:177:ARG:HB2	4:N:221:ASP:HB3	2.03	0.41
4:O:353:ALA:HB3	4:O:397:PHE:HB2	2.03	0.41
4:O:570:GLY:HA3	4:P:170:ARG:NH1	2.35	0.41
4:P:26:HIS:NE2	4:P:114:ASP:OD2	2.53	0.41
4:P:49:VAL:HG11	4:P:77:ARG:HH21	1.84	0.41
4:P:300:ASP:OD1	4:P:301:GLN:N	2.54	0.41
1:A:271:ASP:HB2	4:P:334:ARG:HB2	2.02	0.40
1:D:82:THR:OG1	1:D:85:VAL:HB	2.21	0.40
3:F:7:ASP:HA	3:F:10:LYS:HE2	2.04	0.40
1:G:254:LEU:HD13	1:G:288:LEU:HB3	2.03	0.40
2:K:390:LYS:HA	2:K:390:LYS:HD3	1.91	0.40
3:L:54:HIS:HA	3:L:55:PRO:HD3	1.89	0.40
4:M:108:THR:HG21	5:Q:27:A:H4'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:201:LYS:HE3	4:M:238:GLU:OE1	2.20	0.40
4:N:300:ASP:OD1	4:N:301:GLN:N	2.54	0.40
4:N:492:HIS:ND1	4:N:528:PRO:HA	2.36	0.40
4:O:33:GLY:HA3	5:S:33:U:C6	2.56	0.40
4:O:340:TYR:OH	4:O:419:ASP:OD2	2.39	0.40
1:A:82:THR:O	1:A:99:SER:OG	2.39	0.40
1:G:265:TYR:CD2	1:G:399:GLY:HA3	2.56	0.40
1:G:336:ASN:H	1:G:339:ASP:HB3	1.86	0.40
2:H:332:LYS:O	2:H:336:ILE:HG13	2.21	0.40
1:J:44:SER:HB2	1:J:86:ARG:HE	1.85	0.40
1:J:74:ILE:O	1:J:116:THR:HA	2.22	0.40
1:J:82:THR:HA	1:J:102:ASP:OD1	2.22	0.40
2:K:295:LEU:HA	2:K:296:PRO:HD3	1.87	0.40
4:M:273:MET:HE1	4:M:282:TYR:CE2	2.57	0.40
4:N:357:VAL:HB	4:N:360:ARG:NH1	2.36	0.40
4:P:589:LYS:HE3	4:P:589:LYS:HB2	1.91	0.40
2:B:78:ARG:HD2	2:B:273:PHE:CZ	2.56	0.40
1:G:415:ASP:HA	1:G:416:PRO:HD3	1.89	0.40
2:H:164:LYS:H	2:H:164:LYS:HD3	1.85	0.40
1:J:202:ILE:HG12	2:K:45:PRO:HB2	2.03	0.40
2:K:320:LEU:HD21	2:K:330:PHE:CG	2.57	0.40
4:M:585:ARG:HH21	4:N:578:ARG:HA	1.86	0.40
4:N:492:HIS:CE1	4:N:528:PRO:HB3	2.56	0.40
4:P:252:GLU:CD	4:P:270:PHE:HB2	2.41	0.40
1:A:427:ILE:HD12	1:A:427:ILE:HA	1.82	0.40
2:B:58:MET:HE3	2:B:182:ILE:HA	2.04	0.40
1:G:176:SER:O	1:G:176:SER:OG	2.39	0.40
1:G:336:ASN:HD21	3:I:95:GLU:HB2	1.86	0.40
1:J:186:LEU:O	1:J:440:PRO:HD3	2.21	0.40
1:J:187:THR:HG22	1:J:439:MET:HG2	2.02	0.40
1:J:190:LYS:HE2	1:J:190:LYS:H	1.87	0.40
2:K:7:ILE:HB	2:K:198:VAL:HG12	2.03	0.40
4:N:383:ILE:O	4:N:387:VAL:HG13	2.22	0.40
4:O:343:PHE:CZ	4:O:415:LYS:HG3	2.56	0.40
4:P:51:ASP:N	4:P:52:PRO:HD3	2.36	0.40
4:P:111:PHE:HE1	4:P:127:TYR:HB2	1.86	0.40
4:P:492:HIS:CE1	4:P:528:PRO:HB3	2.57	0.40
2:B:303:ARG:O	2:B:307:GLU:HG2	2.21	0.40
1:D:130:SER:OG	1:D:132:GLN:OE1	2.33	0.40
3:I:10:LYS:HE2	3:I:10:LYS:HB3	1.95	0.40
1:J:56:ALA:HA	1:J:59:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:290:ARG:HB3	4:M:423:LEU:HB2	2.04	0.40
4:O:252:GLU:HG2	4:O:256:ARG:HE	1.85	0.40

All (2) 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:G:268:ALA:O	4:O:335:SER:OG[1_455]	2.12	0.08
1:J:268:ALA:O	4:M:335:SER:OG[1_455]	2.14	0.06

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	481/484 (99%)	446 (93%)	35 (7%)	0	100	100
1	D	481/484 (99%)	446 (93%)	35 (7%)	0	100	100
1	G	481/484 (99%)	447 (93%)	34 (7%)	0	100	100
1	J	481/484 (99%)	445 (92%)	36 (8%)	0	100	100
2	B	395/481 (82%)	358 (91%)	35 (9%)	2 (0%)	29	66
2	E	395/481 (82%)	362 (92%)	33 (8%)	0	100	100
2	H	395/481 (82%)	360 (91%)	34 (9%)	1 (0%)	41	74
2	K	395/481 (82%)	357 (90%)	37 (9%)	1 (0%)	41	74
3	C	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
3	F	94/104 (90%)	90 (96%)	4 (4%)	0	100	100
3	I	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
3	L	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
4	M	587/599 (98%)	542 (92%)	43 (7%)	2 (0%)	41	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	N	587/599 (98%)	541 (92%)	44 (8%)	2 (0%)	41 74
4	O	587/599 (98%)	543 (92%)	43 (7%)	1 (0%)	47 78
4	P	587/599 (98%)	542 (92%)	43 (7%)	2 (0%)	41 74
All	All	6228/6672 (93%)	5752 (92%)	465 (8%)	11 (0%)	47 78

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	337	CYS
2	K	337	CYS
2	H	337	CYS
4	P	298	VAL
4	P	450	HIS
4	N	298	VAL
4	O	298	VAL
4	M	298	VAL
4	N	173	PRO
2	B	366	PRO
4	M	173	PRO

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	377/378 (100%)	367 (97%)	10 (3%)	44 68
1	D	377/378 (100%)	364 (97%)	13 (3%)	37 64
1	G	377/378 (100%)	361 (96%)	16 (4%)	30 59
1	J	377/378 (100%)	359 (95%)	18 (5%)	25 56
2	B	329/333 (99%)	319 (97%)	10 (3%)	41 66
2	E	329/333 (99%)	325 (99%)	4 (1%)	71 84
2	H	329/333 (99%)	324 (98%)	5 (2%)	65 81
2	K	329/333 (99%)	313 (95%)	16 (5%)	25 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	81/88 (92%)	79 (98%)	2 (2%)	47 70
3	F	81/88 (92%)	80 (99%)	1 (1%)	71 84
3	I	81/88 (92%)	75 (93%)	6 (7%)	13 44
3	L	81/88 (92%)	77 (95%)	4 (5%)	25 56
4	M	493/502 (98%)	472 (96%)	21 (4%)	29 58
4	N	493/502 (98%)	471 (96%)	22 (4%)	27 57
4	O	493/502 (98%)	468 (95%)	25 (5%)	24 55
4	P	493/502 (98%)	469 (95%)	24 (5%)	25 56
All	All	5120/5204 (98%)	4923 (96%)	197 (4%)	33 61

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	61	ARG
1	A	119	LYS
1	A	131	ASN
1	A	209	ASP
1	A	220	ASP
1	A	240	GLU
1	A	349	PHE
1	A	407	TRP
1	A	439	MET
2	B	74	ASN
2	B	109	LEU
2	B	110	GLU
2	B	208	PHE
2	B	264	LYS
2	B	266	GLU
2	B	345	ASN
2	B	357	LYS
2	B	363	GLU
2	B	388	LEU
3	C	1	MET
3	C	26	ARG
1	D	34	GLN
1	D	53	GLN
1	D	59	GLU
1	D	119	LYS

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Mol	Chain	Res	Type
1	D	131	ASN
1	D	204	TYR
1	D	209	ASP
1	D	220	ASP
1	D	343	ARG
1	D	349	PHE
1	D	408	LYS
1	D	411	GLU
1	D	439	MET
2	E	334	GLN
2	E	378	ARG
2	E	380	LYS
2	E	394	GLU
3	F	32	ASN
1	G	19	PHE
1	G	26	ARG
1	G	33	ARG
1	G	122	MET
1	G	124	GLU
1	G	131	ASN
1	G	147	ARG
1	G	163	ARG
1	G	178	ARG
1	G	244	ASP
1	G	266	PHE
1	G	349	PHE
1	G	407	TRP
1	G	452	GLN
1	G	460	GLU
1	G	468	HIS
2	H	116	ARG
2	H	265	GLU
2	H	360	LEU
2	H	363	GLU
2	H	370	GLU
3	I	1	MET
3	I	5	ARG
3	I	26	ARG
3	I	61	ARG
3	I	65	ASP
3	I	69	GLU
1	J	36	ASP

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Mol	Chain	Res	Type
1	J	46	THR
1	J	55	LYS
1	J	58	ASP
1	J	61	ARG
1	J	95	ASP
1	J	121	ASN
1	J	163	ARG
1	J	190	LYS
1	J	198	ARG
1	J	266	PHE
1	J	270	LEU
1	J	284	GLU
1	J	354	LYS
1	J	407	TRP
1	J	424	ILE
1	J	459	GLN
1	J	479	ARG
2	K	95	MET
2	K	96	ASP
2	K	110	GLU
2	K	203	LYS
2	K	218	ASN
2	K	277	ASP
2	K	292	ARG
2	K	302	LYS
2	K	345	ASN
2	K	358	ASP
2	K	360	LEU
2	K	371	GLN
2	K	382	ASN
2	K	387	LYS
2	K	388	LEU
2	K	393	PHE
3	L	5	ARG
3	L	60	GLN
3	L	69	GLU
3	L	92	LYS
4	M	21	LEU
4	M	58	PHE
4	M	111	PHE
4	M	115	GLU
4	M	125	LEU

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Mol	Chain	Res	Type
4	M	153	ARG
4	M	170	ARG
4	M	212	TYR
4	M	225	ARG
4	M	300	ASP
4	M	307	PHE
4	M	360	ARG
4	M	373	LYS
4	M	381	ASN
4	M	390	VAL
4	M	425	ARG
4	M	450	HIS
4	M	483	GLU
4	M	517	PHE
4	M	563	ASP
4	M	587	GLN
4	N	3	ARG
4	N	21	LEU
4	N	42	ARG
4	N	51	ASP
4	N	54	ARG
4	N	58	PHE
4	N	115	GLU
4	N	125	LEU
4	N	170	ARG
4	N	185	THR
4	N	212	TYR
4	N	307	PHE
4	N	334	ARG
4	N	362	LYS
4	N	373	LYS
4	N	439	GLU
4	N	483	GLU
4	N	498	GLN
4	N	517	PHE
4	N	563	ASP
4	N	586	GLU
4	N	587	GLN
4	O	3	ARG
4	O	21	LEU
4	O	56	GLU
4	O	58	PHE

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Mol	Chain	Res	Type
4	O	62	ASP
4	O	73	THR
4	O	115	GLU
4	O	119	VAL
4	O	125	LEU
4	O	153	ARG
4	O	211	ARG
4	O	212	TYR
4	O	354	TYR
4	O	360	ARG
4	O	425	ARG
4	O	427	TRP
4	O	441	ASN
4	O	483	GLU
4	O	490	ARG
4	O	503	VAL
4	O	510	GLU
4	O	517	PHE
4	O	559	GLN
4	O	563	ASP
4	O	589	LYS
4	P	3	ARG
4	P	21	LEU
4	P	29	ARG
4	P	53	ASP
4	P	58	PHE
4	P	125	LEU
4	P	126	ARG
4	P	185	THR
4	P	212	TYR
4	P	223	ASP
4	P	276	GLU
4	P	304	GLU
4	P	307	PHE
4	P	334	ARG
4	P	391	ASP
4	P	425	ARG
4	P	439	GLU
4	P	467	PRO
4	P	483	GLU
4	P	508	GLU
4	P	517	PHE

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Mol	Chain	Res	Type
4	P	563	ASP
4	P	586	GLU
4	P	589	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	141	ASN
2	H	345	ASN
1	J	185	ASN
4	M	47	GLN
4	M	451	HIS
4	M	511	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	Q	75/76 (98%)	10 (13%)	1 (1%)
5	R	75/76 (98%)	10 (13%)	1 (1%)
5	S	75/76 (98%)	11 (14%)	0
5	T	75/76 (98%)	11 (14%)	1 (1%)
All	All	300/304 (98%)	42 (14%)	3 (1%)

All (42) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	Q	9	A
5	Q	18	G
5	Q	19	G
5	Q	20	U
5	Q	21	A
5	Q	33	U
5	Q	37	A
5	Q	47	U
5	Q	48	C
5	Q	76	A
5	R	9	A
5	R	18	G
5	R	19	G
5	R	20	U

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Mol	Chain	Res	Type
5	R	21	A
5	R	33	U
5	R	37	A
5	R	47	U
5	R	48	C
5	R	76	A
5	S	9	A
5	S	18	G
5	S	19	G
5	S	20	U
5	S	21	A
5	S	22	G
5	S	33	U
5	S	37	A
5	S	47	U
5	S	48	C
5	S	76	A
5	T	9	A
5	T	18	G
5	T	19	G
5	T	20	U
5	T	21	A
5	T	22	G
5	T	33	U
5	T	37	A
5	T	47	U
5	T	48	C
5	T	76	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	Q	47	U
5	R	47	U
5	T	47	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	483/484 (99%)	0.20	14 (2%) 51 39	45, 68, 100, 138	0
1	D	483/484 (99%)	0.07	7 (1%) 75 64	25, 51, 82, 110	0
1	G	483/484 (99%)	1.36	133 (27%) 0 0	85, 159, 207, 235	0
1	J	483/484 (99%)	1.68	171 (35%) 0 0	98, 173, 227, 253	0
2	B	399/481 (82%)	0.15	11 (2%) 53 40	37, 68, 135, 151	0
2	E	399/481 (82%)	0.17	15 (3%) 40 30	33, 69, 140, 156	0
2	H	399/481 (82%)	0.43	30 (7%) 14 10	58, 95, 164, 185	0
2	K	399/481 (82%)	0.62	36 (9%) 9 7	57, 115, 170, 202	0
3	C	96/104 (92%)	0.44	8 (8%) 11 9	49, 91, 131, 172	0
3	F	96/104 (92%)	0.02	3 (3%) 49 36	34, 73, 113, 152	0
3	I	96/104 (92%)	0.69	12 (12%) 3 4	84, 128, 163, 174	0
3	L	96/104 (92%)	0.80	13 (13%) 3 3	103, 137, 165, 169	0
4	M	589/599 (98%)	0.32	32 (5%) 25 19	39, 76, 173, 209	0
4	N	589/599 (98%)	0.08	10 (1%) 70 59	36, 69, 118, 140	0
4	O	589/599 (98%)	0.36	40 (6%) 17 12	39, 80, 196, 249	0
4	P	589/599 (98%)	0.07	12 (2%) 65 53	30, 69, 120, 159	0
5	Q	76/76 (100%)	0.42	3 (3%) 39 28	76, 126, 163, 182	0
5	R	76/76 (100%)	0.46	4 (5%) 26 20	65, 112, 149, 175	0
5	S	76/76 (100%)	0.19	2 (2%) 56 43	64, 94, 137, 188	0
5	T	76/76 (100%)	0.44	3 (3%) 39 28	84, 123, 160, 187	0
All	All	6572/6976 (94%)	0.45	559 (8%) 10 8	25, 85, 183, 253	0

All (559) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	27	THR	9.2
1	J	73	PRO	8.8
2	K	359	GLY	8.8
1	G	36	ASP	8.7
1	J	419	GLN	7.7
1	G	346	ALA	7.6
1	G	121	ASN	7.4
1	J	212	GLY	7.4
1	J	170	GLY	7.4
1	J	74	ILE	7.4
4	O	315	ASN	7.3
1	J	416	PRO	7.1
1	J	116	THR	7.1
1	J	3	HIS	6.8
2	K	267	ALA	6.6
1	G	118	GLY	6.6
1	J	2	LEU	6.5
1	J	213	PRO	6.5
2	K	368	SER	6.2
4	M	371	ILE	6.1
4	O	443	ASP	6.1
3	C	94	ILE	6.0
3	C	72	HIS	5.9
4	O	371	ILE	5.9
1	J	329	TYR	5.9
1	J	75	ALA	5.8
1	G	146	ASP	5.5
3	C	74	ASP	5.5
1	G	194	GLY	5.5
4	O	373	LYS	5.4
3	I	18	GLY	5.4
1	J	84	GLY	5.4
2	B	266	GLU	5.4
1	G	38	GLN	5.3
1	J	322	PHE	5.2
1	G	347	GLU	5.2
1	G	481	PRO	5.2
1	J	169	THR	5.1
1	J	44	SER	5.1
2	E	267	ALA	4.9
2	H	381	ASP	4.9
4	O	374	PHE	4.9
1	J	141	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	J	76	HIS	4.9
1	G	73	PRO	4.9
1	G	142	PRO	4.8
1	J	195	ARG	4.8
2	B	382	ASN	4.8
4	O	588	PRO	4.8
2	K	30	GLY	4.8
1	J	241	GLN	4.7
1	G	449	VAL	4.7
1	G	276	ASP	4.7
1	J	165	LEU	4.7
3	F	94	ILE	4.7
1	G	454	LEU	4.7
1	J	260	GLY	4.6
1	J	194	GLY	4.6
4	O	293	LEU	4.6
1	G	355	ASN	4.6
1	J	20	SER	4.6
1	G	148	VAL	4.5
1	J	345	ARG	4.5
1	J	445	ASP	4.5
1	G	170	GLY	4.5
1	G	453	LEU	4.5
1	J	324	GLY	4.5
1	G	185	ASN	4.4
1	J	351	SER	4.4
3	I	91	PRO	4.4
1	J	346	ALA	4.4
2	H	335	GLY	4.4
5	S	17	C	4.4
1	J	478	THR	4.4
5	R	17	C	4.4
1	G	37	PRO	4.4
1	G	9	GLU	4.3
4	O	308	LYS	4.3
1	J	418	SER	4.3
1	J	242	PRO	4.3
1	J	1	MET	4.3
4	O	313	PRO	4.3
1	J	399	GLY	4.3
1	J	204	TYR	4.3
1	J	392	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	J	21	ALA	4.2
1	J	149	PRO	4.2
2	K	397	ALA	4.2
1	J	398	LEU	4.2
1	G	166	PRO	4.2
2	E	381	ASP	4.2
1	J	87	THR	4.2
1	G	445	ASP	4.1
1	G	446	GLY	4.1
2	K	381	ASP	4.1
1	J	45	ILE	4.1
4	O	355	ILE	4.1
1	J	34	GLN	4.1
4	M	588	PRO	4.1
1	J	93	MET	4.1
1	J	86	ARG	4.0
5	T	17	C	4.0
1	G	440	PRO	4.0
1	J	390	ALA	4.0
1	G	188	GLY	4.0
1	G	122	MET	4.0
2	B	381	ASP	4.0
4	M	355	ILE	4.0
5	R	76	A	4.0
1	G	418	SER	4.0
1	J	142	PRO	3.9
2	K	45	PRO	3.9
4	N	590	ALA	3.9
1	J	37	PRO	3.9
1	J	53	GLN	3.9
1	G	328	GLY	3.9
1	G	189	ILE	3.9
3	C	95	GLU	3.9
1	J	305	PRO	3.8
4	M	295	LEU	3.8
1	J	240	GLU	3.8
1	G	345	ARG	3.8
1	J	186	LEU	3.8
4	M	395	VAL	3.8
1	G	149	PRO	3.8
1	J	85	VAL	3.8
2	K	39	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	6	THR	3.7
1	G	15	ALA	3.7
1	G	483	GLY	3.7
1	D	413	ASN	3.7
2	K	130	LYS	3.7
2	E	266	GLU	3.7
4	N	175	GLY	3.7
1	J	36	ASP	3.7
1	G	169	THR	3.6
4	O	587	GLN	3.6
1	J	215	ALA	3.6
1	J	202	ILE	3.6
1	J	411	GLU	3.6
1	J	23	GLU	3.6
1	G	214	LEU	3.6
1	G	434	LEU	3.5
4	M	303	LYS	3.5
4	M	586	GLU	3.5
1	G	213	PRO	3.5
4	O	295	LEU	3.5
1	G	43	ILE	3.5
1	G	240	GLU	3.5
1	J	209	ASP	3.5
4	O	367	LEU	3.5
4	M	298	VAL	3.5
2	H	401	GLY	3.5
4	P	175	GLY	3.5
1	G	165	LEU	3.5
1	J	348	GLY	3.5
1	G	437	LEU	3.5
2	B	398	ASN	3.5
1	G	42	PHE	3.5
4	M	391	ASP	3.5
1	J	79	LEU	3.4
2	K	191	SER	3.4
1	J	54	ALA	3.4
1	G	86	ARG	3.4
3	L	88	TYR	3.4
1	G	167	ALA	3.4
1	J	129	SER	3.4
2	K	265	GLU	3.4
2	K	332	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	412	LYS	3.4
1	G	2	LEU	3.3
1	G	74	ILE	3.3
1	G	439	MET	3.3
4	M	397	PHE	3.3
2	H	353	SER	3.3
1	J	355	ASN	3.3
3	L	12	ALA	3.3
1	J	65	GLU	3.3
1	G	435	PRO	3.3
1	J	18	GLN	3.3
3	L	10	LYS	3.3
1	G	45	ILE	3.3
2	H	336	ILE	3.3
1	G	413	ASN	3.3
1	J	22	GLU	3.3
1	D	481	PRO	3.2
1	J	277	ALA	3.2
1	G	444	VAL	3.2
4	O	299	ALA	3.2
2	H	387	LYS	3.2
2	E	385	SER	3.2
1	G	237	THR	3.2
1	G	168	ALA	3.2
4	N	443	ASP	3.2
1	G	470	TYR	3.2
1	J	31	ARG	3.2
2	E	265	GLU	3.2
4	M	441	ASN	3.2
4	O	368	GLN	3.2
1	J	429	ALA	3.2
4	M	299	ALA	3.2
1	G	223	LEU	3.2
2	K	14	GLN	3.2
3	I	80	ALA	3.2
1	J	367	GLY	3.2
1	G	153	SER	3.1
1	A	481	PRO	3.1
1	G	482	ALA	3.1
2	K	244	VAL	3.1
1	G	416	PRO	3.1
1	J	148	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
4	M	308	LYS	3.1
2	H	337	CYS	3.1
1	G	318	ASN	3.1
1	G	92	LYS	3.1
1	J	155	GLY	3.1
4	M	442	ASP	3.1
2	E	141	GLY	3.0
4	O	294	GLU	3.0
1	J	214	LEU	3.0
1	G	278	VAL	3.0
1	G	177	ILE	3.0
1	J	26	ARG	3.0
4	O	307	PHE	3.0
1	G	79	LEU	3.0
5	T	45	G	3.0
4	O	304	GLU	3.0
1	J	437	LEU	3.0
2	H	257	GLU	3.0
1	G	351	SER	3.0
1	G	414	ASP	3.0
1	A	187	THR	3.0
3	C	78	THR	3.0
4	O	353	ALA	3.0
1	J	40	ASN	3.0
1	D	415	ASP	3.0
2	H	260	SER	3.0
2	H	37	ALA	3.0
3	I	88	TYR	3.0
3	L	93	VAL	3.0
1	J	415	ASP	3.0
1	J	72	ALA	2.9
1	G	89	CYS	2.9
2	E	387	LYS	2.9
1	G	162	ALA	2.9
1	J	436	GLY	2.9
1	J	153	SER	2.9
2	E	391	MET	2.9
1	G	56	ALA	2.9
3	F	95	GLU	2.9
1	J	327	TYR	2.9
4	N	83	ALA	2.9
1	J	342	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	K	219	SER	2.9
1	J	205	ALA	2.9
1	J	328	GLY	2.9
4	O	303	LYS	2.9
2	K	266	GLU	2.9
2	H	34	ASN	2.9
1	A	66	ASN	2.9
1	J	94	LEU	2.9
1	J	210	GLN	2.9
1	J	221	CYS	2.9
1	J	143	TRP	2.9
1	G	54	ALA	2.9
2	H	263	GLY	2.9
3	C	93	VAL	2.9
1	J	461	GLY	2.9
1	J	160	VAL	2.9
4	O	359	GLU	2.9
2	H	31	ALA	2.9
1	A	41	SER	2.8
1	G	156	SER	2.8
3	L	94	ILE	2.8
4	N	586	GLU	2.8
1	G	398	LEU	2.8
2	H	386	GLY	2.8
1	J	7	LEU	2.8
2	K	84	PRO	2.8
1	J	216	ARG	2.8
1	G	294	ASP	2.8
4	O	389	ALA	2.8
4	M	334	ARG	2.8
1	J	406	ALA	2.8
2	K	255	LYS	2.8
1	J	434	LEU	2.8
1	G	394	VAL	2.8
2	H	38	SER	2.8
1	J	92	LYS	2.8
1	J	402	THR	2.8
4	N	60	LYS	2.8
1	J	386	ASP	2.8
1	G	163	ARG	2.8
1	J	190	LYS	2.8
2	K	345	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	396	VAL	2.7
1	D	480	THR	2.7
1	J	80	PHE	2.7
1	G	405	PRO	2.7
2	K	210	THR	2.7
1	J	57	ALA	2.7
1	G	141	ASN	2.7
1	J	438	SER	2.7
2	H	33	PRO	2.7
2	K	43	ALA	2.7
1	G	260	GLY	2.7
1	D	416	PRO	2.7
1	G	277	ALA	2.7
1	G	415	ASP	2.7
4	M	373	LYS	2.7
4	M	349	ALA	2.7
1	G	120	LEU	2.7
1	J	77	LYS	2.7
3	L	11	ILE	2.7
3	L	53	ALA	2.7
1	G	93	MET	2.7
2	B	401	GLY	2.7
1	J	289	GLY	2.6
4	O	334	ARG	2.6
5	Q	74	C	2.6
2	K	393	PHE	2.6
1	A	22	GLU	2.6
2	E	371	GLN	2.6
1	G	44	SER	2.6
1	J	332	ASP	2.6
2	H	385	SER	2.6
4	M	374	PHE	2.6
1	G	174	GLY	2.6
1	J	412	LYS	2.6
4	M	306	GLU	2.6
4	M	307	PHE	2.6
1	J	405	PRO	2.6
1	G	296	SER	2.6
1	J	285	LEU	2.6
1	G	329	TYR	2.6
4	M	359	GLU	2.6
5	S	21	A	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	388	VAL	2.6
1	G	193	TYR	2.6
1	J	4	GLN	2.6
3	I	17	LEU	2.6
4	O	298	VAL	2.6
1	J	17	LYS	2.5
3	I	95	GLU	2.5
1	G	212	GLY	2.5
1	J	225	LEU	2.5
1	J	193	TYR	2.5
2	K	402	SER	2.5
1	J	290	ALA	2.5
1	J	173	THR	2.5
4	O	504	LEU	2.5
1	J	460	GLU	2.5
4	N	510	GLU	2.5
1	A	450	GLY	2.5
3	F	96	SER	2.5
1	G	285	LEU	2.5
1	J	294	ASP	2.5
1	J	168	ALA	2.5
1	J	222	ALA	2.5
2	H	364	GLN	2.5
2	H	265	GLU	2.5
1	G	34	GLN	2.5
4	O	314	ALA	2.5
1	G	474	SER	2.5
1	J	133	SER	2.5
4	O	397	PHE	2.5
4	O	586	GLU	2.5
1	G	16	ASP	2.5
1	G	341	TYR	2.5
1	G	452	GLN	2.5
1	J	38	GLN	2.5
3	L	80	ALA	2.5
1	G	80	PHE	2.5
1	J	393	GLU	2.4
4	P	588	PRO	2.4
1	G	227	VAL	2.4
2	K	361	GLU	2.4
2	E	264	LYS	2.4
1	G	119	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	417	VAL	2.4
1	G	471	GLN	2.4
4	P	298	VAL	2.4
1	J	47	ASP	2.4
1	J	304	ILE	2.4
2	K	35	THR	2.4
1	J	154	GLY	2.4
1	J	323	ASP	2.4
1	J	354	LYS	2.4
1	J	440	PRO	2.4
4	O	442	ASP	2.4
1	J	228	MET	2.4
1	G	132	GLN	2.4
1	J	69	LEU	2.4
1	G	5	LEU	2.4
1	J	480	THR	2.4
2	K	44	MET	2.4
1	J	89	CYS	2.4
2	K	388	LEU	2.4
3	L	91	PRO	2.4
1	G	202	ILE	2.4
1	J	211	GLY	2.4
4	O	352	LEU	2.4
1	A	360	GLY	2.4
4	P	367	LEU	2.4
1	J	122	MET	2.4
1	J	42	PHE	2.4
1	D	483	GLY	2.4
1	A	406	ALA	2.4
2	H	25	SER	2.4
2	B	400	GLU	2.4
1	A	65	GLU	2.3
3	I	12	ALA	2.3
4	N	367	LEU	2.3
1	J	349	PHE	2.3
4	N	115	GLU	2.3
4	M	319	GLY	2.3
1	J	162	ALA	2.3
2	H	389	ALA	2.3
4	O	486	GLY	2.3
1	J	56	ALA	2.3
4	O	386	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	288	LEU	2.3
4	P	174	GLU	2.3
4	M	487	GLY	2.3
1	G	397	ILE	2.3
1	D	294	ASP	2.3
4	O	467	PRO	2.3
1	J	362	TYR	2.3
1	J	29	LEU	2.3
4	O	306	GLU	2.3
4	P	580	LEU	2.3
2	B	387	LYS	2.3
1	J	439	MET	2.3
2	H	59	ALA	2.3
2	H	216	ASN	2.3
1	J	166	PRO	2.3
4	N	47	GLN	2.3
4	P	300	ASP	2.3
1	G	155	GLY	2.3
2	B	267	ALA	2.3
2	H	139	MET	2.3
4	P	371	ILE	2.3
1	G	426	THR	2.3
2	K	370	GLU	2.3
1	J	295	ILE	2.3
3	I	56	LEU	2.3
4	P	16	GLY	2.3
5	R	47	U	2.3
4	M	372	VAL	2.3
3	L	16	ARG	2.3
1	J	30	GLY	2.3
2	K	348	MET	2.3
3	C	19	LEU	2.3
1	J	178	ARG	2.2
1	G	160	VAL	2.2
1	G	393	GLU	2.2
3	L	18	GLY	2.2
1	G	22	GLU	2.2
1	J	179	GLN	2.2
1	G	133	SER	2.2
1	J	479	ARG	2.2
1	J	128	GLY	2.2
3	I	86	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
4	P	322	ALA	2.2
2	B	140	SER	2.2
4	M	318	LYS	2.2
3	L	52	LEU	2.2
1	J	432	ALA	2.2
2	K	331	GLU	2.2
1	J	203	ALA	2.2
1	G	95	ASP	2.2
2	K	146	ARG	2.2
1	G	326	ARG	2.2
1	J	264	GLU	2.2
1	G	293	LYS	2.2
1	J	246	TYR	2.2
2	K	198	VAL	2.2
1	G	392	ALA	2.2
1	J	183	LEU	2.2
3	L	8	VAL	2.2
1	G	114	ALA	2.2
1	G	332	ASP	2.2
2	K	391	MET	2.2
4	M	548	SER	2.2
1	J	139	VAL	2.2
1	A	64	GLY	2.2
2	E	334	GLN	2.2
2	K	341	LYS	2.2
3	I	41	MET	2.1
1	G	35	LEU	2.1
1	G	96	ASN	2.1
2	E	346	TRP	2.1
4	P	590	ALA	2.1
1	G	164	LEU	2.1
1	G	144	SER	2.1
2	H	361	GLU	2.1
4	M	470	ALA	2.1
5	Q	17	C	2.1
2	H	363	GLU	2.1
5	R	34	G	2.1
2	E	187	MET	2.1
4	O	284	SER	2.1
1	J	43	ILE	2.1
1	J	146	ASP	2.1
1	J	223	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	326	ARG	2.1
1	J	417	VAL	2.1
2	K	31	ALA	2.1
3	I	62	LEU	2.1
4	M	370	PRO	2.1
1	A	478	THR	2.1
1	J	325	VAL	2.1
4	O	311	SER	2.1
1	G	399	GLY	2.1
1	J	373	TYR	2.1
3	C	10	LYS	2.1
1	G	226	GLY	2.1
1	G	289	GLY	2.1
4	P	84	ARG	2.1
4	O	46	ALA	2.1
1	G	20	SER	2.1
1	J	152	SER	2.1
2	H	354	LEU	2.1
2	B	264	LYS	2.1
1	G	324	GLY	2.1
1	J	175	GLY	2.1
3	I	87	LEU	2.1
1	A	221	CYS	2.1
1	A	443	PHE	2.1
1	J	95	ASP	2.1
1	J	358	MET	2.1
1	G	1	MET	2.1
1	J	397	ILE	2.1
1	G	63	ASN	2.1
1	J	318	ASN	2.1
4	M	315	ASN	2.1
4	M	320	ARG	2.1
1	J	35	LEU	2.1
2	E	242	GLY	2.1
4	M	313	PRO	2.0
1	G	279	LEU	2.0
2	B	388	LEU	2.0
4	M	390	VAL	2.0
2	E	369	ALA	2.0
2	H	396	MET	2.0
1	J	220	ASP	2.0
2	H	310	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	211	GLY	2.0
1	J	107	GLU	2.0
2	K	295	LEU	2.0
1	A	413	ASN	2.0
5	Q	21	A	2.0
4	O	585	ARG	2.0
1	G	420	TYR	2.0
4	O	354	TYR	2.0
5	T	73	G	2.0
1	J	81	CYS	2.0
2	H	140	SER	2.0
4	O	365	GLU	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.