Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 10:03 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

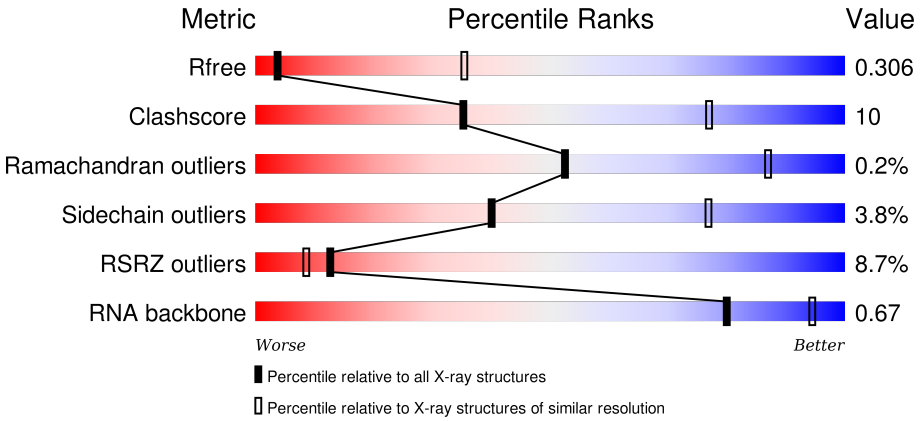
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)
RNA backbone	2183	1067 (4.60-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 76% 23%
1	G	484	28% 70% 28%
1	J	484	36% 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	8% 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	13% 68% 21% 8%
4	M	599	6% 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	3% 70% 25% 5%

2 Entry composition

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.

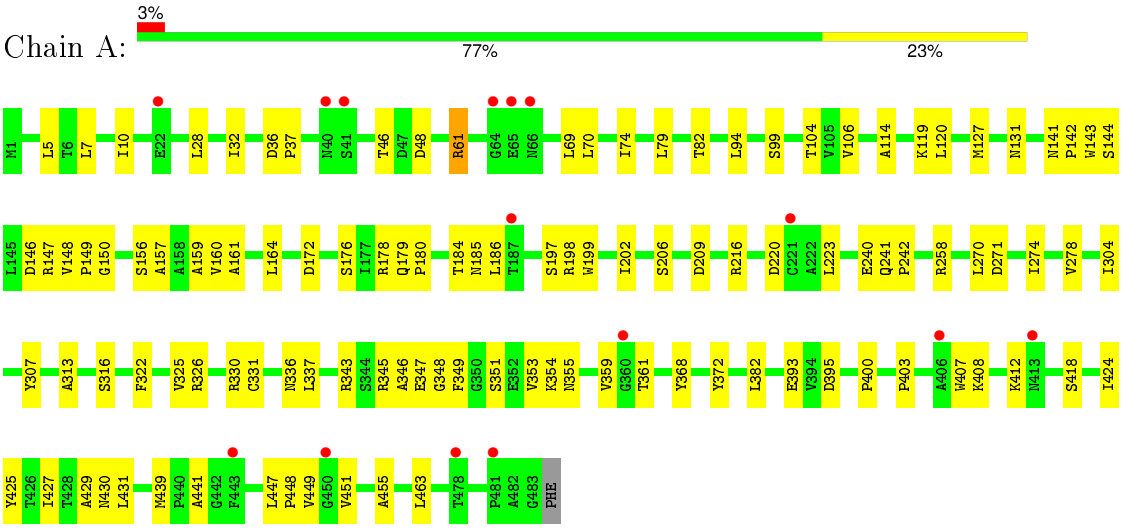
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	76	Total	C	N	O	P	0	0	0
			1622	723	288	535	76			
5	R	76	Total	C	N	O	P	0	0	0
			1622	723	288	535	76			
5	S	76	Total	C	N	O	P	0	0	0
			1622	723	288	535	76			
5	T	76	Total	C	N	O	P	0	0	0
			1622	723	288	535	76			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

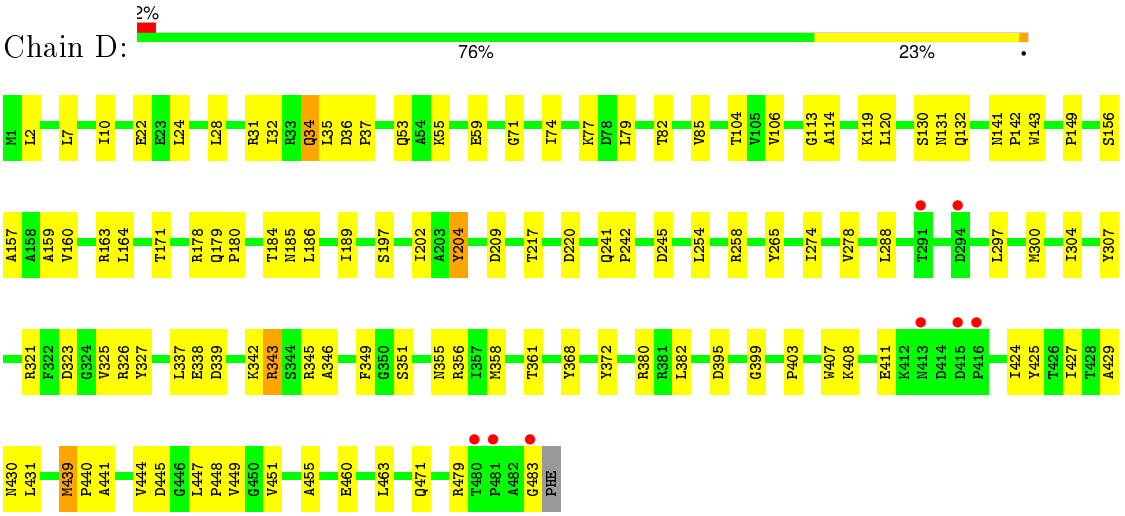
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain A:



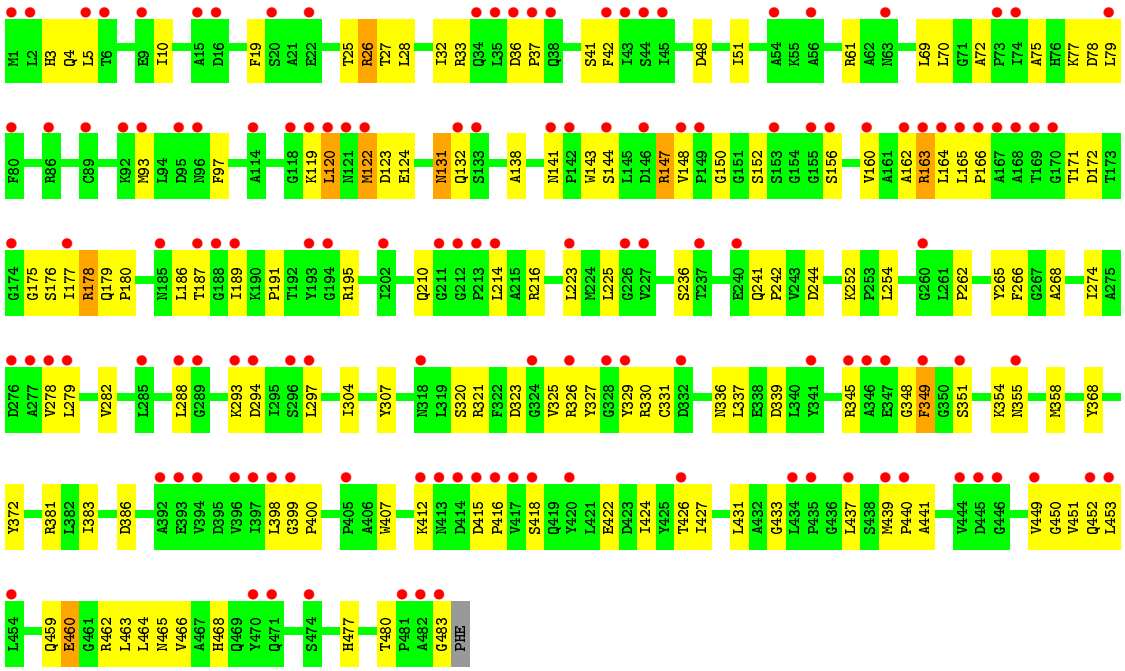
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain D:



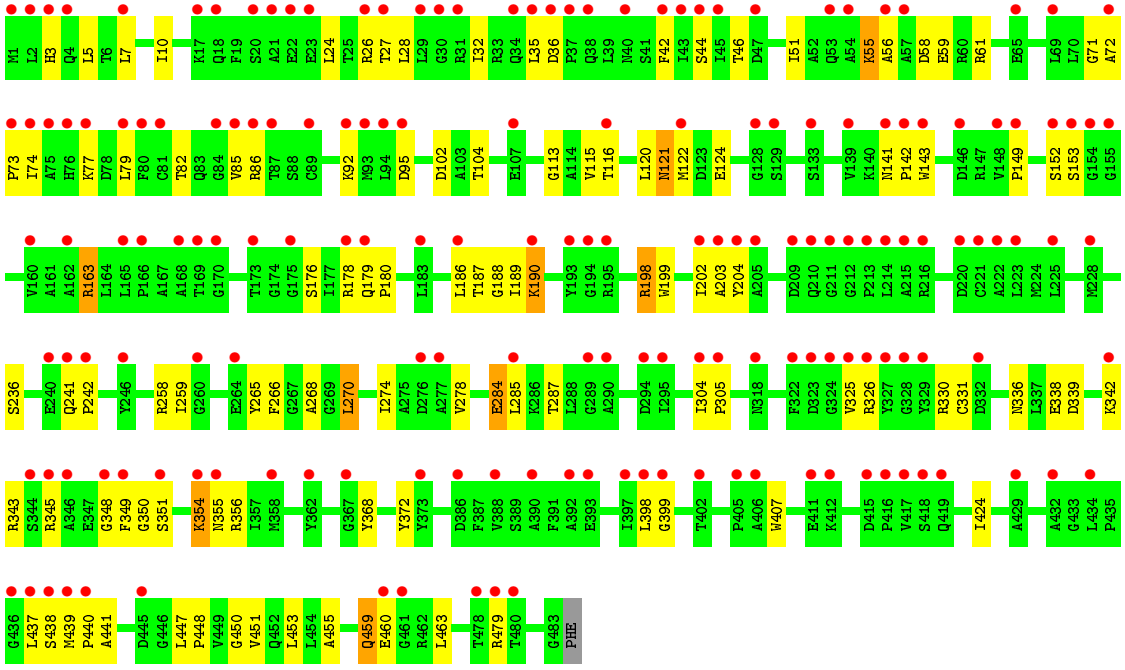
- Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

Chain G:



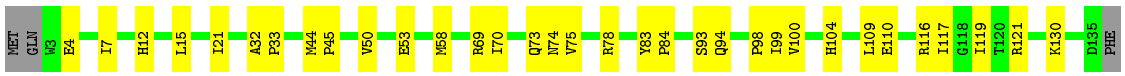
• Molecule 1: Glutamyl-tRNA(Gln) amidotransferase subunit A

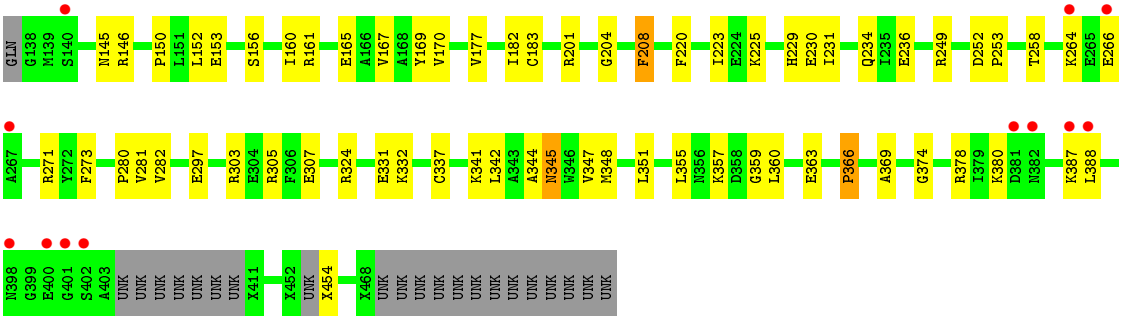
Chain J:



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

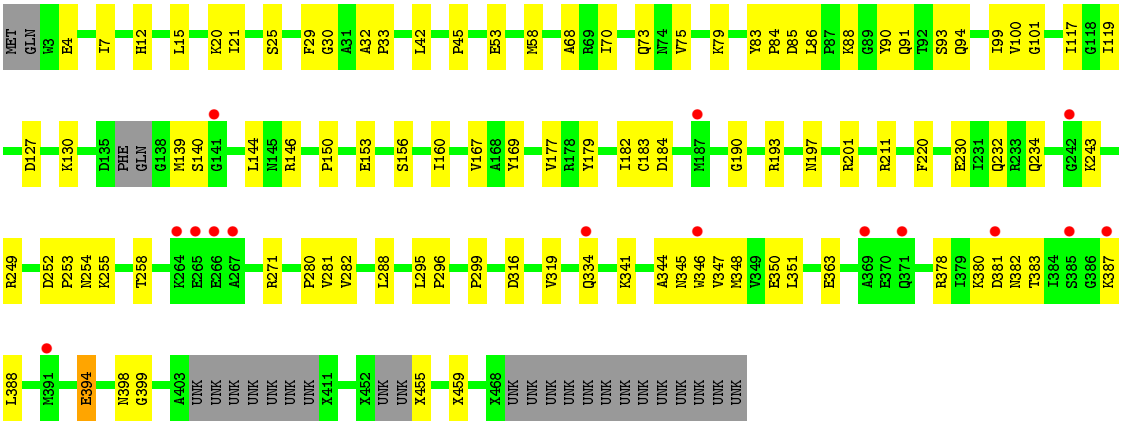
Chain B:





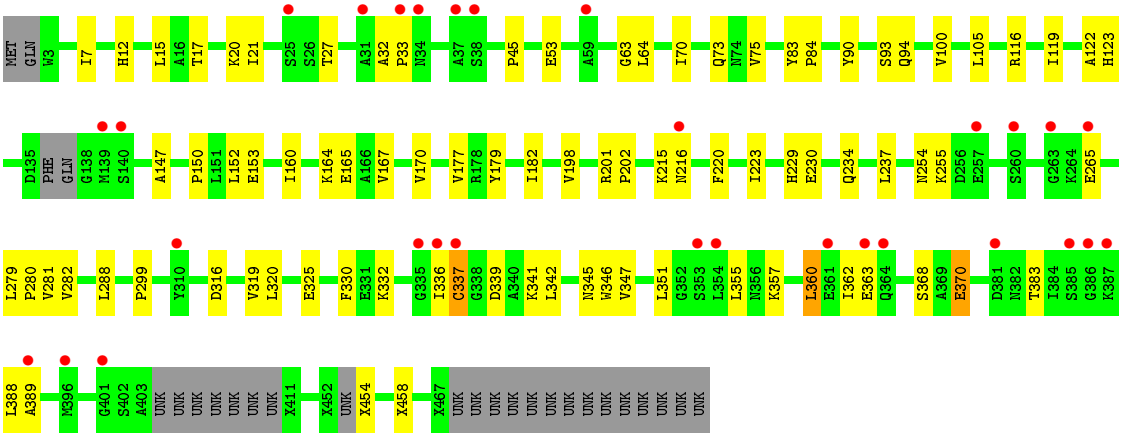
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

Chain E:



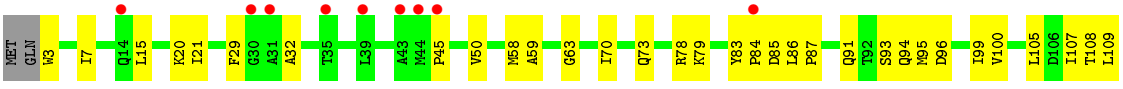
• Molecule 2: Aspartyl/glutamyl-tRNA(Asn/Gln) amidotransferase subunit B

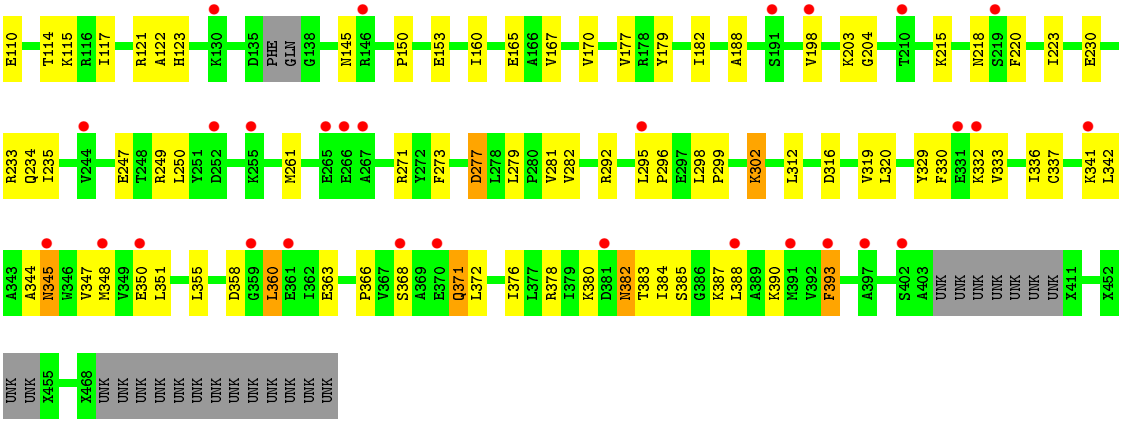
Chain H:



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

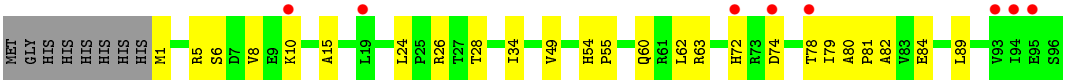
Chain K:





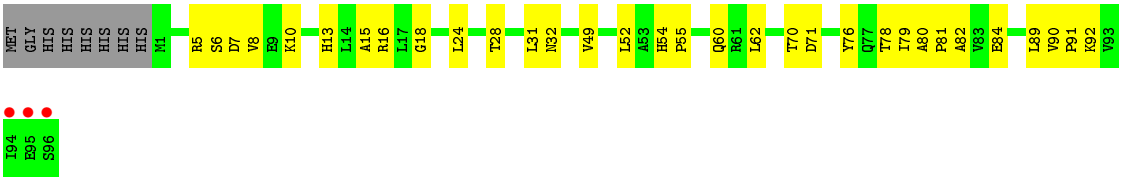
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain C:



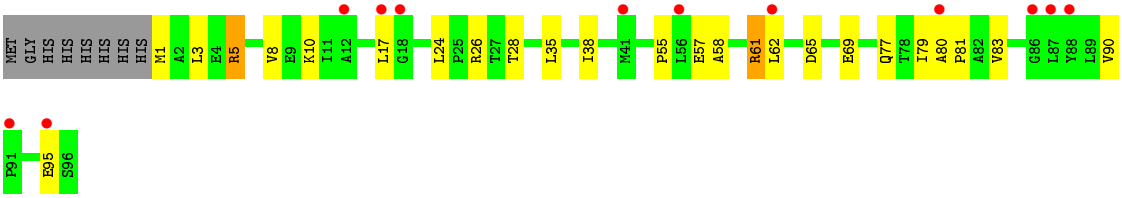
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain F:



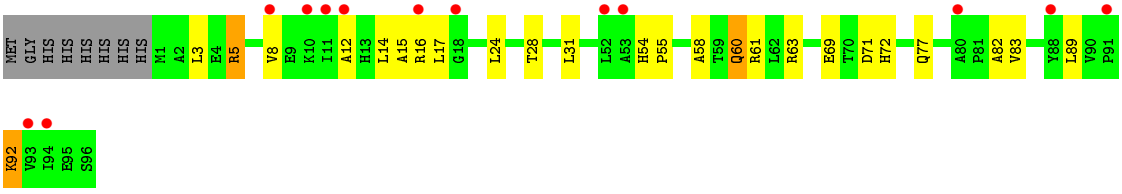
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain I:



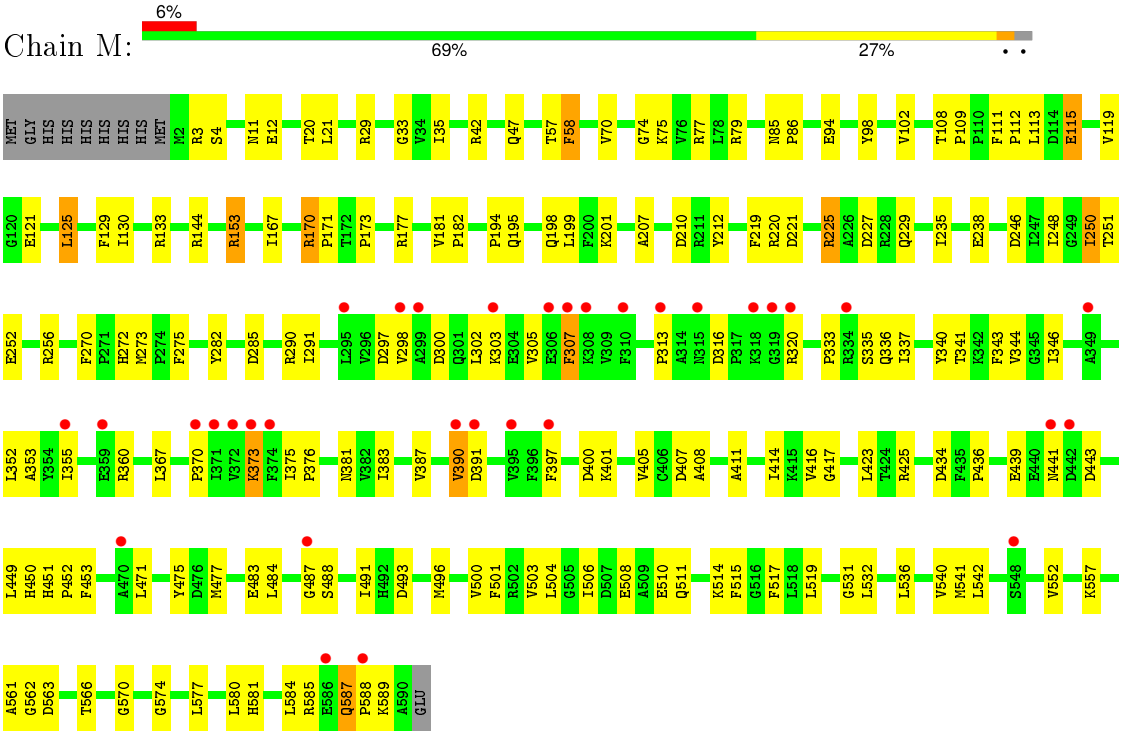
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit C

Chain L:



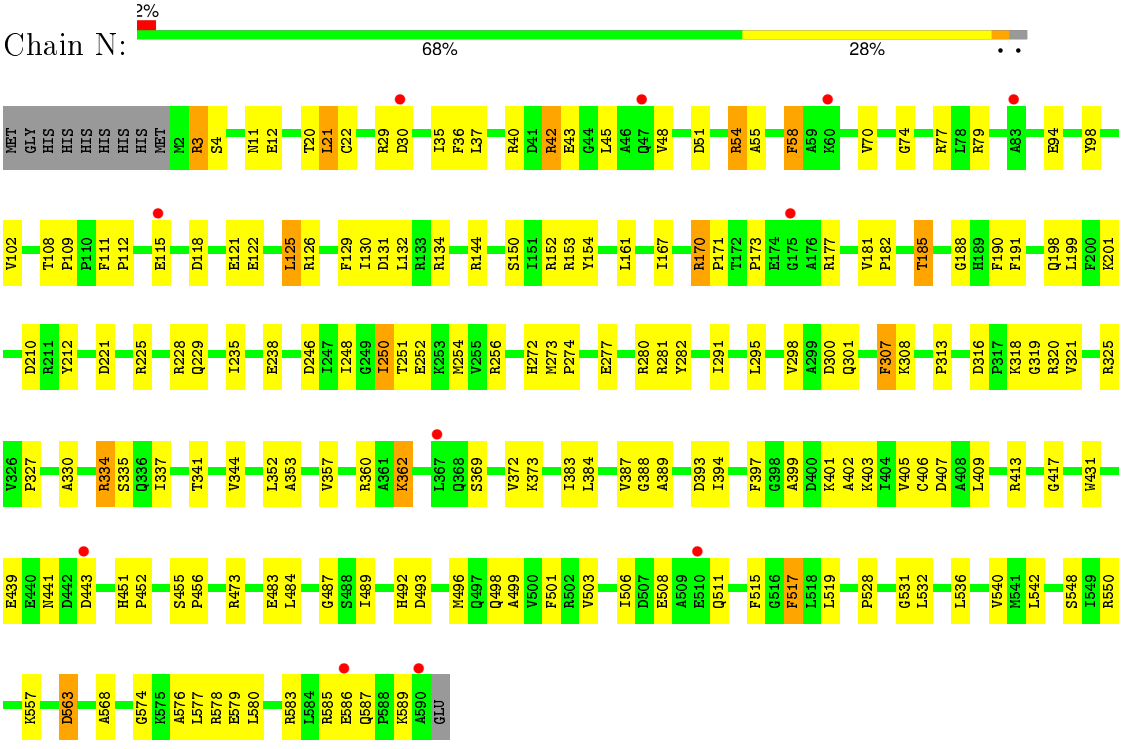
• Molecule 4: Aspartate--tRNA(Asp/Asn) ligase

Chain M:



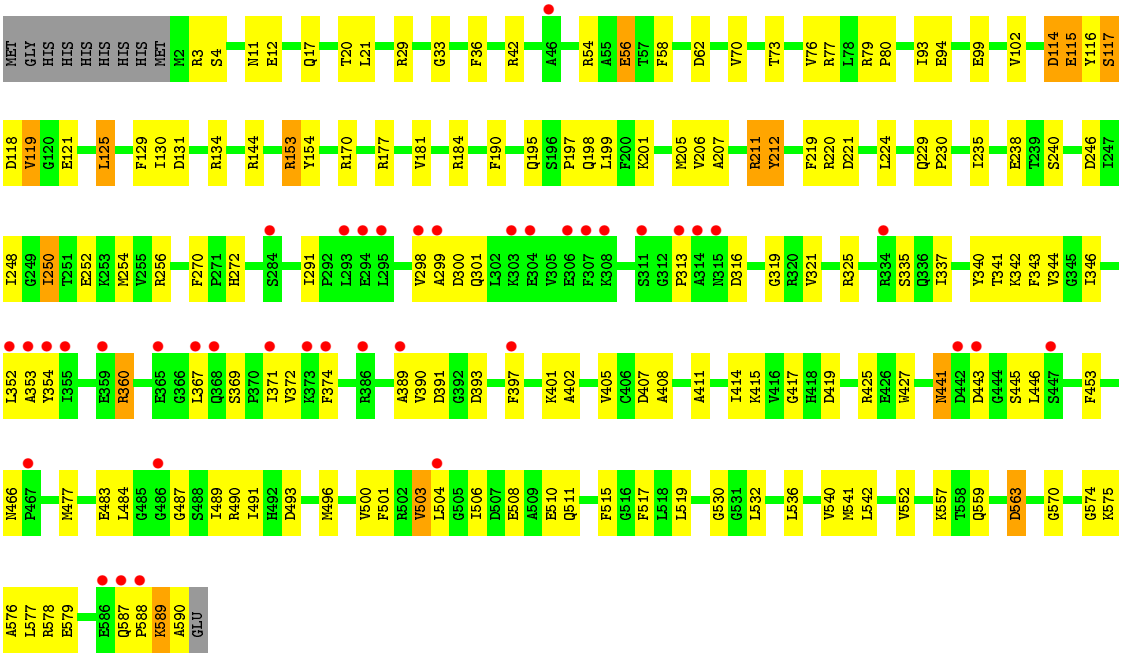
• Molecule 4: Aspartate--tRNA(Asp/Asn) ligase

Chain N:



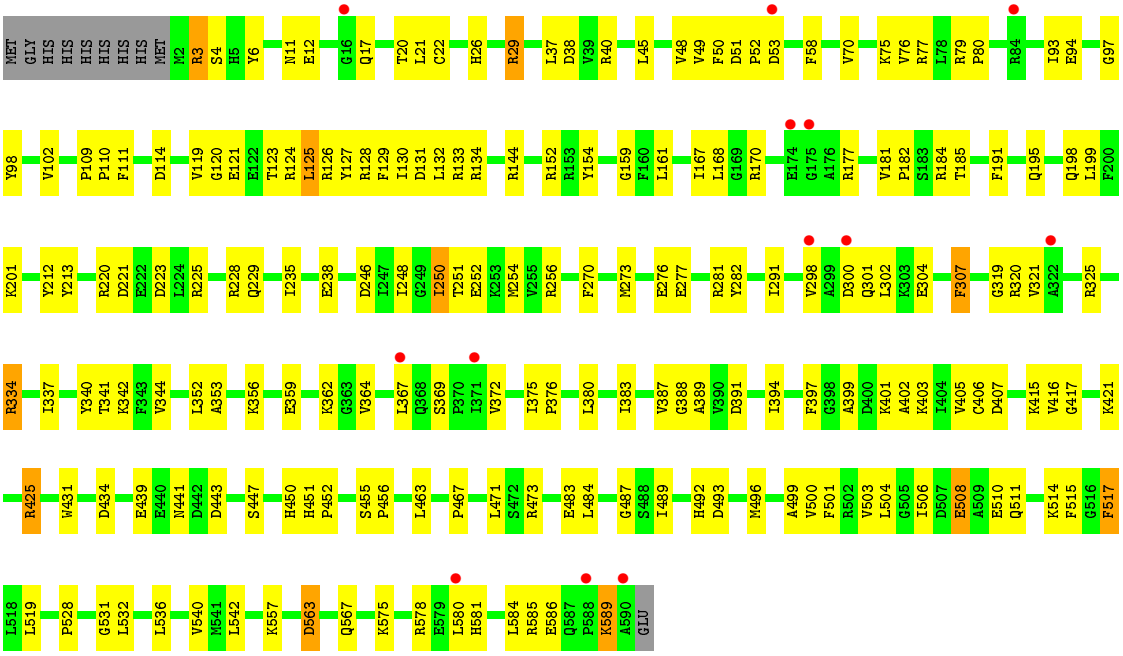
• Molecule 4: Aspartate--tRNA(Asp/Asn) ligase

Chain O:



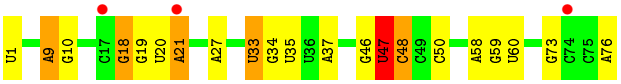
• Molecule 4: Aspartate--tRNA(Asp/Asn) ligase

Chain P:



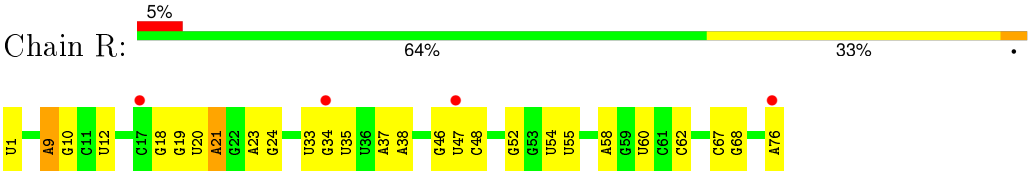
• Molecule 5: 76mer-tRNA

Chain Q:



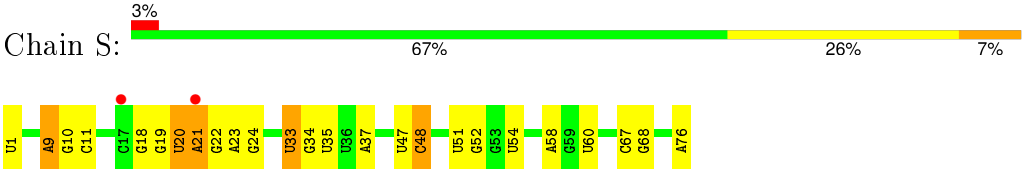
• Molecule 5: 76mer-tRNA

Chain R:



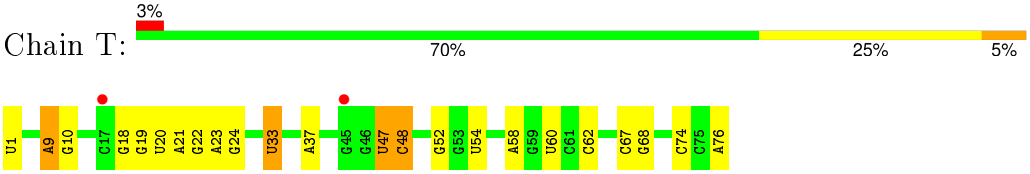
• Molecule 5: 76mer-tRNA

Chain S:



• Molecule 5: 76mer-tRNA

Chain T:



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 0.287 , 0.306	Depositor DCC
R_{free} test set	4824 reflections (5.00%)	DCC
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
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 96489 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:P:79:ARG:NH2	4:P:93:ILE:O	2.13	0.80
4:M:584:LEU:HD13	4:N:188:GLY:HA2	1.62	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
4:N:3:ARG:HD3	4:N:22:CYS:H	1.50	0.73
2:B:4:GLU:HG3	2:B:201:ARG:HG3	1.69	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
4:O:489:ILE:HD13	4:O:530:GLY:HA3	1.71	0.72
1:G:325:VAL:HG13	1:G:326:ARG:HG3	1.71	0.72
4:O:229:GLN:NE2	4:O:557:LYS:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:77:LYS:HG3	1:J:122:MET:HG3	1.72	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
1:J:51:ILE:HG12	1:J:55:LYS:HE2	1.74	0.70
3:C:78:THR:HG23	3:C:79:ILE:HG13	1.73	0.70
4:P:403:LYS:NZ	4:P:407:ASP:OD2	2.22	0.70
4:P:201:LYS:HE2	4:P:238:GLU:HB2	1.74	0.70
1:D:160:VAL:HB	1:D:186:LEU:HD21	1.73	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:440:PRO:HA	1:G:450:GLY:HA2	1.77	0.67
1:G:195:ARG:HH21	1:G:225:LEU:HD11	1.60	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
5:Q:47:U:O2'	5:Q:48:C:OP1	2.09	0.67
4:N:369:SER:HB3	4:N:372:VAL:HG23	1.76	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
4:N:77:ARG:HG2	4:N:94:GLU:HG3	1.77	0.65
1:J:270:LEU:HB2	1:J:274:ILE:HD11	1.78	0.65
4:P:447:SER:HA	4:P:504:LEU:HD11	1.78	0.65
4:N:493:ASP:HB3	4:N:496:MET:HB3	1.76	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:K:355:LEU:HA	2:K:360:LEU:HD11	1.79	0.64
2:E:140:SER:HB2	3:F:92:LYS:HB2	1.78	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
5:R:58:A:O2'	5:R:60:U:OP2	2.14	0.64
4:P:487:GLY:HA3	4:P:532:LEU:HA	1.80	0.64
1:A:351:SER:O	1:A:355:ASN:ND2	2.23	0.64
4:M:210:ASP:OD2	4:N:3:ARG:NH2	2.31	0.63
1:A:5:LEU:O	1:A:216:ARG:NH1	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
4:N:229:GLN:HE22	4:N:557:LYS:H	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ARG:NH1	1:A:395:ASP:OD1	2.32	0.63
4:O:493:ASP:HB3	4:O:496:MET:HB3	1.81	0.63
4:N:144:ARG:HG3	4:N:540:VAL:HG21	1.81	0.63
1:A:141:ASN:HD22	1:A:149:PRO:HA	1.64	0.62
4:O:201:LYS:HE2	4:O:238:GLU:HB2	1.79	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:N:499:ALA:O	4:N:503:VAL:HG13	1.98	0.62
4:M:508:GLU:OE2	4:M:511:GLN:NE2	2.32	0.62
1:D:439:MET:HE2	1:D:440:PRO:HD2	1.82	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
5:R:9:A:O2'	5:R:10:G:N7	2.32	0.62
4:O:390:VAL:HG22	4:O:391:ASP:H	1.64	0.62
2:H:100:VAL:HB	2:H:122:ALA:HB3	1.81	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
1:G:148:VAL:HG22	1:G:150:GLY:H	1.63	0.62
2:B:305:ARG:NH2	2:B:331:GLU:OE1	2.31	0.62
1:A:157:ALA:HB1	1:A:184:THR:HG21	1.80	0.62
2:E:12:HIS:HB2	2:E:193:ARG:HG3	1.82	0.62
4:O:77:ARG:HH21	5:S:34:G:H1	1.45	0.62
1:J:326:ARG:NH1	2:K:87:PRO:O	2.33	0.61
2:E:127:ASP:OD2	2:E:193:ARG:NH2	2.33	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
4:M:561:ALA:HB3	4:N:185:THR:HG21	1.82	0.61
1:G:61:ARG:HG3	1:G:70:LEU:HB3	1.82	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
4:O:590:ALA:O	4:P:578:ARG:NH1	2.34	0.61
1:G:32:ILE:HD12	1:G:42:PHE:HE2	1.64	0.61
4:P:131:ASP:OD1	4:P:134:ARG:NH1	2.33	0.61
2:H:73:GLN:HG2	2:H:282:VAL:HG22	1.81	0.61
4:O:177:ARG:NH1	4:O:221:ASP:O	2.34	0.61
4:N:357:VAL:HG11	4:N:384:LEU:HD21	1.82	0.61
1:A:346:ALA:C	1:A:348:GLY:HA3	2.21	0.61
2:K:32:ALA:O	2:K:145:ASN:ND2	2.34	0.61
4:O:170:ARG:HH21	4:P:567:GLN:HB3	1.66	0.61
4:M:574:GLY:HA2	4:M:577:LEU:HD12	1.83	0.61
2:B:44:MET:HG3	2:B:45:PRO:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:338:GLU:HG3	3:L:16:ARG:HH21	1.66	0.61
2:E:249:ARG:NH1	2:E:258:THR:O	2.34	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
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:H:17:THR:O	2:H:27:THR:OG1	2.10	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
4:N:353:ALA:HB3	4:N:397:PHE:HB2	1.83	0.60
4:M:320:ARG:HG3	4:M:405:VAL:HG11	1.84	0.60
3:F:78:THR:HG23	3:F:79:ILE:HG13	1.83	0.60
3:C:5:ARG:HD2	3:C:24:LEU:HD13	1.82	0.60
2:K:188:ALA:O	5:Q:73:G:O2'	2.18	0.60
2:H:21:ILE:HB	2:H:150:PRO:HB3	1.82	0.60
4:O:369:SER:HB3	4:O:372:VAL:HG23	1.83	0.60
2:K:250:LEU:HD23	2:K:261:MET:HB2	1.84	0.60
2:K:73:GLN:HG2	2:K:282:VAL:HG22	1.83	0.60
4:O:195:GLN:OE1	4:O:220:ARG:HG3	2.01	0.60
3:F:5:ARG:HB2	3:F:24:LEU:HD21	1.82	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
4:M:219:PHE:HZ	4:N:167:ILE:HD12	1.67	0.59
3:F:84:GLU:HG3	3:F:89:LEU:HD11	1.83	0.59
2:K:378:ARG:O	2:K:382:ASN:ND2	2.34	0.59
5:Q:58:A:O2'	5:Q:60:U:OP2	2.19	0.59
4:P:344:VAL:HG21	4:P:352:LEU:HB2	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:H:355:LEU:HA	2:H:360:LEU:HD11	1.84	0.59
2:E:146:ARG:NH2	2:E:190:GLY:O	2.36	0.59
2:K:360:LEU:HD12	2:K:366:PRO:HG2	1.82	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:E:197:ASN:HB3	2:E:211:ARG:HD3	1.85	0.59
4:P:229:GLN:HE22	4:P:557:LYS:H	1.50	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

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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:J:141:ASN:HD22	1:J:149:PRO:HA	1.67	0.58
1:D:441:ALA:HB2	1:D:451:VAL:HG23	1.85	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
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
2:E:398:ASN:OD1	2:E:399:GLY:N	2.37	0.58
2:B:387:LYS:HG3	2:B:454:UNK:HA	1.85	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:O:201:LYS:HG2	4:O:212:TYR:HE2	1.69	0.57
4:M:407:ASP:OD1	4:M:408:ALA:N	2.36	0.57
3:F:82:ALA:HB1	3:F:89:LEU:HB2	1.86	0.57
1:J:398:LEU:HG	1:J:453:LEU:HB3	1.87	0.57
1:J:345:ARG:NH1	3:L:15:ALA:O	2.37	0.57
2:K:342:LEU:HD23	2:K:380:LYS:HE3	1.85	0.57
1:J:236:SER:O	3:L:61:ARG:NE	2.29	0.57
4:P:11:ASN:OD1	4:P:12:GLU:N	2.34	0.57
3:I:8:VAL:HG21	3:I:28:THR:HG22	1.86	0.57
1:D:361:THR:HG23	2:E:271:ARG:HH11	1.68	0.57
1:D:104:THR:HG21	1:D:197:SER:HB2	1.87	0.57
4:M:434:ASP:HB3	4:M:471:LEU:HD23	1.86	0.57
4:M:42:ARG:HH21	4:N:161:LEU:HB2	1.70	0.57
1:G:345:ARG:HB3	3:I:17:LEU:HD23	1.85	0.57
4:O:344:VAL:HG21	4:O:352:LEU:HB2	1.86	0.57
1:J:336:ASN:H	1:J:339:ASP:HB3	1.69	0.57
1:A:198:ARG:NH2	1:A:206:SER:O	2.38	0.57
4:P:79:ARG:HG3	4:P:80:PRO:HD2	1.87	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
1:A:178:ARG:NH2	1:A:430:ASN:OD1	2.38	0.57
1:A:7:LEU:HD23	1:A:10:ILE:HD12	1.87	0.57
4:P:506:ILE:O	4:P:506:ILE:HD12	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
4:O:576:ALA:HA	4:O:579:GLU:HG2	1.87	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
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
5:T:58:A:O2'	5:T:60:U:OP2	2.22	0.56
1:D:351:SER:O	1:D:355:ASN:ND2	2.25	0.56
1:D:274:ILE:HD12	1:D:449:VAL:HG11	1.86	0.56
4:N:334:ARG:HD2	4:N:335:SER:N	2.20	0.56
4:M:77:ARG:HH21	5:Q:34:G:H1	1.52	0.56
4:O:219:PHE:HZ	4:P:167:ILE:HD12	1.71	0.56
4:N:273:MET:HE2	4:N:277:GLU:HG2	1.88	0.56
2:H:7:ILE:HG22	2:H:198:VAL:HG13	1.87	0.56
4:P:367:LEU:HD12	4:P:380:LEU:HD23	1.86	0.56
4:P:121:GLU:O	4:P:125:LEU:HD13	2.06	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:575:LYS:O	4:P:578:ARG:HG2	2.05	0.56
4:P:144:ARG:HG3	4:P:540:VAL:HG21	1.88	0.56
4:O:4:SER:HB3	4:O:20:THR:H	1.69	0.56
1:G:178:ARG:HH11	1:G:178:ARG:HB2	1.70	0.56
4:N:330:ALA:HA	4:N:394:ILE:HG13	1.88	0.56
4:M:4:SER:HB3	4:M:20:THR:H	1.70	0.56
2:K:123:HIS:NE2	2:K:153:GLU:OE1	2.38	0.56
1:J:354:LYS:HG3	3:L:17:LEU:HD23	1.88	0.56
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
1:A:455:ALA:HB2	1:A:463:LEU:HD13	1.88	0.55
4:P:320:ARG:HG3	4:P:405:VAL:HG11	1.87	0.55
2:E:344:ALA:O	2:E:348:MET:HG3	2.05	0.55
4:M:225:ARG:HD2	4:M:227:ASP:H	1.71	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:356:LYS:NZ	4:P:394:ILE:HD11	2.22	0.55
4:P:184:ARG:O	4:P:581:HIS:NE2	2.37	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: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
1:A:69:LEU:HD21	1:A:223:LEU:HB3	1.88	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
3:C:84:GLU:HB2	3:C:89:LEU:HD21	1.90	0.54
1:A:258:ARG:NH1	1:A:393:GLU:O	2.41	0.54
2:K:382:ASN:HD22	2:K:383:THR:HG23	1.71	0.54
2:E:177:VAL:HG13	2:E:182:ILE:HB	1.89	0.54
4:N:131:ASP:OD1	4:N:134:ARG:NH1	2.40	0.54
2:H:230:GLU:HG3	2:H:234:GLN:HE21	1.71	0.54
1:G:265:TYR:HD2	1:G:400:PRO:HD2	1.72	0.54
1:G:141:ASN:HD21	1:G:143:TRP:HB2	1.72	0.54
4:O:79:ARG:NE	4:O:94:GLU:HG3	2.21	0.54
1:D:278:VAL:HG22	1:D:451:VAL:HG22	1.88	0.54
4:N:121:GLU:O	4:N:125:LEU:HD13	2.08	0.54
1:G:144:SER:OG	1:G:147:ARG:NE	2.40	0.54
3:F:71:ASP:O	3:F:76:TYR:OH	2.25	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
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
1:A:185:ASN:HB2	1:A:448:PRO:HB3	1.89	0.54
4:P:50:PHE:CE2	4:P:97:GLY:HA3	2.43	0.54
4:M:344:VAL:HG21	4:M:352:LEU:HB2	1.89	0.54
4:P:177:ARG:HB2	4:P:221:ASP:HB3	1.90	0.54
2:K:378:ARG:HG3	2:K:382:ASN:HD21	1.73	0.54
4:M:451:HIS:HD2	4:M:453:PHE:HB2	1.73	0.53
4:N:401:LYS:O	4:N:405:VAL:HG12	2.08	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
2:B:73:GLN:HG2	2:B:282:VAL:HG22	1.89	0.53
4:N:252:GLU:HG2	4:N:256:ARG:HE	1.74	0.53
2:H:345:ASN:HD21	5:S:54:U:H5"	1.72	0.53
4:M:585:ARG:HH22	4:N:578:ARG:HG2	1.72	0.53
1:D:254:LEU:HD13	1:D:288:LEU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ARG:HB2	1:D:395:ASP:H	1.74	0.53
4:P:456:PRO:O	4:P:473:ARG:NH1	2.42	0.53
2:E:79:LYS:HB3	2:E:91:GLN:HB3	1.90	0.53
1:G:77:LYS:NZ	1:G:152:SER:O	2.41	0.53
4:O:197:PRO:O	4:O:201:LYS:HG3	2.09	0.53
2:B:236:GLU:OE1	4:N:585:ARG:HD2	2.07	0.53
4:M:121:GLU:O	4:M:125:LEU:HD13	2.09	0.53
2:H:12:HIS:NE2	2:H:153:GLU:OE2	2.42	0.53
1:D:143:TRP:CH2	1:D:479:ARG:HB3	2.43	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
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
1:D:245:ASP:OD1	1:D:245:ASP:N	2.39	0.52
2:K:79:LYS:HB3	2:K:91:GLN:HB3	1.91	0.52
4:P:198:GLN:HG3	4:P:199:LEU:H	1.75	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
1:G:381:ARG:NH2	3:I:57:GLU:OE2	2.40	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
2:H:216:ASN:O	2:H:216:ASN:ND2	2.42	0.52
5:Q:47:U:O2'	5:Q:50:C:OP1	2.27	0.52
4:P:401:LYS:O	4:P:405:VAL:HG12	2.09	0.52
4:P:252:GLU:HG2	4:P:256:ARG:HE	1.73	0.52
1:J:441:ALA:HB2	1:J:451:VAL:HG13	1.92	0.52
4:N:77:ARG:NE	4:N:94:GLU:OE2	2.40	0.52
1:G:162:ALA:O	1:G:163:ARG:HG2	2.08	0.52
1:D:382:LEU:HD12	3:F:49:VAL:HG21	1.92	0.52
2:K:100:VAL:HB	2:K:122:ALA:HB3	1.90	0.52
1:G:437:LEU:HD12	1:G:453:LEU:HD11	1.91	0.52
4:O:341:THR:HG22	4:O:352:LEU:HB3	1.92	0.52
2:K:94:GLN:O	2:K:121:ARG:NH2	2.43	0.52
2:H:281:VAL:HG13	3:I:61:ARG:HH21	1.75	0.52
1:D:82:THR:HG22	1:D:106:VAL:HG11	1.92	0.52
1:D:31:ARG:HH11	1:D:163:ARG:HD2	1.74	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)
2:K:108:THR:HA	2:K:114:THR:HG23	1.91	0.52
1:G:274:ILE:HG23	1:G:449:VAL:HG11	1.92	0.52
4:O:79:ARG:HG3	4:O:80:PRO:HD2	1.91	0.51
1:J:198:ARG:HH12	1:J:203:ALA:HB2	1.73	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
1:G:325:VAL:HG23	3:I:90:VAL:HG21	1.92	0.51
1:G:41:SER:O	1:G:120:LEU:HD22	2.11	0.51
1:J:204:TYR:OH	1:J:356:ARG:NH1	2.36	0.51
2:E:232:GLN:OE1	4:P:585:ARG:NH1	2.42	0.51
4:N:456:PRO:O	4:N:473:ARG:NH1	2.43	0.51
4:P:220:ARG:HH22	4:P:228:ARG:HD3	1.76	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
1:G:441:ALA:HB2	1:G:451:VAL:HG23	1.92	0.51
4:M:514:LYS:HG3	4:M:515:PHE:CE2	2.46	0.51
4:M:170:ARG:HG2	4:M:171:PRO:HD2	1.92	0.51
1:A:403:PRO:HD3	1:A:425:TYR:CE1	2.46	0.51
4:N:501:PHE:CD1	4:N:506:ILE:HD11	2.45	0.51
4:N:198:GLN:O	4:N:201:LYS:HG2	2.11	0.51
4:O:487:GLY:HA3	4:O:532:LEU:HA	1.92	0.51
1:G:330:ARG:NH1	1:G:331:CYS:O	2.43	0.51
5:T:23:A:H2'	5:T:24:G:C8	2.46	0.51
3:C:8:VAL:HG21	3:C:28:THR:HG22	1.92	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:P:182:PRO:HB2	4:P:580:LEU:HG	1.92	0.51
4:M:370:PRO:HA	4:M:373:LYS:HE2	1.92	0.51
4:P:369:SER:HB3	4:P:372:VAL:HG23	1.93	0.51
2:H:170:VAL:HG21	2:H:223:ILE:HD13	1.93	0.51
1:G:79:LEU:HD22	1:G:171:THR:HG21	1.92	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
2:B:177:VAL:HG11	2:B:183:CYS:HB3	1.93	0.51
4:O:201:LYS:HG2	4:O:212:TYR:CE2	2.46	0.50
4:M:297:ASP:OD1	4:M:320:ARG:NH1	2.43	0.50
1:A:307:TYR:CD1	1:A:427:ILE:HD11	2.45	0.50
1:D:274:ILE:HG23	1:D:449:VAL:HG11	1.92	0.50
2:K:105:LEU:HD22	2:K:107:ILE:HD13	1.92	0.50
2:K:50:VAL:O	3:L:63:ARG:NH1	2.44	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:H:237:LEU:HD11	4:O:590:ALA:HB2	1.94	0.50
4:N:252:GLU:OE2	4:N:256:ARG:NH2	2.44	0.50
2:B:167:VAL:HG13	2:B:220:PHE:HB3	1.94	0.50
4:N:487:GLY:HA3	4:N:532:LEU:HA	1.94	0.50
2:K:230:GLU:HG3	2:K:234:GLN:HE21	1.76	0.50
5:T:52:G:H1	5:T:62:C:H42	1.58	0.50
4:N:574:GLY:O	4:N:578:ARG:HG3	2.11	0.50
4:M:584:LEU:HD21	4:N:190:PHE:CZ	2.46	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:N:30:ASP:O	5:R:38:A:N6	2.43	0.50
2:E:316:ASP:OD1	2:E:316:ASP:N	2.39	0.50
4:N:182:PRO:HB2	4:N:580:LEU:HG	1.92	0.50
4:N:70:VAL:HG12	4:N:102:VAL:HA	1.93	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:557:LYS:HB3	4:M:562:GLY:H	1.75	0.50
4:M:500:VAL:HA	4:M:503:VAL:HG12	1.94	0.50
4:P:421:LYS:HE2	4:P:425:ARG:NH1	2.26	0.50
1:J:368:TYR:HB3	1:J:372:TYR:HD2	1.77	0.50
2:B:32:ALA:O	2:B:145:ASN:ND2	2.43	0.50
5:R:21:A:H2'	5:R:46:G:H1	1.76	0.50
2:B:341:LYS:O	2:B:345:ASN:HB2	2.12	0.50
4:P:4:SER:HB3	4:P:20:THR:H	1.76	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
4:M:514:LYS:HG3	4:M:515:PHE:CD2	2.46	0.50
4:P:79:ARG:NE	4:P:94:GLU:HG3	2.27	0.50
1:A:143:TRP:CZ3	1:A:161:ALA:HB1	2.40	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
4:P:29:ARG:HH11	4:P:29:ARG:HB2	1.77	0.49
2:K:360:LEU:H	2:K:360:LEU:HD22	1.77	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
4:O:411:ALA:O	4:O:414:ILE:HG13	2.13	0.49
4:M:589:LYS:HB3	4:N:578:ARG:HG2	1.92	0.49
2:H:360:LEU:HD13	2:H:360:LEU:H	1.78	0.49
1:A:427:ILE:HG13	1:A:431:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:17:GLN:O	4:P:76:VAL:HG12	2.12	0.49
4:O:198:GLN:HG3	4:O:199:LEU:H	1.76	0.49
4:O:360:ARG:HH12	4:O:390:VAL:HG23	1.78	0.49
3:F:84:GLU:HB2	3:F:89:LEU:HD21	1.93	0.49
1:D:380:ARG:HG2	3:F:52:LEU:HD23	1.94	0.49
4:O:119:VAL:HG23	5:S:11:C:O2'	2.11	0.49
1:J:26:ARG:HG3	1:J:27:THR:N	2.28	0.49
1:D:297:LEU:HB3	1:D:300:MET:HB2	1.95	0.49
4:P:484:LEU:HD21	4:P:542:LEU:HD12	1.94	0.49
2:B:69:ARG:NH1	2:B:70:ILE:O	2.46	0.49
4:N:441:ASN:O	4:N:443:ASP:N	2.44	0.49
4:P:75:LYS:HB2	4:P:98:TYR:HE2	1.78	0.49
1:D:307:TYR:CD1	1:D:427:ILE:HD11	2.48	0.49
4:N:325:ARG:HH21	4:N:327:PRO:HB3	1.78	0.49
1:J:104:THR:HG23	1:J:199:TRP:HE3	1.78	0.49
1:G:75:ALA:H	1:G:165:LEU:HD21	1.78	0.49
4:O:501:PHE:CD1	4:O:506:ILE:HD11	2.47	0.49
2:K:247:GLU:OE2	2:K:249:ARG:NH2	2.45	0.49
2:B:297:GLU:HG2	2:B:324:ARG:HH12	1.78	0.49
4:M:307:PHE:HD1	4:M:307:PHE:O	1.96	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: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
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
4:M:182:PRO:HB2	4:M:580:LEU:HG	1.93	0.49
1:A:48:ASP:OD1	1:A:48:ASP:N	2.46	0.49
1:G:143:TRP:NE1	1:G:483:GLY:O	2.46	0.49
1:G:69:LEU:H	1:G:69:LEU:HD23	1.78	0.49
4:M:373:LYS:HD2	4:M:373:LYS:H	1.77	0.48
4:N:11:ASN:OD1	4:N:12:GLU:N	2.41	0.48
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
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
4:M:198:GLN:HG3	4:M:199:LEU:H	1.77	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: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:D:143:TRP:CD1	1:D:448:PRO:HG3	2.48	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:A:331:CYS:SG	1:A:343:ARG:NE	2.64	0.48
2:K:333:VAL:HG13	2:K:376:ILE:HG21	1.95	0.48
4:M:585:ARG:HD3	4:N:583:ARG:HB3	1.94	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
2:B:117:ILE:HG21	2:B:169:TYR:CD1	2.49	0.48
4:N:321:VAL:HG13	4:N:399:ALA:HB2	1.94	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
1:J:304:ILE:HG13	1:J:305:PRO:CD	2.43	0.48
1:D:28:LEU:O	1:D:32:ILE:HG12	2.13	0.48
1:G:437:LEU:HD11	1:G:439:MET:HG3	1.95	0.48
4:N:280:ARG:NH2	4:N:281:ARG:HE	2.12	0.48
1:G:320:SER:HA	1:G:345:ARG:HH21	1.77	0.48
1:G:236:SER:HB3	3:I:61:ARG:HD2	1.95	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:441:ALA:HB2	1:A:451:VAL:HG23	1.94	0.48
3:F:71:ASP:HB2	3:F:76:TYR:CE1	2.49	0.48
1:A:74:ILE:HG12	1:A:114:ALA:HB1	1.95	0.48
4:O:252:GLU:OE2	4:O:256:ARG:NH2	2.47	0.48
4:O:70:VAL:HG12	4:O:102:VAL:HA	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
1:A:304:ILE:HD11	1:A:424:ILE:HG23	1.95	0.48
4:M:153:ARG:HH22	4:N:152:ARG:HB3	1.78	0.47
4:O:224:LEU:HD21	4:O:230:PRO:HD3	1.96	0.47
4:N:515:PHE:O	4:N:519:LEU:HG	2.13	0.47
2:K:179:TYR:CZ	2:K:299:PRO:HB3	2.49	0.47
2:B:249:ARG:HD2	2:B:258:THR:HG22	1.96	0.47
4:P:557:LYS:HG2	4:P:563:ASP:HB3	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
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
2:E:42:LEU:HD12	2:E:144:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:401:LYS:O	4:O:405:VAL:HG12	2.13	0.47
3:L:5:ARG:HB2	3:L:24:LEU:HD21	1.96	0.47
4:N:229:GLN:HE22	4:N:557:LYS:N	2.12	0.47
4:N:181:VAL:HB	4:N:191:PHE:HB2	1.96	0.47
1:J:7:LEU:HD22	1:J:72:ALA:HB1	1.97	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:G:172:ASP:HB2	1:G:177:ILE:HD12	1.97	0.47
4:M:515:PHE:O	4:M:519:LEU:HG	2.14	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
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
2:H:339:ASP:HB3	2:H:342:LEU:HG	1.97	0.47
4:O:42:ARG:NH2	4:P:161:LEU:HD13	2.29	0.47
4:N:357:VAL:HG22	4:N:393:ASP:O	2.14	0.47
4:N:129:PHE:CD1	4:N:130:ILE:HG23	2.50	0.47
5:T:67:C:H2'	5:T:68:G:C8	2.50	0.47
4:N:225:ARG:HB2	4:N:228:ARG:HD2	1.97	0.47
1:D:346:ALA:HB2	3:F:18:GLY:HA3	1.96	0.47
4:P:340:TYR:CZ	4:P:416:VAL:HG22	2.49	0.47
2:B:117:ILE:HD11	2:B:160:ILE:HA	1.95	0.47
1:J:178:ARG:NE	1:J:190:LYS:HD3	2.30	0.47
1:G:32:ILE:HD13	1:G:164:LEU:HD23	1.97	0.47
4:M:401:LYS:O	4:M:405:VAL:HG12	2.14	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:427:ILE:HG13	1:G:431:LEU:HD13	1.97	0.47
4:N:344:VAL:HG21	4:N:352:LEU:HB2	1.97	0.47
2:H:105:LEU:HB2	2:H:119:ILE:HD11	1.97	0.47
4:O:557:LYS:HG2	4:O:563:ASP:HB3	1.97	0.47
4:M:337:ILE:O	4:M:341:THR:HG23	2.15	0.47
2:K:368:SER:H	2:K:371:GLN:HE21	1.62	0.47
4:P:321:VAL:HG13	4:P:399:ALA:HB2	1.95	0.47
4:O:246:ASP:O	4:O:250:ILE:HD13	2.15	0.47
2:E:230:GLU:HG3	2:E:234:GLN:HE21	1.79	0.47
1:J:77:LYS:HG2	1:J:79:LEU:H	1.80	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
2:E:93:SER:OG	2:E:94:GLN:N	2.46	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)
4:N:273:MET:HE1	4:N:282:TYR:CE2	2.50	0.46
4:M:400:ASP:OD1	4:M:401:LYS:N	2.39	0.46
4:N:201:LYS:HE3	4:N:238:GLU:OE1	2.15	0.46
4:M:510:GLU:O	4:M:514:LYS:HG2	2.15	0.46
5:T:67:C:H2'	5:T:68:G:H8	1.81	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:O:131:ASP:OD1	4:O:134:ARG:NH1	2.48	0.46
1:A:278:VAL:HG21	1:A:400:PRO:HB3	1.97	0.46
2:H:177:VAL:HG13	2:H:182:ILE:HB	1.96	0.46
4:N:548:SER:OG	4:N:550:ARG:HG2	2.14	0.46
3:L:77:GLN:HG2	3:L:83:VAL:HG21	1.96	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
4:M:453:PHE:O	4:M:491:ILE:HG12	2.14	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:G:254:LEU:HD21	1:G:466:VAL:HG23	1.97	0.46
4:O:353:ALA:HB1	4:O:371:ILE:HD13	1.96	0.46
4:M:113:LEU:HD21	4:M:133:ARG:CB	2.45	0.46
4:P:251:THR:OG1	4:P:532:LEU:HD21	2.15	0.46
4:O:506:ILE:HD12	4:O:506:ILE:O	2.15	0.46
1:J:152:SER:H	1:J:176:SER:HB3	1.80	0.46
1:A:127:MET:SD	1:A:353:VAL:HA	2.55	0.46
1:J:241:GLN:HA	1:J:242:PRO:HD3	1.79	0.46
1:D:189:ILE:HD11	1:D:460:GLU:HB3	1.98	0.46
1:A:172:ASP:HA	1:A:176:SER:HB2	1.97	0.46
2:K:3:TRP:CZ2	2:K:235:ILE:HG23	2.50	0.46
2:K:78:ARG:HD2	2:K:273:PHE:CZ	2.51	0.46
1:A:202:ILE:HG12	2:B:45:PRO:HB2	1.98	0.46
2:E:394:GLU:O	2:E:398:ASN:ND2	2.49	0.46
2:K:347:VAL:HA	2:K:351:LEU:HD21	1.97	0.46
2:B:170:VAL:HG21	2:B:223:ILE:HD13	1.97	0.46
4:P:451:HIS:CG	4:P:452:PRO:HD2	2.51	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
1:G:25:THR:HA	1:G:28:LEU:HG	1.97	0.46
4:P:510:GLU:O	4:P:514:LYS:HG2	2.15	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

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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:O:299:ALA:HB2	4:O:321:VAL:HG13	1.98	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
2:H:279:LEU:HD22	3:I:58:ALA:HB3	1.98	0.46
4:P:341:THR:HG22	4:P:352:LEU:HB3	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
2:H:383:THR:HG21	2:H:388:LEU:HD22	1.97	0.46
4:P:375:ILE:HG23	4:P:380:LEU:HD11	1.97	0.46
3:L:71:ASP:OD2	3:L:72:HIS:N	2.49	0.46
1:G:120:LEU:HD11	1:G:156:SER:N	2.30	0.46
4:P:376:PRO:O	4:P:380:LEU:HD13	2.16	0.46
1:D:130:SER:HB3	1:D:407:TRP:CH2	2.49	0.46
1:J:460:GLU:O	1:J:463:LEU:HG	2.15	0.46
2:E:179:TYR:CZ	2:E:299:PRO:HB3	2.50	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
1:J:440:PRO:HA	1:J:450:GLY:HA2	1.98	0.46
2:K:170:VAL:HG21	2:K:223:ILE:HD13	1.97	0.46
1:J:349:PHE:CG	1:J:350:GLY:N	2.84	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
4:N:307:PHE:HD1	4:N:308:LYS:N	2.13	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
4:M:353:ALA:HB3	4:M:397:PHE:HB2	1.98	0.46
1:A:361:THR:HG23	2:B:271:ARG:HH11	1.81	0.46
1:D:321:ARG:HB3	2:E:88:LYS:HA	1.98	0.46
4:N:318:LYS:HA	4:N:318:LYS:HD2	1.60	0.46
4:N:362:LYS:HD2	4:N:362:LYS:HA	1.46	0.46
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
1:A:82:THR:HG22	1:A:106:VAL:HG11	1.98	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:B:347:VAL:HA	2:B:351:LEU:HD21	1.96	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)
4:M:566:THR:O	4:N:170:ARG:HD3	2.15	0.45
1:J:330:ARG:NH1	1:J:331:CYS:O	2.50	0.45
5:S:20:U:H2'	5:S:21:A:H5"	1.98	0.45
1:J:265:TYR:CD2	1:J:399:GLY:HA3	2.50	0.45
4:N:451:HIS:CG	4:N:452:PRO:HD2	2.51	0.45
2:K:85:ASP:OD1	2:K:86:LEU:N	2.50	0.45
4:O:441:ASN:O	4:O:443:ASP:N	2.48	0.45
4:O:153:ARG:HD3	4:O:153:ARG:HA	1.59	0.45
3:C:5:ARG:HH11	3:C:24:LEU:HD13	1.82	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
2:H:347:VAL:HA	2:H:351:LEU:HD21	1.99	0.45
1:G:216:ARG:NH2	1:G:477:HIS:O	2.50	0.45
4:M:35:ILE:HG13	4:M:58:PHE:CZ	2.52	0.45
3:F:80:ALA:HA	3:F:81:PRO:HD3	1.86	0.45
4:N:229:GLN:NE2	4:N:557:LYS:H	2.14	0.45
3:F:6:SER:O	3:F:10:LYS:HG2	2.17	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
2:B:252:ASP:HA	2:B:253:PRO:HD3	1.86	0.45
4:P:514:LYS:HG3	4:P:515:PHE:CE2	2.51	0.45
4:O:371:ILE:HG23	4:O:374:PHE:CE2	2.52	0.45
1:A:160:VAL:HB	1:A:186:LEU:HD11	1.99	0.45
1:J:42:PHE:HA	1:J:120:LEU:HA	1.98	0.45
2:B:344:ALA:O	2:B:348:MET:HG3	2.17	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
1:J:189:ILE:HB	1:J:437:LEU:HD13	1.99	0.45
4:O:466:ASN:OD1	4:O:466:ASN:N	2.48	0.45
4:O:589:LYS:CB	4:P:578:ARG:HB2	2.47	0.45
4:O:367:LEU:O	4:O:372:VAL:HG21	2.17	0.45
4:M:74:GLY:HA2	4:M:98:TYR:HD2	1.82	0.45
1:G:412:LYS:HD2	1:G:418:SER:HB3	1.98	0.45
2:B:355:LEU:O	2:B:359:GLY:HA2	2.16	0.45
1:J:179:GLN:HB3	1:J:180:PRO:HD3	1.98	0.45
4:N:35:ILE:HG13	4:N:58:PHE:CZ	2.52	0.45
1:A:354:LYS:HE2	1:A:354:LYS:HB3	1.72	0.45
1:A:270:LEU:HD11	1:A:274:ILE:HB	1.97	0.45
4:N:320:ARG:HG3	4:N:405:VAL:HG11	1.99	0.45
4:N:29:ARG:HD2	5:R:35:U:O2'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:278:VAL:HG22	1:G:451:VAL:HG22	1.99	0.45
4:N:313:PRO:HA	4:N:316:ASP:HB3	1.99	0.45
4:P:70:VAL:HG12	4:P:102:VAL:HA	1.97	0.45
2:K:341:LYS:O	2:K:345:ASN:HB2	2.17	0.45
1:G:351:SER:O	1:G:355:ASN:ND2	2.31	0.45
1:A:179:GLN:HB3	1:A:180:PRO:HD3	1.99	0.45
3:C:6:SER:O	3:C:10:LYS:HG2	2.17	0.44
2:B:332:LYS:HD3	2:B:369:ALA:HB3	1.99	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
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: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:H:179:TYR:CZ	2:H:299:PRO:HB3	2.52	0.44
1:A:79:LEU:HA	1:A:79:LEU:HD23	1.82	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:K:378:ARG:HA	2:K:382:ASN:OD1	2.18	0.44
1:A:447:LEU:HA	1:A:448:PRO:HD3	1.78	0.44
4:P:340:TYR:HE1	4:P:415:LYS:HZ2	1.66	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:M:75:LYS:HB2	4:M:98:TYR:HE2	1.83	0.44
2:K:350:GLU:HB3	2:K:393:PHE:CE2	2.53	0.44
1:G:179:GLN:HB3	1:G:180:PRO:HD3	1.99	0.44
4:M:47:GLN:NE2	4:M:94:GLU:OE1	2.50	0.44
1:D:339:ASP:O	1:D:343:ARG:HB2	2.17	0.44
5:S:67:C:H2'	5:S:68:G:H8	1.81	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
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
2:B:50:VAL:O	3:C:63:ARG:NH1	2.51	0.44
1:D:74:ILE:HG12	1:D:114:ALA:HB1	1.99	0.44
4:O:154:TYR:CE1	4:O:254:MET:HB2	2.53	0.44
1:G:383:ILE:HA	1:G:386:ASP:OD2	2.17	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
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
1:A:359:VAL:HG11	3:C:34:ILE:HG21	2.00	0.44
2:H:15:LEU:HD21	2:H:152:LEU:HB2	2.00	0.44
2:B:360:LEU:HD12	2:B:366:PRO:HG3	1.99	0.44
4:O:29:ARG:HD2	5:S:35:U:O2'	2.17	0.44
2:K:115:LYS:HA	2:K:115:LYS:HD3	1.80	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: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: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
4:M:313:PRO:HA	4:M:316:ASP:CG	2.38	0.44
2:E:117:ILE:HG21	2:E:169:TYR:CD1	2.52	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
4:M:581:HIS:HA	4:N:585:ARG:HE	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
1:G:368:TYR:HB3	1:G:372:TYR:HD2	1.83	0.44
5:Q:48:C:H2'	5:Q:59:G:H4'	2.00	0.43
2:B:160:ILE:HD11	2:B:165:GLU:C	2.39	0.43
1:D:304:ILE:HD12	1:D:304:ILE:H	1.83	0.43
1:G:162:ALA:O	1:G:164:LEU:HD12	2.18	0.43
4:N:307:PHE:HD1	4:N:308:LYS:H	1.66	0.43
2:E:88:LYS:HD2	2:E:90:TYR:CE1	2.53	0.43
2:E:281:VAL:HA	3:F:60:GLN:HB3	2.00	0.43
2:K:344:ALA:O	2:K:348:MET:HG2	2.18	0.43
1:G:293:LYS:HD3	1:G:294:ASP:H	1.83	0.43
4:N:295:LEU:HD21	4:N:409:LEU:HB3	1.99	0.43
1:D:79:LEU:HA	1:D:79:LEU:HD23	1.83	0.43
2:E:243:LYS:HB3	2:E:243:LYS:HE2	1.75	0.43
4:O:589:LYS:HB3	4:P:578:ARG:HB2	2.00	0.43
2:E:341:LYS:O	2:E:345:ASN:HB2	2.17	0.43
4:M:251:THR:OG1	4:M:532:LEU:HD21	2.18	0.43
5:S:67:C:H2'	5:S:68:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:TYR:CZ	2:E:45:PRO:HD3	2.52	0.43
4:P:120:GLY:O	4:P:123:THR:OG1	2.34	0.43
4:N:111:PHE:HA	4:N:112:PRO:HD3	1.67	0.43
1:J:142:PRO:HB2	1:J:143:TRP:CE3	2.53	0.43
4:N:108:THR:HA	4:N:109:PRO:HD2	1.86	0.43
1:J:72:ALA:HA	1:J:73:PRO:HD3	1.83	0.43
4:O:300:ASP:OD1	4:O:301:GLN:HG3	2.18	0.43
4:M:541:MET:HA	4:M:552:VAL:HG11	2.00	0.43
4:M:375:ILE:HA	4:M:376:PRO:HD2	1.82	0.43
2:E:363:GLU:OE2	2:E:363:GLU:N	2.51	0.43
4:M:303:LYS:HG2	4:M:303:LYS:H	1.62	0.43
1:G:163:ARG:HD2	1:G:480:THR:HB	1.99	0.43
2:K:20:LYS:O	3:L:63:ARG:NH2	2.41	0.43
3:C:54:HIS:HA	3:C:55:PRO:HD3	1.90	0.43
1:A:144:SER:OG	1:A:146:ASP:OD1	2.36	0.43
4:N:154:TYR:CE1	4:N:254:MET:HB2	2.53	0.43
1:J:82:THR:OG1	1:J:85:VAL:HB	2.19	0.43
4:O:445:SER:OG	4:O:446:LEU:N	2.52	0.43
4:N:54:ARG:HA	4:N:54:ARG:HD2	1.70	0.43
1:A:141:ASN:HA	1:A:142:PRO:HD3	1.92	0.43
2:H:83:TYR:CG	2:H:84:PRO:HD2	2.54	0.43
1:G:327:TYR:CZ	2:H:45:PRO:HD3	2.54	0.43
4:O:589:LYS:HG3	4:O:590:ALA:N	2.29	0.43
2:K:299:PRO:HA	2:K:302:LYS:HG2	1.99	0.43
2:B:98:PRO:HB3	2:B:121:ARG:HH21	1.82	0.43
3:F:54:HIS:HA	3:F:55:PRO:HD3	1.88	0.43
2:K:316:ASP:HA	2:K:319:VAL:HG22	2.00	0.43
2:K:59:ALA:HB1	2:K:99:ILE:HG21	2.00	0.43
2:E:254:ASN:OD1	2:E:255:LYS:N	2.52	0.43
4:P:229:GLN:HE22	4:P:557:LYS:N	2.16	0.43
4:M:275:PHE:CD2	4:M:436:PRO:HD3	2.53	0.43
2:H:123:HIS:NE2	2:H:153:GLU:OE1	2.51	0.43
1:D:185:ASN:HB2	1:D:448:PRO:HB3	2.01	0.43
2:E:346:TRP:O	2:E:350:GLU:HB2	2.19	0.43
4:M:439:GLU:HB2	4:M:449:LEU:HD21	2.01	0.43
2:E:99:ILE:HG22	2:E:100:VAL:HG12	2.00	0.43
1:J:121:ASN:N	1:J:121:ASN:OD1	2.51	0.43
1:A:313:ALA:O	1:A:316:SER:OG	2.20	0.43
4:P:273:MET:HE1	4:P:282:TYR:CD2	2.53	0.43
4:O:42:ARG:NH1	4:P:159:GLY:O	2.44	0.43
4:O:360:ARG:NH1	4:O:390:VAL:HG23	2.33	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:259:ILE:HD13	1:J:285:LEU:HD23	2.00	0.43
4:O:116:TYR:CE2	4:O:118:ASP:HB2	2.53	0.43
1:G:241:GLN:HA	1:G:242:PRO:HD3	1.83	0.43
2:B:204:GLY:HA3	2:K:204:GLY:HA3	1.99	0.43
5:R:67:C:H2'	5:R:68:G:C8	2.54	0.43
1:J:455:ALA:HB1	1:J:459:GLN:OE1	2.18	0.43
1:G:354:LYS:O	1:G:358:MET:HG2	2.19	0.43
1:G:69:LEU:HD12	1:G:72:ALA:HB3	2.00	0.43
2:H:179:TYR:CE1	2:H:299:PRO:HB3	2.54	0.43
4:O:270:PHE:HE2	4:O:477:MET:HE3	1.84	0.43
4:O:56:GLU:H	4:O:56:GLU:HG3	1.54	0.43
2:K:233:ARG:HG3	4:M:588:PRO:O	2.18	0.43
4:O:325:ARG:NH1	4:O:393:ASP:OD2	2.52	0.43
4:O:205:MET:SD	4:O:240:SER:OG	2.72	0.43
2:H:64:LEU:HD11	2:H:288:LEU:HA	2.01	0.43
1:G:36:ASP:HB3	1:G:37:PRO:HD3	2.01	0.43
4:M:108:THR:HA	4:M:109:PRO:HD2	1.87	0.43
2:H:368:SER:HB3	2:H:370:GLU:OE2	2.19	0.43
1:G:179:GLN:NE2	1:G:422:GLU:OE2	2.39	0.42
2:B:93:SER:OG	2:B:94:GLN:N	2.49	0.42
4:O:248:ILE:HD12	4:O:272:HIS:NE2	2.34	0.42
4:M:129:PHE:CD1	4:M:130:ILE:HG23	2.54	0.42
4:M:451:HIS:CG	4:M:452:PRO:HD2	2.53	0.42
1:A:368:TYR:HB3	1:A:372:TYR:CD2	2.54	0.42
4:N:3:ARG:CD	4:N:22:CYS:H	2.28	0.42
1:D:163:ARG:NH2	1:D:483:GLY:HA2	2.34	0.42
2:K:312:LEU:HG	2:K:316:ASP:OD1	2.19	0.42
1:G:336:ASN:OD1	1:G:337:LEU:N	2.49	0.42
1:A:241:GLN:HA	1:A:242:PRO:HD3	1.72	0.42
4:M:441:ASN:O	4:M:443:ASP:N	2.49	0.42
2:K:83:TYR:CG	2:K:84:PRO:HD2	2.54	0.42
1:G:132:GLN:HA	1:G:138:ALA:HB2	2.00	0.42
2:E:316:ASP:HA	2:E:319:VAL:HG12	2.02	0.42
2:K:15:LEU:HB3	2:K:58:MET:HE1	2.01	0.42
4:O:29:ARG:HB2	4:O:36:PHE:HB2	2.01	0.42
1:G:78:ASP:OD2	1:G:119:LYS:HE3	2.19	0.42
4:M:340:TYR:CZ	4:M:416:VAL:HG12	2.54	0.42
2:H:20:LYS:NZ	2:H:147:ALA:O	2.48	0.42
5:R:52:G:H1	5:R:62:C:H42	1.67	0.42
1:G:252:LYS:HB3	1:G:465:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:492:HIS:ND1	4:P:528:PRO:HA	2.34	0.42
4:O:369:SER:HB3	4:O:372:VAL:CG2	2.50	0.42
4:M:57:THR:HG21	4:M:98:TYR:O	2.19	0.42
2:E:29:PHE:HA	2:E:30:GLY:HA3	1.80	0.42
2:K:384:ILE:HG22	2:K:385:SER:H	1.84	0.42
2:H:336:ILE:O	2:H:337:CYS:HB2	2.20	0.42
5:T:47:U:HO2'	5:T:48:C:P	2.42	0.42
1:J:447:LEU:HA	1:J:448:PRO:HD3	1.93	0.42
2:E:119:ILE:HA	2:E:156:SER:HA	2.02	0.42
4:O:504:LEU:O	4:O:504:LEU:HD13	2.20	0.42
1:D:159:ALA:O	1:D:164:LEU:HB2	2.20	0.42
4:P:277:GLU:O	4:P:281:ARG:HG2	2.20	0.42
1:J:178:ARG:HG3	1:J:190:LYS:NZ	2.34	0.42
3:I:80:ALA:HA	3:I:81:PRO:HD3	1.89	0.42
2:K:390:LYS:HE3	5:Q:18:G:C6	2.54	0.42
1:A:104:THR:HG22	1:A:199:TRP:O	2.20	0.42
4:M:115:GLU:H	4:M:115:GLU:HG3	1.48	0.42
1:G:189:ILE:HG13	1:G:464:LEU:HD21	2.02	0.42
1:D:31:ARG:NH1	1:D:163:ARG:HD2	2.35	0.42
2:B:70:ILE:HG23	2:B:99:ILE:O	2.19	0.42
2:K:58:MET:HE2	2:K:182:ILE:HG23	2.02	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
2:K:215:LYS:HB3	2:K:215:LYS:HE2	1.91	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: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: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:H:215:LYS:HB2	2:H:215:LYS:HE2	1.91	0.42
2:B:208:PHE:HE1	5:T:33:U:OP2	2.03	0.42
4:O:367:LEU:HD23	4:O:367:LEU:HA	1.88	0.42
4:N:337:ILE:O	4:N:341:THR:HG23	2.20	0.42
4:P:319:GLY:HA2	4:P:402:ALA:N	2.34	0.42
4:M:207:ALA:HB1	4:N:132:LEU:HB2	2.01	0.42
1:G:131:ASN:ND2	1:G:131:ASN:O	2.51	0.42
1:J:190:LYS:N	1:J:190:LYS:HE2	2.35	0.42
2:E:139:MET:HA	3:F:91:PRO:HA	2.01	0.42
3:C:80:ALA:HA	3:C:81:PRO:HD3	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:68:ALA:HB1	2:E:101:GLY:O	2.19	0.42
1:G:279:LEU:O	1:G:282:VAL:HG22	2.19	0.42
4:M:383:ILE:O	4:M:387:VAL:HG13	2.19	0.42
1:D:338:GLU:OE2	1:D:342:LYS:NZ	2.43	0.42
2:E:130:LYS:NZ	5:T:74:C:OP2	2.36	0.42
2:K:7:ILE:HD11	2:K:160:ILE:HG12	2.01	0.41
1:G:399:GLY:O	1:G:451:VAL:HG13	2.20	0.41
2:B:345:ASN:HD21	5:R:54:U:H4'	1.83	0.41
4:M:113:LEU:HD21	4:M:133:ARG:HB2	2.02	0.41
2:H:164:LYS:HE2	2:H:164:LYS:HB2	1.91	0.41
4:N:3:ARG:HD3	4:N:21:LEU:HA	2.02	0.41
4:P:37:LEU:HD12	4:P:50:PHE:HE1	1.85	0.41
1:G:165:LEU:HA	1:G:166:PRO:HD3	1.87	0.41
4:N:55:ALA:HA	4:N:58:PHE:HB2	2.01	0.41
1:D:265:TYR:HD2	1:D:399:GLY:HA3	1.84	0.41
2:B:12:HIS:NE2	2:B:153:GLU:OE2	2.53	0.41
1:D:337:LEU:HD13	3:F:90:VAL:HG11	2.02	0.41
4:N:74:GLY:HA2	4:N:98:TYR:HD2	1.85	0.41
1:G:177:ILE:HG23	1:G:214:LEU:HD21	2.02	0.41
4:O:319:GLY:HA2	4:O:402:ALA:H	1.83	0.41
4:N:225:ARG:HD3	4:N:225:ARG:HA	1.68	0.41
1:D:338:GLU:HG2	1:D:342:LYS:HD2	2.02	0.41
4:P:463:LEU:HD21	4:P:500:VAL:HG22	2.03	0.41
2:E:32:ALA:HA	2:E:33:PRO:HD3	1.87	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
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
4:M:313:PRO:HA	4:M:316:ASP:OD2	2.20	0.41
1:D:204:TYR:OH	1:D:356:ARG:NH1	2.54	0.41
4:P:383:ILE:O	4:P:387:VAL:HG13	2.19	0.41
3:L:3:LEU:HD22	3:L:31:LEU:HD22	2.03	0.41
1:G:48:ASP:O	1:G:51:ILE:HG13	2.20	0.41
2:E:252:ASP:HA	2:E:253:PRO:HD3	1.83	0.41
4:P:168:LEU:HB3	4:P:191:PHE:CD1	2.54	0.41
2:K:363:GLU:N	2:K:363:GLU:OE2	2.52	0.41
3:L:92:LYS:HD2	3:L:92:LYS:HA	1.68	0.41
1:G:323:ASP:OD1	1:G:325:VAL:HG12	2.20	0.41
1:G:398:LEU:HB3	1:G:453:LEU:HB3	2.01	0.41
4:N:273:MET:CE	4:N:277:GLU:HG2	2.50	0.41
1:G:3:HIS:CE1	1:G:4:GLN:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:79:ARG:HG2	4:M:94:GLU:HG3	2.02	0.41
1:A:61:ARG:HD2	1:A:70:LEU:HD13	2.02	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
2:H:357:LYS:HB3	2:H:357:LYS:HE2	1.84	0.41
4:P:342:LYS:HD2	4:P:342:LYS:HA	1.85	0.41
1:D:444:VAL:HG12	1:D:445:ASP:OD2	2.20	0.41
4:O:93:ILE:HG22	4:O:94:GLU:N	2.35	0.41
1:A:427:ILE:HD12	1:A:430:ASN:HB2	2.03	0.41
4:M:504:LEU:HD13	4:M:504:LEU:O	2.21	0.41
4:N:248:ILE:HG21	4:N:272:HIS:NE2	2.36	0.41
1:A:336:ASN:OD1	1:A:337:LEU:N	2.49	0.41
1:G:459:GLN:OE1	1:G:462:ARG:NH2	2.40	0.41
1:A:382:LEU:HD12	3:C:49:VAL:HG21	2.03	0.41
2:H:201:ARG:HA	2:H:202:PRO:HD3	1.97	0.41
1:D:141:ASN:HA	1:D:142:PRO:HD3	1.93	0.41
4:P:337:ILE:O	4:P:341:THR:HG23	2.21	0.41
4:P:364:VAL:HG13	4:P:372:VAL:HG12	2.03	0.41
4:O:337:ILE:O	4:O:341:THR:HG23	2.21	0.41
4:N:29:ARG:HB2	4:N:36:PHE:HB2	2.03	0.41
4:P:356:LYS:HZ3	4:P:394:ILE:HD11	1.86	0.41
1:D:447:LEU:HA	1:D:448:PRO:HD3	1.94	0.41
2:B:32:ALA:HA	2:B:33:PRO:HD3	1.76	0.41
1:G:433:GLY:HA3	3:I:55:PRO:HB3	2.03	0.41
4:P:359:GLU:OE2	4:P:362:LYS:HG3	2.20	0.41
4:O:342:LYS:HA	4:O:342:LYS:HD2	1.82	0.41
2:H:160:ILE:HD11	2:H:165:GLU:C	2.41	0.41
4:N:341:THR:HG22	4:N:352:LEU:HB3	2.02	0.41
1:J:188:GLY:O	1:J:437:LEU:HD12	2.21	0.41
2:E:20:LYS:HE3	2:E:25:SER:HB2	2.03	0.41
4:O:207:ALA:HB1	4:P:132:LEU:HB2	2.02	0.41
3:C:72:HIS:CE1	3:C:74:ASP:HB2	2.55	0.41
2:E:295:LEU:HA	2:E:296:PRO:HD3	1.82	0.41
2:B:15:LEU:HD11	2:B:152:LEU:HB2	2.02	0.41
4:M:85:ASN:HA	4:M:86:PRO:HD3	1.80	0.41
2:H:346:TRP:CZ2	2:H:389:ALA:HB1	2.55	0.41
4:P:225:ARG:HA	4:P:225:ARG:HD2	1.72	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:P:578:ARG:HB3	4:P:578:ARG:HE	1.49	0.41
1:G:453:LEU:HD12	1:G:463:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:ARG:HH22	1:G:460:GLU:HG3	1.86	0.41
4:N:273:MET:HA	4:N:274:PRO:HD3	1.94	0.41
5:R:55:U:N3	5:R:58:A:OP2	2.36	0.41
1:A:159:ALA:O	1:A:164:LEU:HB2	2.21	0.41
4:P:325:ARG:HD2	4:P:389:ALA:HA	2.03	0.41
1:D:31:ARG:HH11	1:D:163:ARG:HH11	1.67	0.41
2:B:99:ILE:HG22	2:B:100:VAL:HG12	2.02	0.41
4:M:252:GLU:OE2	4:M:256:ARG:NH2	2.54	0.41
2:K:371:GLN:H	2:K:371:GLN:HG2	1.53	0.41
1:A:104:THR:HG21	1:A:197:SER:HB3	2.03	0.41
4:N:455:SER:HB3	4:N:489:ILE:HG23	2.02	0.41
2:E:83:TYR:CG	2:E:84:PRO:HD2	2.56	0.41
4:M:475:TYR:CE2	4:M:488:SER:HA	2.56	0.41
4:P:154:TYR:CE1	4:P:254:MET:HB2	2.56	0.41
2:K:332:LYS:O	2:K:336:ILE:HG13	2.21	0.41
1:J:258:ARG:H	1:J:258:ARG:HG2	1.66	0.41
1:A:412:LYS:HD2	1:A:418:SER:HB2	2.02	0.41
2:H:320:LEU:HD21	2:H:330:PHE:CG	2.56	0.41
2:B:342:LEU:HD23	2:B:380:LYS:NZ	2.35	0.41
1:A:36:ASP:N	1:A:37:PRO:HD2	2.36	0.41
1:G:191:PRO:HG2	1:G:210:GLN:HG3	2.03	0.41
1:D:241:GLN:HA	1:D:242:PRO:HD3	1.73	0.41
4:O:541:MET:HA	4:O:552:VAL:HG11	2.02	0.41
4:O:353:ALA:HB3	4:O:397:PHE:HB2	2.03	0.41
1:J:284:GLU:O	1:J:287:THR:OG1	2.27	0.41
1:A:94:LEU:HD13	1:A:322:PHE:HE2	1.85	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: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:G:5:LEU:HD13	1:G:10:ILE:HG12	2.02	0.41
4:O:570:GLY:HA3	4:P:170:ARG:NH1	2.35	0.41
1:D:36:ASP:N	1:D:37:PRO:HD2	2.36	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
4:M:201:LYS:HE3	4:M:238:GLU:OE1	2.20	0.40
1:G:254:LEU:HD13	1:G:288:LEU:HB3	2.03	0.40
3:F:7:ASP:HA	3:F:10:LYS:HE2	2.04	0.40
4:M:108:THR:HG21	5:Q:27:A:H4'	2.03	0.40
2:K:390:LYS:HA	2:K:390:LYS:HD3	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:300:ASP:OD1	4:N:301:GLN:N	2.54	0.40
4:O:340:TYR:OH	4:O:419:ASP:OD2	2.39	0.40
3:L:54:HIS:HA	3:L:55:PRO:HD3	1.89	0.40
4:O:33:GLY:HA3	5:S:33:U:C6	2.56	0.40
4:N:492:HIS:ND1	4:N:528:PRO:HA	2.36	0.40
4:N:357:VAL:HB	4:N:360:ARG:NH1	2.36	0.40
1:J:44:SER:HB2	1:J:86:ARG:HE	1.85	0.40
1:G:265:TYR:CD2	1:G:399:GLY:HA3	2.56	0.40
1:A:82:THR:O	1:A:99:SER:OG	2.39	0.40
1:J:82:THR:HA	1:J:102:ASP:OD1	2.22	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:74:ILE:O	1:J:116:THR:HA	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:P:589:LYS:HE3	4:P:589:LYS:HB2	1.91	0.40
4:M:585:ARG:HH21	4:N:578:ARG:HA	1.86	0.40
4:P:252:GLU:CD	4:P:270:PHE:HB2	2.41	0.40
2:H:164:LYS:H	2:H:164:LYS:HD3	1.85	0.40
4:N:492:HIS:CE1	4:N:528:PRO:HB3	2.56	0.40
1:G:415:ASP:HA	1:G:416:PRO:HD3	1.89	0.40
1:J:202:ILE:HG12	2:K:45:PRO:HB2	2.03	0.40
2:B:78:ARG:HD2	2:B:273:PHE:CZ	2.56	0.40
2:K:320:LEU:HD21	2:K:330:PHE:CG	2.57	0.40
1:G:176:SER:OG	1:G:176:SER:O	2.39	0.40
1:J:190:LYS:H	1:J:190:LYS:HE2	1.87	0.40
2:K:7:ILE:HB	2:K:198:VAL:HG12	2.03	0.40
1:A:427:ILE:HA	1:A:427:ILE:HD12	1.82	0.40
4:P:111:PHE:HE1	4:P:127:TYR:HB2	1.86	0.40
4:O:343:PHE:CZ	4:O:415:LYS:HG3	2.56	0.40
1:J:186:LEU:O	1:J:440:PRO:HD3	2.21	0.40
1:G:336:ASN:HD21	3:I:95:GLU:HB2	1.86	0.40
4:P:492:HIS:CE1	4:P:528:PRO:HB3	2.57	0.40
4:P:51:ASP:N	4:P:52:PRO:HD3	2.36	0.40
4:N:383:ILE:O	4:N:387:VAL:HG13	2.22	0.40
2:B:58:MET:HE3	2:B:182:ILE:HA	2.04	0.40
1:J:187:THR:HG22	1:J:439:MET:HG2	2.02	0.40
1:D:130:SER:OG	1:D:132:GLN:OE1	2.33	0.40
4:O:252:GLU:HG2	4:O:256:ARG:HE	1.85	0.40
2:B:303:ARG:O	2:B:307:GLU:HG2	2.21	0.40
4:M:290:ARG:HB3	4:M:423:LEU:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:56:ALA:HA	1:J:59:GLU:HG2	2.03	0.40
3:I:10:LYS:HB3	3:I:10:LYS:HE2	1.95	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%)	34	77
2	E	395/481 (82%)	362 (92%)	33 (8%)	0	100	100
2	H	395/481 (82%)	360 (91%)	34 (9%)	1 (0%)	46	83
2	K	395/481 (82%)	357 (90%)	37 (9%)	1 (0%)	46	83
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%)	46	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	N	587/599 (98%)	541 (92%)	44 (8%)	2 (0%)	46 83
4	O	587/599 (98%)	543 (92%)	43 (7%)	1 (0%)	52 87
4	P	587/599 (98%)	542 (92%)	43 (7%)	2 (0%)	46 83
All	All	6228/6672 (93%)	5752 (92%)	465 (8%)	11 (0%)	52 87

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%)	52 83
1	D	377/378 (100%)	364 (97%)	13 (3%)	44 79
1	G	377/378 (100%)	361 (96%)	16 (4%)	36 75
1	J	377/378 (100%)	359 (95%)	18 (5%)	31 72
2	B	329/333 (99%)	319 (97%)	10 (3%)	48 81
2	E	329/333 (99%)	325 (99%)	4 (1%)	78 91
2	H	329/333 (99%)	324 (98%)	5 (2%)	72 90
2	K	329/333 (99%)	313 (95%)	16 (5%)	31 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	81/88 (92%)	79 (98%)	2 (2%)	55 84
3	F	81/88 (92%)	80 (99%)	1 (1%)	78 91
3	I	81/88 (92%)	75 (93%)	6 (7%)	17 58
3	L	81/88 (92%)	77 (95%)	4 (5%)	31 71
4	M	493/502 (98%)	472 (96%)	21 (4%)	35 74
4	N	493/502 (98%)	471 (96%)	22 (4%)	34 74
4	O	493/502 (98%)	468 (95%)	25 (5%)	29 70
4	P	493/502 (98%)	469 (95%)	24 (5%)	31 71
All	All	5120/5204 (98%)	4923 (96%)	197 (4%)	40 77

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

Some 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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.22	15 (3%) 52 37	45, 68, 100, 138	0
1	D	483/484 (99%)	0.09	8 (1%) 73 58	25, 51, 82, 110	0
1	G	483/484 (99%)	1.38	136 (28%) 1 1	85, 159, 207, 235	0
1	J	483/484 (99%)	1.69	173 (35%) 0 1	98, 173, 227, 253	0
2	B	399/481 (82%)	0.17	12 (3%) 54 37	37, 68, 135, 151	0
2	E	399/481 (82%)	0.19	15 (3%) 44 30	33, 69, 140, 156	0
2	H	399/481 (82%)	0.46	30 (7%) 17 11	58, 95, 164, 185	0
2	K	399/481 (82%)	0.64	38 (9%) 10 6	57, 115, 170, 202	0
3	C	96/104 (92%)	0.46	8 (8%) 14 9	49, 91, 131, 172	0
3	F	96/104 (92%)	0.05	3 (3%) 52 37	34, 73, 113, 152	0
3	I	96/104 (92%)	0.71	12 (12%) 5 5	84, 128, 163, 174	0
3	L	96/104 (92%)	0.82	13 (13%) 4 4	103, 137, 165, 169	0
4	M	589/599 (98%)	0.34	33 (5%) 28 18	39, 76, 173, 209	0
4	N	589/599 (98%)	0.10	11 (1%) 70 55	36, 69, 118, 140	0
4	O	589/599 (98%)	0.38	40 (6%) 20 12	39, 80, 196, 249	0
4	P	589/599 (98%)	0.10	13 (2%) 65 50	30, 69, 120, 159	0
5	Q	76/76 (100%)	0.45	3 (3%) 43 29	76, 126, 163, 182	0
5	R	76/76 (100%)	0.49	4 (5%) 30 20	65, 112, 149, 175	0
5	S	76/76 (100%)	0.23	2 (2%) 59 43	64, 94, 137, 188	0
5	T	76/76 (100%)	0.47	2 (2%) 59 43	84, 123, 160, 187	0
All	All	6572/6976 (94%)	0.47	571 (8%) 13 8	25, 85, 183, 253	0

All (571) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	27	THR	9.2
1	G	36	ASP	8.8
1	J	73	PRO	8.7
2	K	359	GLY	8.7
1	J	419	GLN	7.7
1	G	346	ALA	7.6
1	G	121	ASN	7.5
4	O	315	ASN	7.4
1	J	212	GLY	7.3
1	J	170	GLY	7.3
1	J	74	ILE	7.2
1	J	416	PRO	7.1
1	J	116	THR	7.1
2	K	267	ALA	6.7
1	J	3	HIS	6.6
1	G	118	GLY	6.5
1	J	2	LEU	6.4
1	J	213	PRO	6.4
2	K	368	SER	6.3
4	O	443	ASP	6.2
4	M	371	ILE	6.0
3	C	94	ILE	5.9
1	J	329	TYR	5.9
1	J	75	ALA	5.8
4	O	371	ILE	5.8
3	C	72	HIS	5.7
1	G	146	ASP	5.6
3	C	74	ASP	5.6
2	B	266	GLU	5.5
1	G	194	GLY	5.5
3	I	18	GLY	5.4
1	G	38	GLN	5.4
4	O	373	LYS	5.3
1	J	84	GLY	5.3
1	G	347	GLU	5.3
1	J	322	PHE	5.2
1	J	44	SER	5.2
1	G	481	PRO	5.1
1	J	169	THR	5.1
2	H	381	ASP	5.0
1	J	141	ASN	5.0
2	E	267	ALA	5.0
4	O	374	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	382	ASN	4.9
1	G	276	ASP	4.8
1	G	73	PRO	4.8
1	G	142	PRO	4.8
1	J	241	GLN	4.8
4	O	588	PRO	4.8
1	J	76	HIS	4.7
2	K	30	GLY	4.7
1	G	449	VAL	4.7
1	J	20	SER	4.7
1	J	165	LEU	4.7
1	J	195	ARG	4.7
1	G	355	ASN	4.7
1	G	454	LEU	4.7
3	F	94	ILE	4.6
1	J	445	ASP	4.6
1	J	260	GLY	4.6
4	O	293	LEU	4.6
1	J	194	GLY	4.6
1	J	351	SER	4.5
1	G	148	VAL	4.5
1	G	185	ASN	4.5
1	G	170	GLY	4.5
1	G	453	LEU	4.5
1	J	346	ALA	4.4
1	G	9	GLU	4.4
1	J	324	GLY	4.4
1	J	345	ARG	4.4
1	J	478	THR	4.4
1	J	418	SER	4.4
3	I	91	PRO	4.4
2	H	335	GLY	4.3
1	G	37	PRO	4.3
5	S	17	C	4.3
1	J	204	TYR	4.3
5	R	17	C	4.3
1	J	1	MET	4.3
1	J	392	ALA	4.3
1	J	242	PRO	4.3
1	J	21	ALA	4.3
2	E	381	ASP	4.2
4	O	313	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
2	K	397	ALA	4.2
4	O	308	LYS	4.2
1	J	399	GLY	4.2
1	G	445	ASP	4.2
1	J	149	PRO	4.2
1	J	398	LEU	4.2
1	J	87	THR	4.2
2	K	381	ASP	4.2
1	G	166	PRO	4.1
1	J	34	GLN	4.1
1	J	93	MET	4.1
1	G	418	SER	4.1
2	B	381	ASP	4.1
1	G	446	GLY	4.0
1	J	390	ALA	4.0
4	M	588	PRO	4.0
1	J	45	ILE	4.0
4	O	355	ILE	4.0
1	G	122	MET	4.0
1	G	440	PRO	4.0
4	N	590	ALA	4.0
3	C	95	GLU	4.0
1	G	188	GLY	3.9
5	T	17	C	3.9
1	J	86	ARG	3.9
1	J	53	GLN	3.9
1	J	142	PRO	3.9
2	K	45	PRO	3.9
4	M	355	ILE	3.9
1	J	240	GLU	3.9
5	R	76	A	3.9
1	J	37	PRO	3.9
1	G	328	GLY	3.8
1	G	189	ILE	3.8
1	J	305	PRO	3.8
4	M	295	LEU	3.8
1	J	186	LEU	3.8
1	D	413	ASN	3.8
1	G	15	ALA	3.8
2	E	266	GLU	3.8
1	G	6	THR	3.8
4	M	395	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	149	PRO	3.8
1	J	85	VAL	3.7
2	K	39	LEU	3.7
1	J	36	ASP	3.7
1	G	345	ARG	3.7
1	G	483	GLY	3.7
2	K	130	LYS	3.7
1	J	23	GLU	3.6
1	J	411	GLU	3.6
4	O	587	GLN	3.6
1	G	169	THR	3.6
4	N	175	GLY	3.6
4	M	586	GLU	3.6
1	J	215	ALA	3.6
1	G	240	GLU	3.6
1	J	209	ASP	3.6
1	G	214	LEU	3.5
2	K	191	SER	3.5
4	M	391	ASP	3.5
1	J	202	ILE	3.5
1	G	434	LEU	3.5
2	B	398	ASN	3.5
1	G	213	PRO	3.5
4	O	295	LEU	3.5
4	M	298	VAL	3.5
1	J	129	SER	3.5
4	O	367	LEU	3.5
4	M	303	LYS	3.5
1	G	43	ILE	3.5
2	K	265	GLU	3.5
1	G	42	PHE	3.5
1	G	165	LEU	3.5
2	H	401	GLY	3.5
1	G	437	LEU	3.5
1	J	54	ALA	3.5
4	P	175	GLY	3.4
1	J	348	GLY	3.4
1	J	79	LEU	3.4
3	L	88	TYR	3.4
1	G	167	ALA	3.4
2	H	353	SER	3.4
1	J	65	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	355	ASN	3.4
1	J	22	GLU	3.3
1	G	2	LEU	3.3
1	G	439	MET	3.3
3	L	12	ALA	3.3
4	M	397	PHE	3.3
1	G	86	ARG	3.3
1	G	413	ASN	3.3
1	G	412	LYS	3.3
2	K	332	LYS	3.3
1	J	18	GLN	3.3
2	H	337	CYS	3.3
1	G	74	ILE	3.3
2	E	385	SER	3.3
4	N	443	ASP	3.3
2	E	265	GLU	3.3
1	G	435	PRO	3.3
1	J	277	ALA	3.3
4	O	299	ALA	3.2
1	G	45	ILE	3.2
1	G	168	ALA	3.2
1	G	237	THR	3.2
4	M	441	ASN	3.2
1	G	153	SER	3.2
1	G	444	VAL	3.2
2	H	336	ILE	3.2
1	D	481	PRO	3.2
3	L	10	LYS	3.2
1	G	470	TYR	3.2
4	O	368	GLN	3.2
1	J	429	ALA	3.2
4	M	299	ALA	3.2
3	I	80	ALA	3.2
2	K	14	GLN	3.2
1	G	482	ALA	3.2
1	G	89	CYS	3.2
2	H	387	LYS	3.2
1	G	223	LEU	3.1
1	G	318	ASN	3.1
4	O	294	GLU	3.1
1	A	481	PRO	3.1
4	M	442	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	367	GLY	3.1
2	K	244	VAL	3.1
1	J	31	ARG	3.1
1	J	221	CYS	3.1
1	J	148	VAL	3.1
2	H	257	GLU	3.1
1	G	416	PRO	3.1
4	O	304	GLU	3.1
1	G	351	SER	3.1
1	G	414	ASP	3.1
1	J	155	GLY	3.1
4	M	308	LYS	3.0
1	J	40	ASN	3.0
4	O	307	PHE	3.0
1	D	415	ASP	3.0
1	G	278	VAL	3.0
2	H	260	SER	3.0
1	G	92	LYS	3.0
1	J	214	LEU	3.0
1	J	415	ASP	3.0
2	E	141	GLY	3.0
1	J	153	SER	3.0
1	G	79	LEU	3.0
4	O	353	ALA	3.0
3	C	78	THR	3.0
1	G	177	ILE	3.0
1	J	437	LEU	3.0
3	F	95	GLU	3.0
2	H	37	ALA	3.0
1	A	187	THR	3.0
2	K	266	GLU	3.0
1	J	72	ALA	3.0
2	K	219	SER	3.0
3	I	88	TYR	3.0
1	G	162	ALA	3.0
1	J	26	ARG	3.0
1	G	56	ALA	3.0
4	N	83	ALA	3.0
5	T	45	G	3.0
2	H	34	ASN	3.0
3	L	93	VAL	2.9
1	A	66	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
4	O	359	GLU	2.9
1	J	205	ALA	2.9
1	J	327	TYR	2.9
1	J	143	TRP	2.9
2	E	391	MET	2.9
1	A	41	SER	2.9
1	G	156	SER	2.9
1	J	210	GLN	2.9
4	N	586	GLU	2.9
1	J	436	GLY	2.9
2	E	387	LYS	2.9
1	G	54	ALA	2.9
2	H	31	ALA	2.9
1	J	94	LEU	2.9
1	J	328	GLY	2.9
1	G	294	ASP	2.9
1	J	342	LYS	2.9
1	J	160	VAL	2.9
2	H	38	SER	2.8
3	C	93	VAL	2.8
4	O	303	LYS	2.8
2	H	263	GLY	2.8
1	J	461	GLY	2.8
1	J	386	ASP	2.8
4	O	389	ALA	2.8
1	G	398	LEU	2.8
1	J	7	LEU	2.8
1	J	406	ALA	2.8
3	L	94	ILE	2.8
1	J	402	THR	2.8
2	H	386	GLY	2.8
2	K	345	ASN	2.8
1	J	438	SER	2.8
2	K	84	PRO	2.8
1	G	394	VAL	2.8
1	J	434	LEU	2.8
1	G	141	ASN	2.8
1	D	480	THR	2.8
1	G	415	ASP	2.8
1	J	57	ALA	2.8
1	J	80	PHE	2.8
2	K	210	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	396	VAL	2.7
2	K	43	ALA	2.7
1	J	216	ARG	2.7
2	K	255	LYS	2.7
1	G	405	PRO	2.7
1	J	92	LYS	2.7
4	M	334	ARG	2.7
4	N	60	LYS	2.7
1	J	190	LYS	2.7
1	G	277	ALA	2.7
2	H	33	PRO	2.7
1	A	22	GLU	2.7
4	M	349	ALA	2.7
1	G	163	ARG	2.7
2	H	385	SER	2.7
3	L	53	ALA	2.7
1	G	44	SER	2.7
1	J	332	ASP	2.7
1	D	416	PRO	2.7
4	M	306	GLU	2.7
1	G	120	LEU	2.7
1	G	260	GLY	2.7
2	E	371	GLN	2.7
1	G	93	MET	2.7
2	K	393	PHE	2.7
4	M	359	GLU	2.6
1	G	296	SER	2.6
1	J	289	GLY	2.6
4	M	373	LYS	2.6
4	M	374	PHE	2.6
3	L	11	ILE	2.6
2	B	401	GLY	2.6
3	I	95	GLU	2.6
1	J	77	LYS	2.6
4	M	307	PHE	2.6
1	J	460	GLU	2.6
5	Q	74	C	2.6
2	K	402	SER	2.6
1	G	174	GLY	2.6
1	J	4	GLN	2.6
4	N	510	GLU	2.6
1	G	193	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	329	TYR	2.6
4	O	334	ARG	2.6
1	J	285	LEU	2.6
1	J	405	PRO	2.6
1	J	294	ASP	2.6
1	J	388	VAL	2.6
1	J	412	LYS	2.6
1	J	89	CYS	2.6
3	F	96	SER	2.6
2	H	265	GLU	2.6
1	J	290	ALA	2.6
4	O	298	VAL	2.5
1	G	474	SER	2.5
1	J	133	SER	2.5
3	I	17	LEU	2.5
1	J	173	THR	2.5
1	J	193	TYR	2.5
4	O	586	GLU	2.5
5	S	21	A	2.5
2	H	364	GLN	2.5
1	J	168	ALA	2.5
1	J	222	ALA	2.5
1	J	225	LEU	2.5
1	G	16	ASP	2.5
1	J	393	GLU	2.5
1	G	34	GLN	2.5
1	G	212	GLY	2.5
4	O	314	ALA	2.5
4	O	504	LEU	2.5
2	K	361	GLU	2.5
1	J	17	LYS	2.5
1	A	450	GLY	2.5
1	G	285	LEU	2.5
1	J	47	ASP	2.5
1	G	452	GLN	2.5
1	J	38	GLN	2.5
4	O	397	PHE	2.5
1	G	341	TYR	2.5
1	J	323	ASP	2.5
1	G	80	PHE	2.5
3	L	80	ALA	2.5
4	O	442	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	471	GLN	2.5
2	K	35	THR	2.4
1	G	132	GLN	2.4
1	G	227	VAL	2.4
4	P	588	PRO	2.4
1	G	417	VAL	2.4
4	P	298	VAL	2.4
2	B	400	GLU	2.4
1	A	65	GLU	2.4
2	H	25	SER	2.4
1	J	440	PRO	2.4
1	J	228	MET	2.4
4	N	115	GLU	2.4
1	J	480	THR	2.4
1	J	304	ILE	2.4
1	J	154	GLY	2.4
2	E	264	LYS	2.4
1	J	69	LEU	2.4
2	K	44	MET	2.4
1	G	119	LYS	2.4
1	G	5	LEU	2.4
4	P	174	GLU	2.4
1	A	406	ALA	2.4
2	K	388	LEU	2.4
3	I	12	ALA	2.4
1	J	42	PHE	2.4
3	L	91	PRO	2.4
1	J	354	LYS	2.4
4	O	306	GLU	2.4
4	O	352	LEU	2.4
1	J	122	MET	2.4
1	D	294	ASP	2.4
1	J	162	ALA	2.4
2	H	389	ALA	2.4
4	P	367	LEU	2.4
1	G	202	ILE	2.4
1	J	349	PHE	2.4
1	A	360	GLY	2.4
1	J	211	GLY	2.4
2	K	370	GLU	2.4
4	P	300	ASP	2.4
1	J	56	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	216	ASN	2.3
4	N	367	LEU	2.3
1	D	483	GLY	2.3
1	J	362	TYR	2.3
4	M	319	GLY	2.3
4	N	47	GLN	2.3
1	G	288	LEU	2.3
2	H	59	ALA	2.3
2	B	267	ALA	2.3
1	G	22	GLU	2.3
1	G	393	GLU	2.3
4	O	467	PRO	2.3
1	G	426	THR	2.3
1	J	29	LEU	2.3
4	P	580	LEU	2.3
1	J	439	MET	2.3
2	H	139	MET	2.3
4	M	487	GLY	2.3
4	O	486	GLY	2.3
1	G	133	SER	2.3
1	G	397	ILE	2.3
2	B	140	SER	2.3
1	J	166	PRO	2.3
5	R	47	U	2.3
3	I	56	LEU	2.3
2	K	331	GLU	2.3
1	G	155	GLY	2.3
4	M	372	VAL	2.3
4	O	386	ARG	2.3
1	J	179	GLN	2.3
4	P	371	ILE	2.3
1	G	95	ASP	2.3
1	J	264	GLU	2.3
1	J	295	ILE	2.3
4	P	16	GLY	2.3
2	B	387	LYS	2.3
1	G	160	VAL	2.3
4	P	322	ALA	2.3
2	K	348	MET	2.3
1	J	432	ALA	2.2
1	J	30	GLY	2.2
3	C	19	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	203	ALA	2.2
4	M	548	SER	2.2
1	A	221	CYS	2.2
3	L	18	GLY	2.2
1	G	332	ASP	2.2
3	L	16	ARG	2.2
1	J	246	TYR	2.2
1	J	128	GLY	2.2
2	H	361	GLU	2.2
3	L	52	LEU	2.2
2	E	346	TRP	2.2
1	G	114	ALA	2.2
1	G	392	ALA	2.2
3	I	86	GLY	2.2
1	G	144	SER	2.2
1	J	178	ARG	2.2
1	G	96	ASN	2.2
2	H	363	GLU	2.2
4	M	318	LYS	2.2
2	K	198	VAL	2.2
4	O	284	SER	2.2
1	J	183	LEU	2.2
1	J	479	ARG	2.2
4	O	311	SER	2.2
2	E	334	GLN	2.2
3	L	8	VAL	2.2
1	J	146	ASP	2.2
4	P	590	ALA	2.2
2	K	391	MET	2.2
1	J	81	CYS	2.2
2	K	146	ARG	2.2
1	J	139	VAL	2.2
1	G	293	LYS	2.2
1	G	20	SER	2.2
4	M	470	ALA	2.2
3	I	41	MET	2.2
1	G	326	ARG	2.1
1	A	64	GLY	2.1
2	K	31	ALA	2.1
1	G	35	LEU	2.1
1	G	164	LEU	2.1
1	J	152	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	187	MET	2.1
1	J	95	ASP	2.1
4	O	46	ALA	2.1
1	A	478	THR	2.1
2	K	341	LYS	2.1
1	J	373	TYR	2.1
1	J	417	VAL	2.1
5	Q	17	C	2.1
1	J	223	LEU	2.1
3	I	62	LEU	2.1
1	J	325	VAL	2.1
4	M	315	ASN	2.1
4	M	370	PRO	2.1
5	R	34	G	2.1
1	J	107	GLU	2.1
1	J	318	ASN	2.1
1	J	43	ILE	2.1
1	J	220	ASP	2.1
1	G	226	GLY	2.1
1	G	399	GLY	2.1
1	G	63	ASN	2.1
1	A	443	PHE	2.1
1	J	326	ARG	2.1
1	A	413	ASN	2.1
2	H	140	SER	2.1
4	O	365	GLU	2.1
1	G	289	GLY	2.1
2	H	354	LEU	2.1
3	I	87	LEU	2.1
1	G	1	MET	2.1
1	J	358	MET	2.1
4	N	30	ASP	2.1
2	E	369	ALA	2.1
3	C	10	LYS	2.1
1	J	175	GLY	2.1
2	H	310	TYR	2.1
1	G	324	GLY	2.0
1	J	35	LEU	2.0
1	J	344	SER	2.0
2	B	402	SER	2.0
4	M	313	PRO	2.0
4	M	390	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	396	MET	2.0
1	G	279	LEU	2.0
2	B	388	LEU	2.0
1	G	420	TYR	2.0
4	P	84	ARG	2.0
2	K	295	LEU	2.0
1	J	397	ILE	2.0
2	B	264	LYS	2.0
2	E	242	GLY	2.0
4	O	354	TYR	2.0
1	G	211	GLY	2.0
1	J	276	ASP	2.0
1	D	291	THR	2.0
1	G	187	THR	2.0
4	M	310	PHE	2.0
2	K	252	ASP	2.0
4	P	53	ASP	2.0
5	Q	21	A	2.0
1	A	40	ASN	2.0
4	M	320	ARG	2.0
1	G	349	PHE	2.0
2	K	350	GLU	2.0
4	O	447	SER	2.0
1	G	297	LEU	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 carbohydrates 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.