



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2017 – 01:46 PM EDT

PDB ID : 5N9J  
Title : Core Mediator of transcriptional regulation  
Authors : Nozawa, K.; Schneider, T.R.; Cramer, P.  
Deposited on : unknown  
Resolution : 3.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

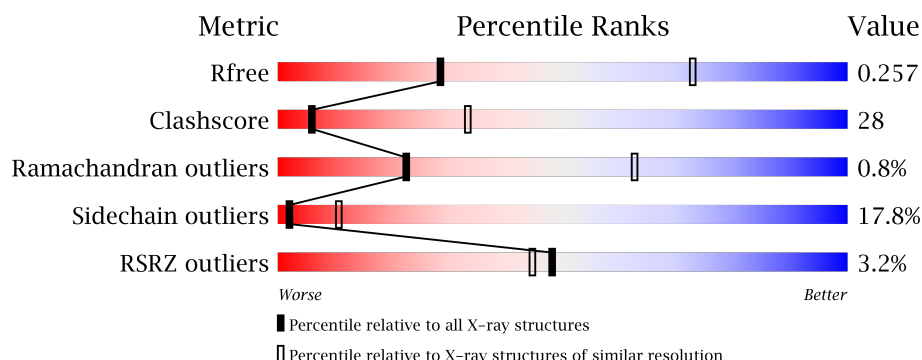
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	591	<div> <div>5%</div> <div>40%</div> <div>41%</div> <div>13%</div> <div>• •</div> </div>
2	B	144	<div> <div>2%</div> <div>47%</div> <div>40%</div> <div>5%</div> <div>8%</div> </div>
3	C	138	<div> <div>•</div> <div>40%</div> <div>35%</div> <div>6%</div> <div>20%</div> </div>
4	D	138	<div> <div>•</div> <div>51%</div> <div>39%</div> <div>7%</div> <div>• •</div> </div>
5	E	376	<div> <div>•</div> <div>30%</div> <div>19%</div> <div>5%</div> <div>•</div> <div>47%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	121	
7	G	239	
8	R	139	
9	S	216	
10	U	200	
11	V	112	
12	W	545	
13	X	210	
14	Y	193	
15	Z	136	

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 23721 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 Mediator of RNA polymerase II transcription subunit 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4597	2979	791	814	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP Q9P7Y4
A	-9	GLY	-	expression tag	UNP Q9P7Y4
A	-8	HIS	-	expression tag	UNP Q9P7Y4
A	-7	HIS	-	expression tag	UNP Q9P7Y4
A	-6	HIS	-	expression tag	UNP Q9P7Y4
A	-5	HIS	-	expression tag	UNP Q9P7Y4
A	-4	HIS	-	expression tag	UNP Q9P7Y4
A	-3	HIS	-	expression tag	UNP Q9P7Y4
A	-2	HIS	-	expression tag	UNP Q9P7Y4
A	-1	HIS	-	expression tag	UNP Q9P7Y4
A	0	HIS	-	expression tag	UNP Q9P7Y4
A	1	HIS	-	expression tag	UNP Q9P7Y4

- Molecule 2 is a protein called Mediator of RNA polymerase II transcription subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1066	673	172	220	1			

- Molecule 3 is a protein called Mediator of RNA polymerase II transcription subunit 19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	111	Total	C	N	O	S	0	0	0
			917	592	158	166	1			

- Molecule 4 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	135	Total	C	N	O	S	0	0	0
			1088	684	187	213	4			

- Molecule 5 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	201	Total	C	N	O	S	0	0	0
			1548	982	271	287	8			

- Molecule 6 is a protein called Mediator Complex Subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	79	Total	C	N	O	S	0	0	0
			632	405	108	116	3			

- Molecule 7 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	163	Total	C	N	O	S	0	0	0
			1319	826	221	265	7			

- Molecule 8 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	R	99	Total	C	N	O	S	0	0	0
			873	576	134	159	4			

- Molecule 9 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	S	171	Total	C	N	O	S	0	0	0
			1410	905	236	260	9			

- Molecule 10 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	U	198	Total	C	N	O	S	0	0	0
			1628	1022	281	322	3			

- Molecule 11 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	V	99	Total	C	N	O	S	0	0	0
			783	494	130	157	2			

- Molecule 12 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	463	Total	C	N	O	S	0	0	0
			3692	2347	619	707	19			

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	X	207	Total	C	N	O	S	0	0	0
			1694	1082	288	316	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	MET	-	initiating methionine	UNP O14198
X	-1	ALA	-	expression tag	UNP O14198
X	0	SER	-	expression tag	UNP O14198

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 20.

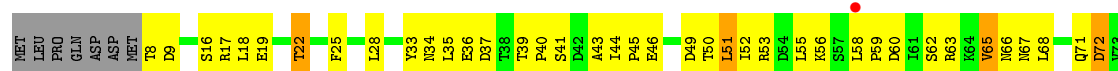
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	Y	185	Total	C	N	O	S	0	0	0
			1515	989	250	271	5			

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	Z	119	Total	C	N	O	S	0	0	0
			959	602	162	193	2			

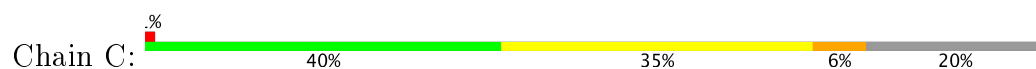
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Chain A:  5% 40% 41% 13% ..





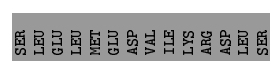
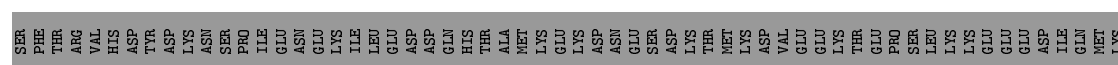
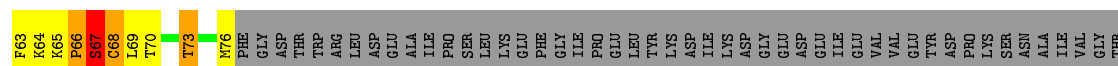
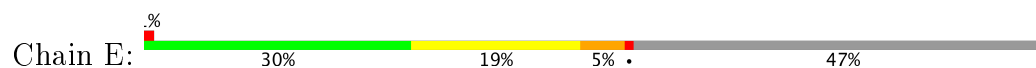
- Molecule 3: Mediator of RNA polymerase II transcription subunit 19



- Molecule 4: Mediator of RNA polymerase II transcription subunit 21



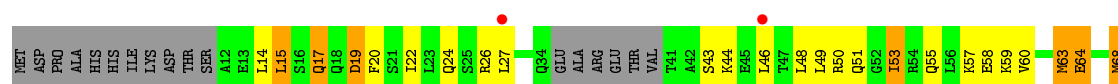
- Molecule 5: Mediator of RNA polymerase II transcription subunit 7



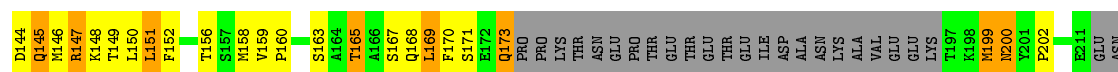
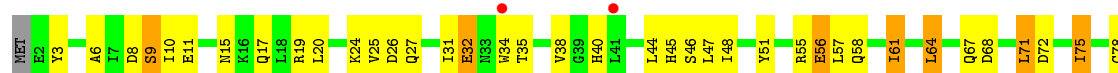
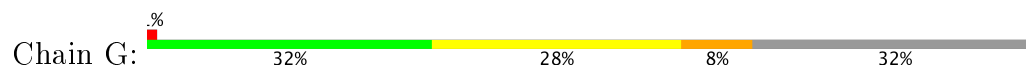
- Molecule 6: Mediator Complex Subunit 9



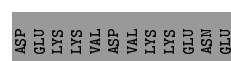
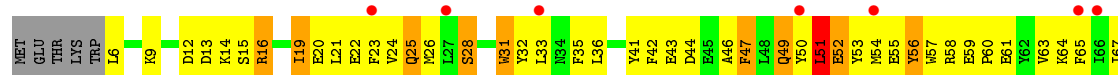
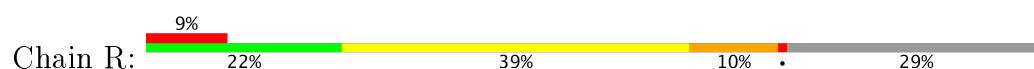




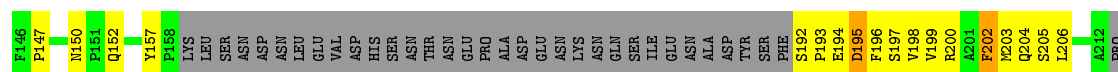
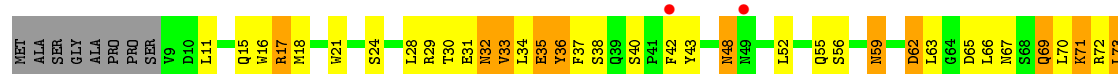
• Molecule 7: Mediator of RNA polymerase II transcription subunit 4



• Molecule 8: Mediator of RNA polymerase II transcription subunit 31

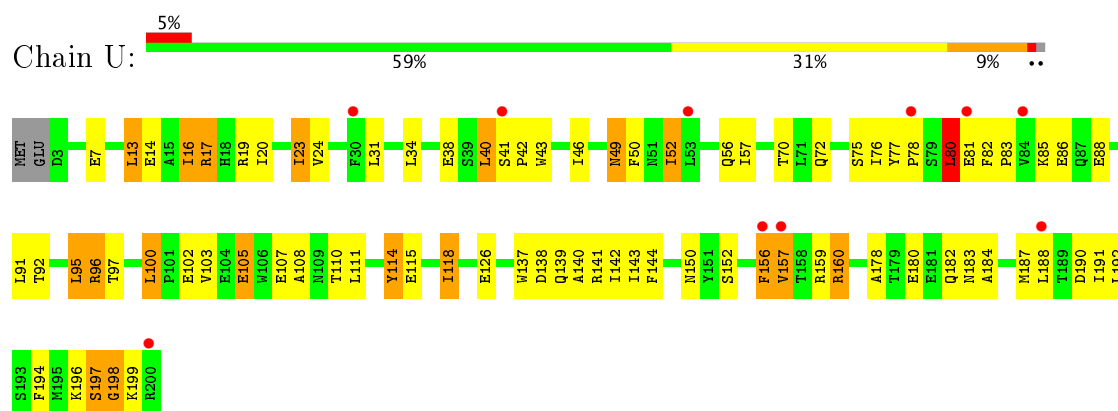


• Molecule 9: Mediator of RNA polymerase II transcription subunit 6

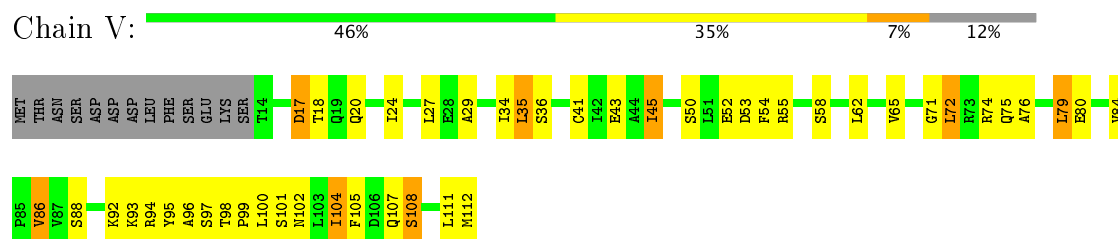


ASP  
VAL  
LYS

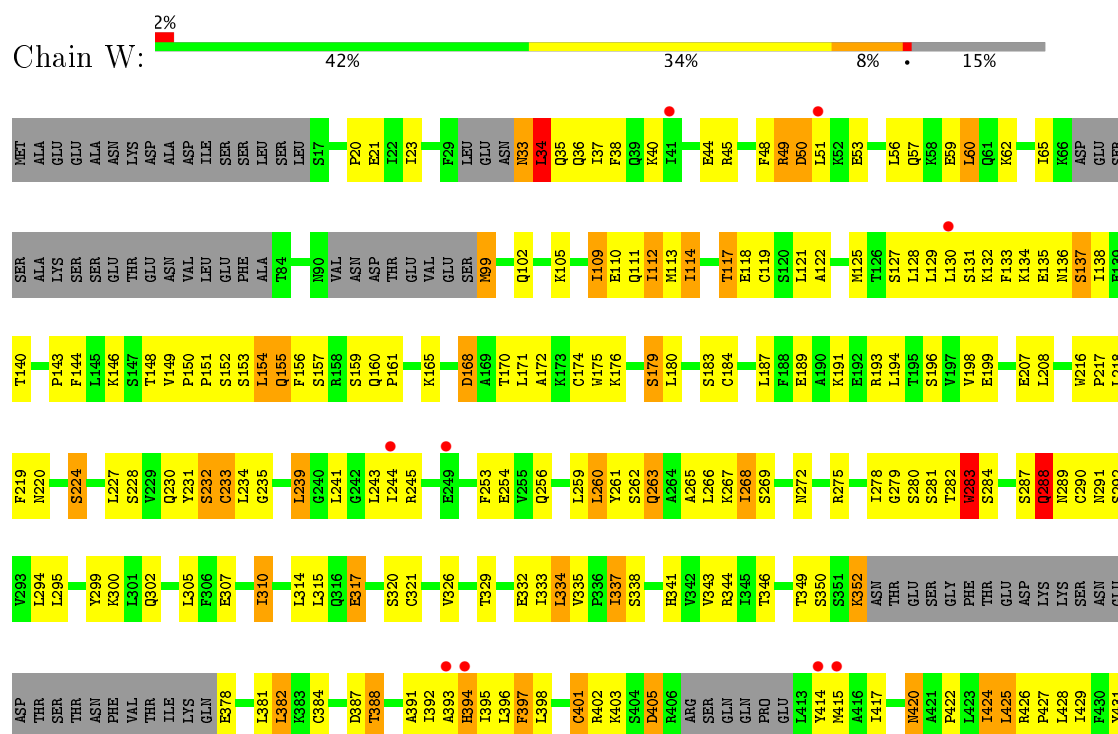
• Molecule 10: Mediator of RNA polymerase II transcription subunit 8

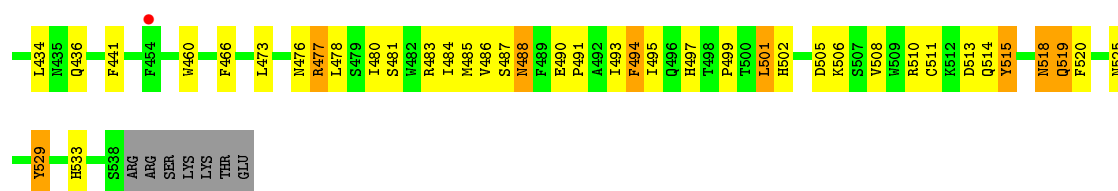


• Molecule 11: Mediator of RNA polymerase II transcription subunit 11

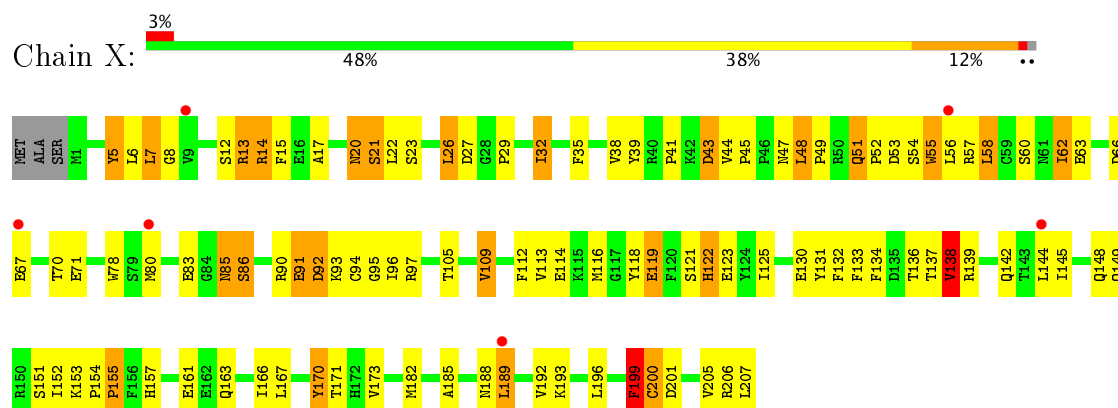


• Molecule 12: Mediator of RNA polymerase II transcription subunit 17

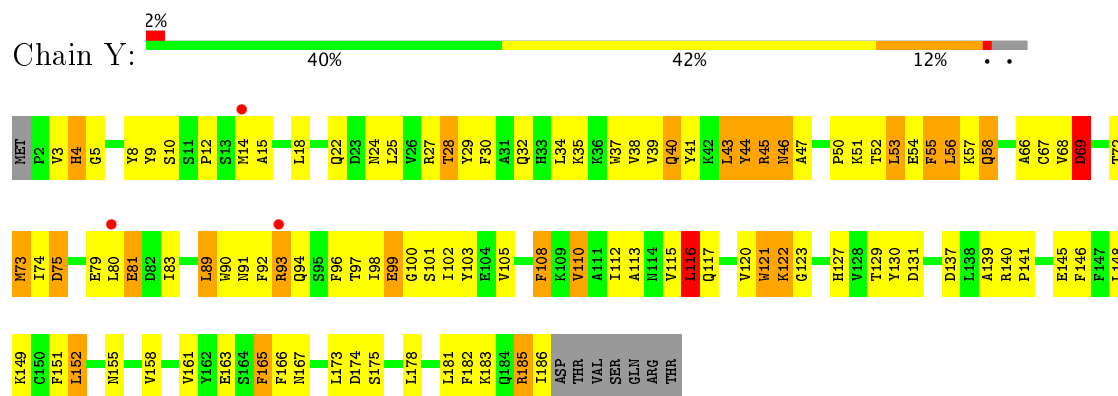




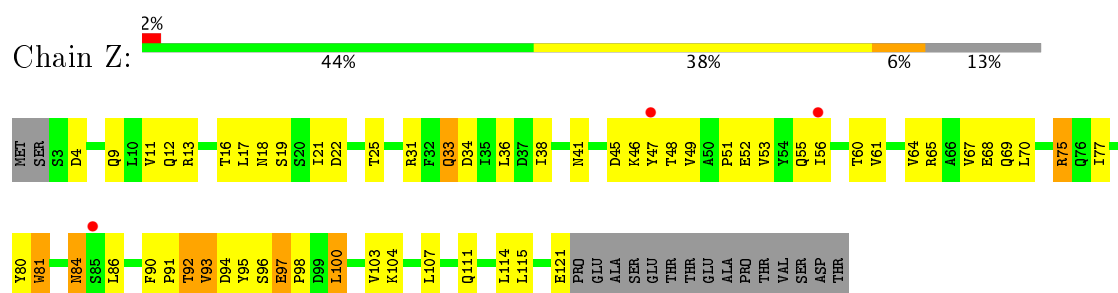
- Molecule 13: Mediator of RNA polymerase II transcription subunit 18



- Molecule 14: Mediator of RNA polymerase II transcription subunit 20



- Molecule 15: Mediator of RNA polymerase II transcription subunit 22



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.86Å 211.77Å 267.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.49 – 3.40 98.49 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (98.49-3.40) 99.2 (98.49-3.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 3.33Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.233 , 0.256 0.236 , 0.257	Depositor DCC
$R_{free}$ test set	5698 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	153.1	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 130.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23721	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 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	0.44	1/4718 (0.0%)	0.67	4/6423 (0.1%)
2	B	0.39	0/1082	0.55	0/1467
3	C	0.38	0/943	0.56	0/1278
4	D	0.40	1/1104 (0.1%)	0.57	1/1486 (0.1%)
5	E	0.33	0/1574	0.59	2/2120 (0.1%)
6	F	0.34	0/634	0.54	0/840
7	G	0.32	0/1339	0.57	0/1804
8	R	0.39	0/901	0.61	1/1222 (0.1%)
9	S	0.35	0/1446	0.54	1/1959 (0.1%)
10	U	0.34	0/1661	0.53	0/2248
11	V	0.41	0/792	0.70	2/1067 (0.2%)
12	W	0.52	6/3761 (0.2%)	0.64	3/5072 (0.1%)
13	X	0.46	1/1739 (0.1%)	0.65	0/2362
14	Y	0.43	0/1554	0.63	1/2108 (0.0%)
15	Z	0.62	2/972 (0.2%)	0.75	4/1320 (0.3%)
All	All	0.43	11/24220 (0.0%)	0.62	19/32776 (0.1%)

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
12	W	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	W	283	TRP	CB-CG	-13.47	1.26	1.50
13	X	199	PHE	CB-CG	-8.11	1.37	1.51
15	Z	96	SER	CA-CB	-7.13	1.42	1.52
12	W	401	CYS	CB-SG	-6.81	1.70	1.82
12	W	283	TRP	CE3-CZ3	-6.18	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	W	288	GLN	CG-CD	-5.79	1.37	1.51
4	D	136	PHE	CB-CG	-5.60	1.41	1.51
12	W	283	TRP	CZ3-CH2	5.44	1.48	1.40
15	Z	96	SER	CB-OG	-5.43	1.35	1.42
12	W	288	GLN	CA-CB	-5.17	1.42	1.53
1	A	217	TRP	CB-CG	-5.02	1.41	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Z	93	VAL	CA-CB-CG2	-7.58	99.54	110.90
8	R	51	LEU	CA-CB-CG	7.51	132.59	115.30
11	V	104	ILE	CG1-CB-CG2	7.00	126.80	111.40
1	A	217	TRP	CA-CB-CG	-6.99	100.42	113.70
4	D	35	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	395	LEU	CA-CB-CG	6.63	130.54	115.30
11	V	79	LEU	CB-CG-CD2	-6.62	99.75	111.00
15	Z	92	THR	C-N-CA	-6.41	105.67	121.70
15	Z	93	VAL	CG1-CB-CG2	6.23	120.87	110.90
1	A	531	LEU	CA-CB-CG	6.23	129.63	115.30
9	S	73	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	266	LEU	CA-CB-CG	6.07	129.25	115.30
12	W	20	PRO	N-CA-CB	6.00	110.51	103.30
15	Z	95	TYR	CA-CB-CG	-5.90	102.19	113.40
5	E	186	PRO	N-CA-CB	5.86	110.33	103.30
14	Y	116	LEU	CA-CB-CG	5.54	128.04	115.30
5	E	312	LEU	CA-CB-CG	5.46	127.85	115.30
12	W	382	LEU	CB-CG-CD1	-5.19	102.17	111.00
12	W	34	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	W	288	GLN	Mainchain

## 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	4597	0	4636	347	1
2	B	1066	0	1050	63	1
3	C	917	0	905	52	1
4	D	1088	0	1099	82	0
5	E	1548	0	1484	107	0
6	F	632	0	697	39	0
7	G	1319	0	1302	83	0
8	R	873	0	832	77	0
9	S	1410	0	1378	96	0
10	U	1628	0	1588	84	0
11	V	783	0	803	77	0
12	W	3692	0	3633	237	0
13	X	1694	0	1670	91	0
14	Y	1515	0	1527	108	1
15	Z	959	0	965	81	0
All	All	23721	0	23569	1307	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 28.

All (1307) 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)
13:X:21:SER:HB3	13:X:199:PHE:CZ	1.89	1.08
1:A:150:SER:HB2	1:A:153:GLN:HB2	1.39	1.03
14:Y:51:LYS:HB3	14:Y:69:ASP:HA	1.38	1.02
10:U:83:PRO:HA	10:U:86:GLU:HB2	1.40	1.00
1:A:208:PRO:HD3	1:A:226:LEU:HG	1.43	0.99
1:A:157:THR:HG22	7:G:91:PRO:HG3	1.43	0.99
5:E:65:LYS:O	8:R:16:ARG:NH2	1.95	0.99
11:V:104:ILE:HG21	12:W:398:LEU:HD12	1.45	0.98
13:X:14:ARG:HH12	13:X:200:CYS:HB2	1.28	0.97
14:Y:39:VAL:HG12	14:Y:57:LYS:HA	1.46	0.94
11:V:79:LEU:HD21	15:Z:13:ARG:NE	1.84	0.93
1:A:206:GLN:O	1:A:226:LEU:HB2	1.67	0.93
4:D:6:THR:HB	5:E:275:ARG:HH22	1.34	0.92
1:A:223:GLN:NE2	1:A:224:PHE:O	2.02	0.92
1:A:114:ARG:HA	5:E:275:ARG:HH21	1.35	0.91
1:A:176:PRO:HD3	1:A:259:LEU:HB3	1.52	0.90
13:X:21:SER:HB3	13:X:199:PHE:HZ	1.26	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:HIS:H	1:A:248:ILE:HD11	1.36	0.88
1:A:168:ARG:HE	1:A:223:GLN:HG3	1.38	0.86
6:F:43:SER:HB2	6:F:46:LEU:HB3	1.57	0.86
11:V:95:TYR:HB2	12:W:235:GLY:HA2	1.58	0.86
9:S:16:TRP:HB3	9:S:115:ILE:HD11	1.56	0.86
10:U:14:GLU:OE2	10:U:17:ARG:NH2	2.09	0.85
1:A:482:GLU:OE1	12:W:525:ASN:ND2	2.10	0.85
3:C:37:LYS:O	3:C:49:ARG:NH1	2.09	0.85
11:V:92:LYS:HG3	11:V:95:TYR:HE1	1.42	0.85
1:A:11:GLU:HB2	7:G:200:ASN:HD21	1.41	0.84
10:U:78:PRO:HB3	12:W:154:LEU:HD22	1.59	0.84
1:A:189:CYS:O	1:A:204:ASN:HA	1.77	0.84
12:W:283:TRP:HZ3	12:W:394:HIS:HB2	1.42	0.84
1:A:171:LEU:HB3	1:A:217:TRP:NE1	1.92	0.84
12:W:193:ARG:NH2	15:Z:68:GLU:OE2	2.11	0.84
14:Y:57:LYS:NZ	14:Y:173:LEU:O	2.11	0.83
12:W:384:CYS:O	12:W:388:THR:OG1	1.95	0.83
1:A:168:ARG:O	1:A:172:TYR:N	2.09	0.83
8:R:25:GLN:HG3	8:R:68:TYR:HD2	1.41	0.83
1:A:112:ARG:HH21	4:D:9:GLN:HB3	1.42	0.83
12:W:477:ARG:NH2	12:W:505:ASP:OD2	2.11	0.83
14:Y:12:PRO:O	14:Y:15:ALA:HB3	1.79	0.83
1:A:212:GLY:O	1:A:216:GLN:N	2.09	0.82
4:D:136:PHE:HZ	6:F:87:LYS:HA	1.43	0.82
5:E:228:LEU:HD11	5:E:270:LEU:HD22	1.60	0.82
1:A:364:HIS:HB3	1:A:367:ILE:HG22	1.61	0.82
2:B:88:ARG:HH21	3:C:41:ARG:HA	1.44	0.82
12:W:310:ILE:HA	12:W:397:PHE:HE2	1.45	0.82
12:W:263:GLN:HE22	12:W:300:LYS:HE2	1.45	0.81
1:A:362:TRP:CZ3	1:A:364:HIS:HB2	2.15	0.81
12:W:224:SER:O	15:Z:75:ARG:NH1	2.13	0.81
10:U:114:TYR:HE2	12:W:170:THR:HB	1.46	0.81
12:W:283:TRP:CZ3	12:W:394:HIS:HB2	2.15	0.81
12:W:288:GLN:HB2	15:Z:93:VAL:HG21	1.62	0.81
1:A:187:GLY:O	1:A:206:GLN:NE2	2.12	0.81
1:A:334:THR:HA	1:A:356:PHE:HB3	1.60	0.81
3:C:19:ARG:HB3	3:C:20:PRO:HD3	1.62	0.81
10:U:157:VAL:HG22	11:V:74:ARG:HB2	1.62	0.81
12:W:176:LYS:NZ	15:Z:52:GLU:OE2	2.13	0.80
10:U:85:LYS:HG2	12:W:149:VAL:HG22	1.64	0.80
1:A:212:GLY:HA2	1:A:215:PHE:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ILE:HG21	1:A:464:PRO:HB2	1.61	0.80
9:S:15:GLN:HB2	9:S:116:TYR:CE1	2.16	0.80
1:A:534:ALA:O	14:Y:27:ARG:NH1	2.15	0.80
9:S:15:GLN:HB2	9:S:116:TYR:HE1	1.45	0.80
6:F:15:LEU:HD11	6:F:59:LYS:HB3	1.62	0.80
11:V:100:LEU:O	11:V:104:ILE:HG13	1.81	0.80
1:A:180:GLN:HG3	4:D:137:GLN:HB3	1.64	0.79
12:W:397:PHE:HE1	12:W:401:CYS:SG	2.06	0.79
1:A:337:ILE:HG23	1:A:355:HIS:HE1	1.47	0.79
1:A:6:ILE:HG12	1:A:7:PRO:HD2	1.65	0.78
2:B:103:GLY:HA3	4:D:31:ASP:O	1.83	0.78
12:W:288:GLN:CD	15:Z:93:VAL:HG11	2.03	0.78
1:A:231:SER:HB3	1:A:233:PRO:HD2	1.63	0.78
10:U:78:PRO:HG3	10:U:91:LEU:HD11	1.65	0.78
6:F:80:LEU:HD21	7:G:64:LEU:HB3	1.64	0.78
12:W:310:ILE:HA	12:W:397:PHE:CE2	2.19	0.78
1:A:132:ARG:NH1	8:R:100:ILE:HB	2.00	0.77
13:X:83:GLU:OE2	13:X:97:ARG:NH1	2.16	0.77
6:F:17:GLN:OE1	7:G:45:HIS:NE2	2.15	0.77
1:A:301:LYS:HB2	1:A:302:PRO:CD	2.15	0.77
14:Y:108:PHE:HD2	14:Y:130:TYR:HD1	1.30	0.77
1:A:209:LYS:HD2	1:A:224:PHE:CD1	2.20	0.77
1:A:435:LEU:HD12	1:A:457:ILE:HG21	1.67	0.77
12:W:132:LYS:HB2	12:W:152:SER:HA	1.68	0.76
11:V:102:ASN:ND2	15:Z:94:ASP:OD1	2.18	0.76
1:A:227:PRO:HD2	1:A:245:ASN:HD21	1.49	0.76
1:A:152:LYS:HG3	12:W:60:LEU:HG	1.66	0.76
12:W:283:TRP:NE1	12:W:307:GLU:OE2	2.13	0.76
1:A:496:TYR:HD2	1:A:502:THR:HG21	1.49	0.76
11:V:20:GLN:HG3	11:V:75:GLN:NE2	2.01	0.76
1:A:395:LEU:HD11	1:A:414:GLY:HA2	1.67	0.76
13:X:86:SER:HB3	13:X:207:LEU:H	1.49	0.75
3:C:76:GLN:OE1	9:S:72:ARG:NH2	2.18	0.75
12:W:422:PRO:O	12:W:426:ARG:NH1	2.20	0.75
14:Y:140:ARG:HE	14:Y:165:PHE:HE1	1.34	0.75
1:A:295:ARG:HD3	1:A:308:TYR:HD2	1.50	0.75
1:A:171:LEU:HB3	1:A:217:TRP:HE1	1.51	0.75
1:A:199:VAL:HG21	1:A:231:SER:HA	1.67	0.74
12:W:405:ASP:N	12:W:405:ASP:OD1	2.20	0.74
13:X:188:ASN:O	13:X:192:VAL:HG12	1.87	0.74
1:A:226:LEU:HD22	1:A:245:ASN:ND2	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:104:ILE:HD13	12:W:394:HIS:CE1	2.22	0.74
1:A:25:HIS:NE2	3:C:84:GLU:O	2.20	0.74
4:D:30:HIS:HB2	4:D:48:PRO:HA	1.68	0.74
7:G:9:SER:OG	7:G:40:HIS:ND1	2.16	0.74
9:S:145:LYS:NZ	12:W:189:GLU:OE1	2.20	0.74
1:A:307:LEU:HD13	1:A:328:ILE:HG23	1.70	0.73
1:A:151:THR:HB	12:W:60:LEU:HD11	1.70	0.73
14:Y:22:GLN:NE2	14:Y:103:TYR:OH	2.20	0.73
9:S:127:THR:O	9:S:131:ASN:ND2	2.21	0.73
11:V:104:ILE:HG21	12:W:398:LEU:CD1	2.17	0.73
14:Y:51:LYS:O	14:Y:69:ASP:N	2.21	0.73
1:A:201:LEU:HD21	1:A:266:LEU:HG	1.70	0.73
1:A:240:ILE:HB	9:S:202:PHE:HE2	1.54	0.73
7:G:11:GLU:HG3	7:G:15:ASN:HD21	1.54	0.73
1:A:528:SER:OG	1:A:530:ARG:NH2	2.22	0.73
14:Y:96:PHE:HE2	14:Y:186:ILE:HG22	1.52	0.73
6:F:77:ILE:HD11	7:G:61:ILE:HG12	1.70	0.73
12:W:245:ARG:NH1	12:W:254:GLU:OE1	2.22	0.73
12:W:495:ILE:HG22	12:W:511:CYS:HA	1.71	0.73
3:C:18:THR:HG23	5:E:249:ALA:HA	1.71	0.72
12:W:228:SER:HA	12:W:243:LEU:HA	1.71	0.72
13:X:133:PHE:HB3	13:X:136:THR:HG23	1.71	0.72
14:Y:24:ASN:O	14:Y:28:THR:OG1	2.07	0.72
14:Y:4:HIS:HB3	14:Y:129:THR:HA	1.71	0.72
12:W:388:THR:O	12:W:392:ILE:HG22	1.89	0.72
1:A:162:ASN:ND2	1:A:185:ALA:O	2.23	0.72
4:D:117:LEU:HD21	5:E:309:THR:HG23	1.70	0.72
4:D:50:SER:HB2	4:D:53:GLU:HB2	1.71	0.72
12:W:315:LEU:HD12	12:W:333:ILE:HD11	1.71	0.72
13:X:137:THR:HB	13:X:170:TYR:HB2	1.72	0.72
1:A:168:ARG:NE	1:A:223:GLN:HG3	2.03	0.72
9:S:122:TYR:OH	15:Z:45:ASP:OD2	2.08	0.72
10:U:82:PHE:HB2	12:W:153:SER:HB3	1.72	0.72
10:U:114:TYR:CE2	12:W:170:THR:HB	2.25	0.72
12:W:281:SER:OG	12:W:387:ASP:OD1	2.08	0.72
13:X:130:GLU:HB3	13:X:139:ARG:HB3	1.71	0.71
1:A:189:CYS:CB	1:A:205:SER:O	2.39	0.71
12:W:262:SER:HB2	12:W:352:LYS:HB3	1.70	0.71
15:Z:93:VAL:HG13	15:Z:93:VAL:O	1.90	0.71
1:A:183:THR:HB	1:A:190:THR:HG23	1.71	0.71
4:D:114:ASN:OD1	5:E:305:ASN:ND2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASP:O	1:A:303:PRO:HA	1.91	0.71
13:X:21:SER:HB3	13:X:199:PHE:CE1	2.24	0.71
1:A:222:PHE:CD2	1:A:252:PHE:HA	2.26	0.71
1:A:518:LEU:HD21	1:A:559:LEU:HB3	1.71	0.71
1:A:47:LYS:NZ	3:C:102:GLY:O	2.22	0.70
11:V:84:VAL:O	15:Z:13:ARG:NH2	2.17	0.70
13:X:148:GLN:H	13:X:151:SER:HB2	1.56	0.70
1:A:17:PRO:HA	2:B:62:SER:OG	1.90	0.70
4:D:34:PRO:HG3	4:D:39:GLU:HB2	1.74	0.70
1:A:146:GLU:O	12:W:40:LYS:NZ	2.24	0.70
12:W:396:LEU:HD12	12:W:424:ILE:HA	1.73	0.70
8:R:31:TRP:HH2	8:R:94:LYS:HA	1.56	0.70
1:A:462:GLN:OE1	1:A:470:ARG:NH2	2.23	0.70
7:G:17:GLN:OE1	7:G:34:TRP:NE1	2.25	0.70
14:Y:98:ILE:HG12	14:Y:115:VAL:HG13	1.74	0.70
1:A:276:ASN:ND2	9:S:197:SER:OG	2.24	0.70
4:D:17:THR:HA	4:D:20:TYR:CE1	2.26	0.70
12:W:288:GLN:NE2	15:Z:93:VAL:HG11	2.06	0.70
1:A:162:ASN:HD21	1:A:187:GLY:H	1.40	0.70
13:X:7:LEU:HD11	13:X:205:VAL:HG22	1.72	0.70
1:A:134:ALA:HA	1:A:140:LYS:HE3	1.74	0.69
12:W:314:LEU:HD11	12:W:424:ILE:HD13	1.73	0.69
12:W:326:VAL:HG12	12:W:335:VAL:HG22	1.74	0.69
1:A:182:PHE:HB3	1:A:191:PHE:CE1	2.27	0.69
1:A:203:THR:HG22	1:A:229:PHE:HB2	1.75	0.69
1:A:153:GLN:NE2	7:G:92:LYS:O	2.25	0.69
13:X:21:SER:CB	13:X:199:PHE:HZ	2.04	0.69
13:X:22:LEU:HA	13:X:199:PHE:HE2	1.56	0.69
5:E:14:PRO:HB3	7:G:152:PHE:HD1	1.57	0.69
14:Y:38:VAL:HG22	14:Y:58:GLN:HE21	1.58	0.69
1:A:132:ARG:NH2	8:R:70:THR:OG1	2.25	0.69
1:A:222:PHE:CD2	1:A:255:GLN:HA	2.28	0.69
4:D:93:ILE:HD11	5:E:284:ILE:HG12	1.75	0.69
11:V:52:GLU:OE1	11:V:55:ARG:NH1	2.26	0.69
14:Y:173:LEU:H	14:Y:173:LEU:HD23	1.57	0.69
7:G:58:GLN:HA	7:G:61:ILE:HG13	1.75	0.69
13:X:52:PRO:O	13:X:55:TRP:NE1	2.26	0.68
12:W:105:LYS:O	12:W:109:ILE:HG22	1.93	0.68
11:V:104:ILE:HG23	12:W:394:HIS:CE1	2.28	0.68
1:A:101:LEU:HB3	4:D:20:TYR:HB3	1.75	0.68
4:D:30:HIS:NE2	4:D:32:PHE:HB2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:79:LEU:HD21	15:Z:13:ARG:HE	1.57	0.68
11:V:79:LEU:HB2	15:Z:81:TRP:CZ3	2.27	0.68
1:A:139:SER:O	1:A:143:MET:N	2.26	0.68
10:U:188:LEU:HD13	13:X:166:ILE:HD13	1.74	0.68
12:W:262:SER:N	12:W:350:SER:O	2.26	0.68
1:A:212:GLY:O	1:A:215:PHE:N	2.27	0.68
1:A:225:HIS:O	1:A:226:LEU:HD23	1.94	0.68
1:A:186:ASN:ND2	12:W:53:GLU:OE1	2.27	0.68
13:X:142:GLN:HE22	13:X:163:GLN:HB3	1.59	0.68
14:Y:46:ASN:OD1	14:Y:47:ALA:N	2.26	0.67
1:A:337:ILE:HG23	1:A:355:HIS:CE1	2.27	0.67
1:A:37:VAL:O	1:A:41:MET:HG3	1.93	0.67
8:R:25:GLN:HG3	8:R:68:TYR:CD2	2.27	0.67
10:U:19:ARG:NH1	10:U:56:GLN:OE1	2.28	0.67
1:A:105:ARG:NH1	4:D:17:THR:OG1	2.26	0.67
1:A:227:PRO:HD2	1:A:245:ASN:ND2	2.08	0.67
2:B:102:ASN:OD1	3:C:23:HIS:ND1	2.28	0.67
12:W:483:ARG:NH2	15:Z:121:GLU:OE1	2.28	0.67
1:A:189:CYS:HB3	1:A:205:SER:O	1.95	0.67
10:U:31:LEU:HD11	12:W:109:ILE:HD12	1.76	0.67
8:R:22:GLU:O	8:R:26:MET:HG2	1.94	0.67
11:V:20:GLN:HG3	11:V:75:GLN:HE21	1.58	0.67
2:B:112:GLN:HA	5:E:243:LEU:HD23	1.77	0.67
1:A:226:LEU:HD22	1:A:245:ASN:HD21	1.59	0.67
1:A:338:SER:HB2	1:A:341:GLU:H	1.59	0.67
12:W:283:TRP:CH2	12:W:394:HIS:HD2	2.12	0.67
12:W:397:PHE:CE1	12:W:401:CYS:SG	2.88	0.66
13:X:17:ALA:O	13:X:21:SER:HB2	1.96	0.66
1:A:544:VAL:HG11	1:A:562:LEU:HD23	1.77	0.66
9:S:28:LEU:HA	9:S:32:ASN:OD1	1.95	0.66
12:W:263:GLN:O	12:W:349:THR:HA	1.95	0.66
1:A:248:ILE:HD12	1:A:258:ILE:HG21	1.77	0.66
1:A:232:THR:HG23	1:A:233:PRO:HD3	1.77	0.66
1:A:278:LEU:O	1:A:282:THR:HG23	1.95	0.66
9:S:48:ASN:HB3	9:S:73:LEU:HD21	1.77	0.66
12:W:266:LEU:HD22	12:W:310:ILE:HD12	1.78	0.66
11:V:79:LEU:HB2	15:Z:81:TRP:CH2	2.31	0.66
1:A:204:ASN:O	1:A:227:PRO:HA	1.96	0.66
7:G:152:PHE:CZ	7:G:169:LEU:HD22	2.30	0.66
7:G:11:GLU:O	7:G:15:ASN:ND2	2.29	0.66
12:W:283:TRP:HE1	12:W:307:GLU:CD	1.98	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:104:ILE:CG1	12:W:394:HIS:HE1	2.08	0.66
12:W:288:GLN:CG	15:Z:93:VAL:HG11	2.25	0.66
9:S:109:PHE:CZ	10:U:78:PRO:HG2	2.32	0.65
12:W:150:PRO:O	12:W:153:SER:OG	2.14	0.65
4:D:136:PHE:CZ	6:F:87:LYS:HA	2.30	0.65
1:A:47:LYS:HG3	3:C:99:VAL:HG11	1.78	0.65
13:X:92:ASP:OD1	13:X:92:ASP:N	2.29	0.65
11:V:27:LEU:HD21	11:V:71:GLY:HA3	1.77	0.65
12:W:501:LEU:HD13	12:W:502:HIS:CE1	2.32	0.65
3:C:71:ASP:OD1	3:C:73:THR:OG1	2.14	0.65
4:D:12:ILE:HG22	4:D:72:ILE:HD13	1.78	0.65
12:W:268:ILE:O	12:W:280:SER:HA	1.96	0.65
12:W:391:ALA:O	12:W:394:HIS:HB3	1.97	0.65
12:W:283:TRP:CZ3	12:W:394:HIS:CD2	2.84	0.65
1:A:222:PHE:CE2	1:A:252:PHE:HA	2.32	0.65
1:A:96:ASN:O	1:A:100:VAL:HG23	1.97	0.65
1:A:375:ASP:OD1	1:A:375:ASP:N	2.29	0.65
8:R:16:ARG:NH2	8:R:53:TYR:OH	2.30	0.65
12:W:283:TRP:CH2	12:W:394:HIS:CD2	2.85	0.65
1:A:155:LEU:HD13	12:W:56:LEU:HD22	1.79	0.65
1:A:113:LEU:HD11	5:E:272:ASN:HA	1.78	0.64
10:U:13:LEU:HA	10:U:16:ILE:HG23	1.79	0.64
15:Z:18:ASN:O	15:Z:21:ILE:N	2.30	0.64
2:B:41:SER:O	2:B:45:PRO:HD2	1.97	0.64
14:Y:108:PHE:HB3	14:Y:130:TYR:HA	1.79	0.64
6:F:19:ASP:HA	6:F:22:ILE:HD12	1.78	0.64
1:A:222:PHE:HD2	1:A:255:GLN:HA	1.62	0.64
12:W:172:ALA:HB1	15:Z:49:VAL:HG21	1.79	0.64
1:A:154:ILE:HA	1:A:157:THR:HG23	1.79	0.64
1:A:54:LEU:HD21	2:B:28:LEU:HD23	1.79	0.64
10:U:20:ILE:O	10:U:24:VAL:HG23	1.97	0.64
14:Y:96:PHE:CD1	14:Y:117:GLN:HB3	2.32	0.64
1:A:272:TYR:CE1	1:A:303:PRO:HG2	2.33	0.64
11:V:76:ALA:O	11:V:79:LEU:HB3	1.97	0.64
12:W:396:LEU:HD12	12:W:424:ILE:HB	1.80	0.64
15:Z:100:LEU:O	15:Z:103:VAL:HG12	1.98	0.63
6:F:60:VAL:O	6:F:63:MET:HB2	1.97	0.63
2:B:79:GLN:NE2	9:S:62:ASP:OD2	2.31	0.63
8:R:86:ASP:HB3	8:R:92:LEU:HD13	1.79	0.63
9:S:143:ILE:O	9:S:147:PRO:HD3	1.98	0.63
1:A:205:SER:HA	1:A:226:LEU:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:63:PHE:O	8:R:16:ARG:NH1	2.24	0.63
1:A:305:LEU:H	1:A:330:ILE:HG22	1.64	0.63
1:A:388:GLN:O	1:A:391:ALA:HB3	1.98	0.63
9:S:48:ASN:ND2	9:S:76:ILE:O	2.32	0.63
11:V:79:LEU:HD12	15:Z:81:TRP:HZ3	1.63	0.63
1:A:194:PRO:O	1:A:195:ASN:ND2	2.21	0.63
8:R:91:ASP:N	8:R:91:ASP:OD1	2.32	0.63
1:A:289:SER:O	1:A:291:LEU:N	2.31	0.63
10:U:110:THR:HG21	12:W:175:TRP:HE1	1.64	0.63
12:W:310:ILE:CA	12:W:397:PHE:HE2	2.10	0.63
12:W:50:ASP:N	12:W:50:ASP:OD1	2.30	0.63
13:X:41:PRO:HG2	13:X:51:GLN:HE21	1.64	0.63
10:U:197:SER:HB2	13:X:55:TRP:HZ2	1.63	0.63
11:V:79:LEU:CA	15:Z:81:TRP:HH2	2.11	0.63
2:B:82:ASN:HB3	2:B:85:VAL:HG23	1.81	0.62
11:V:104:ILE:CB	12:W:394:HIS:HE1	2.12	0.62
1:A:285:LEU:HD21	1:A:380:GLN:HB2	1.81	0.62
5:E:66:PRO:HG3	8:R:56:TYR:CE1	2.34	0.62
12:W:337:ILE:HG22	12:W:341:HIS:HB2	1.81	0.62
14:Y:15:ALA:HA	14:Y:122:LYS:HB2	1.80	0.62
9:S:150:ASN:OD1	9:S:152:GLN:HG2	2.00	0.62
12:W:425:LEU:O	12:W:429:ILE:HG22	2.00	0.62
1:A:301:LYS:HB2	1:A:302:PRO:HD2	1.80	0.62
13:X:67:GLU:HA	13:X:153:LYS:HD2	1.82	0.62
5:E:315:TYR:OH	7:G:81:GLU:OE1	2.17	0.62
13:X:41:PRO:HG2	13:X:51:GLN:HB2	1.82	0.62
13:X:55:TRP:HZ3	13:X:121:SER:HG	1.47	0.62
1:A:157:THR:HG22	7:G:91:PRO:CG	2.24	0.61
11:V:20:GLN:HG2	15:Z:81:TRP:NE1	2.15	0.61
5:E:241:GLU:O	5:E:245:ILE:HG22	1.99	0.61
6:F:49:LEU:O	6:F:53:ILE:HG22	2.00	0.61
1:A:149:LEU:HB3	12:W:40:LYS:HE2	1.80	0.61
14:Y:96:PHE:HD1	14:Y:117:GLN:HB3	1.65	0.61
1:A:114:ARG:HD2	1:A:114:ARG:H	1.64	0.61
1:A:70:TRP:CD1	2:B:83:PRO:HB2	2.36	0.61
14:Y:152:LEU:HA	14:Y:155:ASN:HB2	1.82	0.61
4:D:35:LEU:HB3	4:D:36:PRO:HD2	1.81	0.61
9:S:111:CYS:O	9:S:114:ASN:HB2	1.99	0.61
5:E:14:PRO:HG2	8:R:26:MET:HE1	1.82	0.61
5:E:67:SER:OG	5:E:67:SER:O	2.18	0.61
1:A:222:PHE:CZ	1:A:258:ILE:HG23	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:HD13	1:A:368:VAL:H	1.66	0.61
9:S:109:PHE:HB3	9:S:116:TYR:HB2	1.81	0.61
12:W:128:LEU:HD21	12:W:153:SER:HB2	1.82	0.61
7:G:117:PHE:CD2	8:R:67:ILE:HG23	2.34	0.61
4:D:107:ARG:HB2	5:E:298:VAL:HG22	1.83	0.61
12:W:207:GLU:HG3	12:W:253:PHE:CE2	2.35	0.61
12:W:393:ALA:HB1	12:W:424:ILE:HD11	1.82	0.61
13:X:39:TYR:HB3	13:X:118:TYR:HB3	1.82	0.61
14:Y:15:ALA:CA	14:Y:122:LYS:HB2	2.30	0.61
4:D:124:ARG:NH1	5:E:316:LYS:HE2	2.16	0.61
11:V:112:MET:HG3	15:Z:103:VAL:HG23	1.83	0.60
1:A:132:ARG:NH2	8:R:100:ILE:HD13	2.15	0.60
11:V:92:LYS:HG3	11:V:95:TYR:CE1	2.30	0.60
11:V:104:ILE:HG22	11:V:105:PHE:CD1	2.35	0.60
14:Y:108:PHE:CD2	14:Y:130:TYR:HD1	2.16	0.60
5:E:14:PRO:HB3	7:G:152:PHE:CD1	2.36	0.60
12:W:45:ARG:NH2	12:W:59:GLU:OE2	2.34	0.60
12:W:420:ASN:N	12:W:420:ASN:OD1	2.34	0.60
1:A:164:LEU:HD21	1:A:213:ILE:HG23	1.83	0.60
9:S:82:HIS:H	9:S:90:VAL:HB	1.67	0.60
1:A:195:ASN:HB2	1:A:201:LEU:H	1.65	0.60
2:B:56:LYS:O	2:B:59:PRO:HD2	2.02	0.60
1:A:180:GLN:CG	4:D:137:GLN:HB3	2.32	0.60
5:E:60:ALA:O	5:E:64:LYS:HG2	2.02	0.60
9:S:77:GLN:HE22	9:S:96:ARG:HD2	1.66	0.60
2:B:85:VAL:HA	3:C:51:MET:HE1	1.84	0.59
12:W:392:ILE:HD11	12:W:473:LEU:HD13	1.84	0.59
12:W:488:ASN:OD1	12:W:488:ASN:N	2.33	0.59
1:A:520:TYR:HB2	1:A:527:TRP:CZ3	2.38	0.59
9:S:17:ARG:HB3	9:S:114:ASN:HA	1.84	0.59
10:U:16:ILE:O	10:U:20:ILE:HG22	2.02	0.59
13:X:45:PRO:HD2	13:X:49:PRO:HG2	1.83	0.59
1:A:407:PHE:HD1	1:A:418:HIS:HB2	1.67	0.59
1:A:209:LYS:HD3	1:A:216:GLN:HE22	1.68	0.59
5:E:246:MET:HE3	5:E:253:PHE:HB3	1.84	0.59
6:F:73:LYS:HB3	7:G:57:LEU:HD22	1.84	0.59
12:W:232:SER:O	12:W:232:SER:OG	2.15	0.59
13:X:149:GLN:OE1	13:X:149:GLN:N	2.34	0.59
10:U:196:LYS:HA	13:X:57:ARG:HH22	1.68	0.59
12:W:288:GLN:HB2	15:Z:93:VAL:CG2	2.32	0.59
1:A:309:TYR:HD1	1:A:309:TYR:H	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:120:GLN:OE1	5:E:312:LEU:HD11	2.02	0.59
12:W:501:LEU:HD13	12:W:502:HIS:HE1	1.67	0.59
1:A:225:HIS:HB2	1:A:258:ILE:HD12	1.84	0.59
9:S:110:VAL:HG22	9:S:115:ILE:HG22	1.84	0.59
14:Y:8:TYR:CE2	14:Y:185:ARG:HD3	2.37	0.59
14:Y:38:VAL:HA	14:Y:98:ILE:O	2.03	0.59
9:S:30:THR:HG22	9:S:83:GLU:OE2	2.02	0.59
14:Y:45:ARG:O	14:Y:91:ASN:HB2	2.03	0.59
1:A:297:VAL:HG11	1:A:306:ARG:HE	1.68	0.59
7:G:34:TRP:O	7:G:38:VAL:HG23	2.03	0.59
13:X:86:SER:HB3	13:X:207:LEU:N	2.15	0.59
1:A:63:ARG:HH21	3:C:69:LEU:HG	1.68	0.58
7:G:119:SER:C	8:R:104:TRP:HH2	2.06	0.58
1:A:301:LYS:O	9:S:204:GLN:NE2	2.36	0.58
11:V:107:GLN:NE2	12:W:284:SER:O	2.35	0.58
12:W:396:LEU:HD13	12:W:396:LEU:C	2.23	0.58
1:A:209:LYS:HD2	1:A:224:PHE:CG	2.39	0.58
2:B:137:GLY:HA3	5:E:248:LYS:HD3	1.86	0.58
4:D:121:LEU:HD22	7:G:86:TYR:HB2	1.84	0.58
8:R:33:LEU:HB3	8:R:87:ILE:HD12	1.85	0.58
12:W:329:THR:OG1	12:W:332:GLU:OE1	2.20	0.58
1:A:331:PHE:O	1:A:358:LEU:HD12	2.04	0.58
6:F:68:MET:N	6:F:68:MET:SD	2.76	0.58
9:S:96:ARG:HB3	9:S:102:VAL:HG13	1.85	0.58
12:W:263:GLN:HE21	12:W:263:GLN:HA	1.68	0.58
1:A:204:ASN:OD1	12:W:49:ARG:NH2	2.36	0.58
13:X:125:ILE:HB	13:X:144:LEU:O	2.02	0.58
1:A:138:THR:OG1	8:R:99:GLU:OE1	2.20	0.58
1:A:86:PHE:HD2	1:A:87:LEU:HD12	1.68	0.58
5:E:66:PRO:HG3	8:R:56:TYR:CZ	2.39	0.58
9:S:124:LEU:HD13	10:U:97:THR:HG22	1.86	0.58
11:V:101:SER:O	11:V:104:ILE:HB	2.04	0.58
11:V:108:SER:O	11:V:112:MET:HG2	2.04	0.58
10:U:20:ILE:HD11	12:W:119:CYS:HB3	1.86	0.58
7:G:44:LEU:O	7:G:48:ILE:HG23	2.03	0.57
1:A:237:ARG:O	1:A:240:ILE:HG12	2.03	0.57
1:A:383:LEU:O	1:A:387:THR:OG1	2.18	0.57
6:F:72:GLU:O	6:F:76:ILE:HG23	2.05	0.57
7:G:117:PHE:HD2	8:R:67:ILE:HG23	1.69	0.57
15:Z:51:PRO:O	15:Z:55:GLN:HG3	2.05	0.57
7:G:140:TRP:HB2	7:G:141:PRO:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:32:ASN:O	9:S:32:ASN:ND2	2.37	0.57
1:A:161:LEU:O	1:A:165:ILE:HG13	2.04	0.57
9:S:196:PHE:O	9:S:200:ARG:HG2	2.03	0.57
1:A:162:ASN:ND2	1:A:187:GLY:H	2.02	0.57
9:S:195:ASP:OD1	9:S:195:ASP:N	2.30	0.57
12:W:143:PRO:HA	12:W:146:LYS:HG2	1.85	0.57
12:W:520:PHE:CD2	12:W:525:ASN:HB3	2.39	0.57
14:Y:52:THR:HG22	14:Y:68:VAL:HA	1.85	0.57
4:D:30:HIS:HB2	4:D:49:ILE:H	1.70	0.57
12:W:110:GLU:O	12:W:114:ILE:HG22	2.05	0.57
14:Y:54:GLU:HG2	14:Y:66:ALA:HB1	1.86	0.57
5:E:16:PRO:HA	7:G:151:LEU:HD11	1.86	0.57
7:G:199:MET:SD	7:G:199:MET:N	2.78	0.57
10:U:31:LEU:HA	10:U:34:LEU:HD12	1.87	0.57
11:V:58:SER:O	11:V:62:LEU:HD12	2.03	0.57
12:W:267:LYS:HA	12:W:282:THR:HG22	1.86	0.57
10:U:83:PRO:HA	10:U:86:GLU:CB	2.27	0.57
8:R:41:TYR:HB3	8:R:47:PHE:CD2	2.40	0.56
9:S:77:GLN:NE2	9:S:96:ARG:HD2	2.20	0.56
9:S:131:ASN:OD1	10:U:100:LEU:HB2	2.05	0.56
1:A:129:THR:HG22	8:R:69:PRO:HB2	1.86	0.56
8:R:41:TYR:HB3	8:R:47:PHE:CE2	2.40	0.56
1:A:124:ILE:HD11	8:R:69:PRO:HB3	1.86	0.56
1:A:258:ILE:O	1:A:262:ILE:HG22	2.05	0.56
4:D:118:LYS:HE2	5:E:304:HIS:NE2	2.20	0.56
9:S:81:ILE:HG13	9:S:92:GLN:HB3	1.86	0.56
15:Z:47:TYR:O	15:Z:51:PRO:HD2	2.06	0.56
1:A:209:LYS:HB3	1:A:224:PHE:CD2	2.41	0.56
5:E:290:GLN:OE1	12:W:23:ILE:HA	2.05	0.56
10:U:194:PHE:HD1	10:U:199:LYS:H	1.53	0.56
13:X:38:VAL:HG13	13:X:57:ARG:HB3	1.88	0.56
2:B:25:PHE:CD1	2:B:51:LEU:HD11	2.41	0.56
5:E:246:MET:HE2	5:E:250:PRO:HA	1.88	0.56
13:X:112:PHE:CD2	14:Y:74:ILE:HG13	2.41	0.56
14:Y:15:ALA:HB1	14:Y:122:LYS:HE2	1.87	0.56
1:A:546:THR:HG21	1:A:559:LEU:HD11	1.88	0.56
9:S:29:ARG:HB2	9:S:32:ASN:HB3	1.88	0.56
12:W:397:PHE:C	12:W:397:PHE:CD1	2.79	0.56
1:A:149:LEU:HD13	12:W:44:GLU:HG3	1.87	0.56
1:A:399:ARG:HA	1:A:402:LEU:HD22	1.88	0.56
3:C:64:GLY:O	3:C:66:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:PRO:HB3	5:E:280:ARG:CZ	2.36	0.56
8:R:42:PHE:CD1	8:R:84:ARG:HD3	2.41	0.56
1:A:189:CYS:HB2	1:A:205:SER:O	2.06	0.56
2:B:88:ARG:HE	3:C:41:ARG:HG2	1.71	0.56
13:X:7:LEU:HA	13:X:167:LEU:O	2.06	0.56
14:Y:121:TRP:CH2	14:Y:123:GLY:HA3	2.41	0.56
1:A:357:LEU:HD23	1:A:358:LEU:H	1.71	0.55
1:A:158:LEU:HG	1:A:187:GLY:HA2	1.88	0.55
9:S:30:THR:OG1	9:S:31:GLU:N	2.37	0.55
15:Z:84:ASN:ND2	15:Z:84:ASN:O	2.39	0.55
2:B:33:TYR:CD2	3:C:107:PHE:HE2	2.24	0.55
3:C:65:TYR:HE1	3:C:67:GLU:HG3	1.71	0.55
8:R:70:THR:HG22	8:R:74:MET:HG2	1.87	0.55
12:W:392:ILE:CD1	12:W:473:LEU:HD13	2.36	0.55
14:Y:38:VAL:HG12	14:Y:99:GLU:HB3	1.88	0.55
6:F:87:LYS:NZ	7:G:72:ASP:OD1	2.37	0.55
14:Y:37:TRP:HB2	14:Y:102:ILE:HD12	1.87	0.55
1:A:138:THR:HG21	8:R:95:GLN:HB3	1.89	0.55
1:A:403:HIS:CG	1:A:404:PRO:HD2	2.42	0.55
1:A:20:VAL:HB	2:B:62:SER:OG	2.07	0.55
12:W:307:GLU:HA	12:W:310:ILE:HG22	1.87	0.55
11:V:104:ILE:CG1	12:W:394:HIS:CE1	2.89	0.55
12:W:396:LEU:HD12	12:W:424:ILE:CA	2.36	0.55
1:A:188:ARG:HH12	12:W:48:PHE:HD1	1.55	0.55
1:A:166:ARG:HB2	1:A:184:ILE:HD13	1.88	0.55
1:A:216:GLN:NE2	1:A:223:GLN:HG2	2.22	0.55
6:F:69:THR:HB	6:F:72:GLU:HB2	1.87	0.55
14:Y:5:GLY:CA	14:Y:165:PHE:HB3	2.37	0.55
1:A:502:THR:HB	1:A:517:VAL:HG11	1.89	0.55
2:B:80:GLY:HA2	3:C:55:TYR:CE2	2.41	0.55
14:Y:148:LEU:HA	14:Y:155:ASN:ND2	2.21	0.55
8:R:52:GLU:HA	8:R:55:GLU:HG2	1.89	0.55
1:A:209:LYS:HE2	1:A:212:GLY:H	1.72	0.55
1:A:222:PHE:HE1	1:A:258:ILE:HG12	1.71	0.55
12:W:193:ARG:HG3	12:W:194:LEU:N	2.21	0.55
14:Y:163:GLU:HG3	14:Y:181:LEU:HD11	1.89	0.55
2:B:49:ASP:O	2:B:52:ILE:HG13	2.07	0.55
8:R:28:SER:HB3	8:R:70:THR:HB	1.89	0.55
9:S:81:ILE:CG1	9:S:92:GLN:HB3	2.37	0.55
13:X:47:ASN:HB3	13:X:48:LEU:HD12	1.89	0.55
1:A:189:CYS:O	1:A:204:ASN:CA	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:80:LEU:CD2	7:G:64:LEU:HB3	2.35	0.54
12:W:288:GLN:NE2	12:W:299:TYR:CE2	2.76	0.54
10:U:76:ILE:HG22	10:U:95:LEU:HD11	1.89	0.54
9:S:128:ARG:HD3	12:W:118:GLU:HG3	1.88	0.54
10:U:198:GLY:H	13:X:122:HIS:CE1	2.24	0.54
14:Y:116:LEU:HA	14:Y:121:TRP:CD1	2.43	0.54
11:V:79:LEU:HA	15:Z:81:TRP:CH2	2.42	0.54
4:D:17:THR:HA	4:D:20:TYR:HE1	1.69	0.54
7:G:147:ARG:O	7:G:147:ARG:NE	2.41	0.54
7:G:150:LEU:CB	8:R:19:ILE:HD11	2.38	0.54
1:A:23:PHE:HZ	1:A:61:THR:HG22	1.72	0.54
1:A:513:ASP:HB2	1:A:534:ALA:HB2	1.90	0.54
12:W:266:LEU:HD22	12:W:310:ILE:CD1	2.37	0.54
1:A:516:TRP:CD2	1:A:531:LEU:HB3	2.42	0.54
9:S:193:PRO:HA	9:S:196:PHE:HB3	1.90	0.54
10:U:13:LEU:HA	10:U:16:ILE:CG2	2.38	0.54
1:A:11:GLU:HB2	7:G:200:ASN:ND2	2.18	0.54
1:A:222:PHE:HE2	1:A:251:ALA:C	2.11	0.54
1:A:310:TRP:NE1	1:A:430:SER:O	2.37	0.54
4:D:82:ILE:HG21	5:E:277:HIS:CE1	2.42	0.54
6:F:84:ILE:HA	6:F:87:LYS:HG3	1.89	0.54
11:V:79:LEU:CA	15:Z:81:TRP:CH2	2.91	0.54
1:A:201:LEU:HD21	1:A:266:LEU:CG	2.36	0.54
7:G:6:ALA:O	7:G:10:ILE:HG12	2.08	0.54
9:S:48:ASN:HB3	9:S:73:LEU:CD2	2.38	0.54
9:S:48:ASN:N	9:S:48:ASN:HD22	2.05	0.54
1:A:162:ASN:HD21	1:A:187:GLY:N	2.05	0.53
1:A:222:PHE:CE1	1:A:258:ILE:HG12	2.43	0.53
9:S:63:LEU:O	9:S:66:LEU:HB3	2.09	0.53
10:U:152:SER:HB3	10:U:160:ARG:HH12	1.73	0.53
12:W:53:GLU:O	12:W:57:GLN:HG2	2.07	0.53
13:X:171:THR:HG21	13:X:185:ALA:HB1	1.90	0.53
14:Y:5:GLY:HA2	14:Y:165:PHE:HB3	1.89	0.53
1:A:505:LYS:HD2	1:A:508:TRP:CZ2	2.43	0.53
7:G:114:LEU:HD23	7:G:118:SER:HB2	1.89	0.53
8:R:60:PRO:HA	8:R:63:VAL:HG12	1.89	0.53
12:W:335:VAL:HB	12:W:343:VAL:CG2	2.37	0.53
13:X:35:PHE:HB2	13:X:62:ILE:HD11	1.90	0.53
1:A:199:VAL:HG11	1:A:231:SER:OG	2.07	0.53
1:A:105:ARG:NH2	4:D:13:ASP:HB3	2.23	0.53
9:S:62:ASP:OD1	9:S:62:ASP:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:138:ASP:OD1	10:U:141:ARG:NH1	2.41	0.53
1:A:105:ARG:HH22	4:D:13:ASP:HB3	1.73	0.53
1:A:76:SER:HB2	3:C:35:LEU:HD22	1.91	0.53
4:D:6:THR:HB	5:E:275:ARG:NH2	2.15	0.53
5:E:327:ASP:O	5:E:331:GLN:HG2	2.09	0.53
8:R:21:LEU:O	8:R:25:GLN:NE2	2.39	0.53
9:S:84:ARG:HB3	9:S:88:LEU:HD23	1.91	0.53
3:C:69:LEU:H	3:C:69:LEU:HD23	1.74	0.53
5:E:294:GLU:O	5:E:298:VAL:HG23	2.08	0.53
5:E:319:ASP:OD1	5:E:319:ASP:N	2.41	0.53
1:A:9:ILE:HD11	1:A:85:ALA:HB2	1.91	0.53
5:E:65:LYS:O	8:R:53:TYR:OH	2.26	0.53
12:W:493:ILE:HG13	12:W:513:ASP:HB3	1.91	0.53
13:X:32:ILE:HG13	13:X:32:ILE:O	2.08	0.53
4:D:125:ILE:HD11	7:G:82:MET:HB3	1.90	0.53
10:U:107:GLU:O	10:U:111:LEU:HG	2.09	0.53
10:U:31:LEU:HD21	12:W:113:MET:HG2	1.91	0.53
12:W:220:ASN:HA	12:W:227:LEU:HD23	1.91	0.53
1:A:186:ASN:OD1	12:W:53:GLU:N	2.41	0.52
1:A:390:HIS:O	1:A:394:ILE:HG22	2.09	0.52
6:F:73:LYS:HB3	7:G:57:LEU:CD2	2.39	0.52
11:V:104:ILE:CG2	12:W:394:HIS:HE1	2.22	0.52
1:A:28:LEU:HB3	3:C:86:VAL:HG21	1.89	0.52
4:D:82:ILE:HG21	5:E:277:HIS:NE2	2.24	0.52
7:G:147:ARG:HH11	7:G:173:GLN:CD	2.12	0.52
6:F:57:LYS:NZ	7:G:8:ASP:OD1	2.31	0.52
12:W:130:LEU:O	12:W:134:LYS:N	2.42	0.52
3:C:11:GLY:N	5:E:241:GLU:OE1	2.34	0.52
1:A:221:ASP:OD1	1:A:222:PHE:HB2	2.10	0.52
2:B:139:VAL:HG22	3:C:17:PRO:HD2	1.91	0.52
5:E:12:ALA:HB1	7:G:165:THR:HG23	1.90	0.52
12:W:33:ASN:O	12:W:37:ILE:HG13	2.10	0.52
5:E:253:PHE:N	5:E:254:PRO:HD2	2.24	0.52
6:F:22:ILE:O	6:F:26:ARG:HG3	2.10	0.52
1:A:11:GLU:OE1	7:G:200:ASN:ND2	2.41	0.52
8:R:81:PRO:HA	8:R:84:ARG:HG3	1.92	0.52
9:S:195:ASP:O	9:S:199:VAL:HG23	2.09	0.52
12:W:128:LEU:HD11	12:W:153:SER:HB2	1.92	0.52
14:Y:53:LEU:HD11	14:Y:183:LYS:HZ2	1.75	0.52
2:B:112:GLN:HB2	5:E:243:LEU:HB3	1.91	0.52
1:A:215:PHE:CD1	1:A:215:PHE:N	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TRP:O	1:A:220:VAL:HG22	2.09	0.52
5:E:275:ARG:O	5:E:278:GLN:N	2.43	0.52
14:Y:80:LEU:O	14:Y:83:ILE:HB	2.10	0.52
14:Y:81:GLU:HG3	14:Y:93:ARG:HH22	1.74	0.52
14:Y:39:VAL:HG22	14:Y:98:ILE:HB	1.91	0.52
15:Z:97:GLU:HA	15:Z:97:GLU:OE2	2.09	0.52
4:D:114:ASN:HD21	4:D:118:LYS:HE3	1.74	0.52
13:X:90:ARG:CZ	13:X:96:ILE:HD11	2.39	0.52
1:A:484:ALA:HB2	1:A:556:PHE:CZ	2.44	0.52
6:F:76:ILE:HA	6:F:79:ILE:HG22	1.92	0.52
7:G:90:LEU:HD22	7:G:90:LEU:H	1.75	0.52
10:U:82:PHE:CZ	10:U:91:LEU:HB2	2.44	0.52
12:W:230:GLN:O	12:W:233:CYS:HB3	2.09	0.52
12:W:283:TRP:CZ3	12:W:394:HIS:HD2	2.24	0.52
14:Y:37:TRP:HA	14:Y:58:GLN:HE22	1.75	0.52
11:V:79:LEU:HD12	15:Z:81:TRP:CZ3	2.44	0.52
1:A:186:ASN:ND2	12:W:53:GLU:HB2	2.25	0.52
1:A:86:PHE:CD2	1:A:87:LEU:HD12	2.45	0.52
12:W:171:LEU:HD23	15:Z:46:LYS:HD2	1.92	0.52
12:W:288:GLN:NE2	12:W:299:TYR:CZ	2.78	0.52
12:W:491:PRO:HG3	12:W:514:GLN:NE2	2.24	0.52
14:Y:15:ALA:HA	14:Y:122:LYS:O	2.10	0.52
8:R:58:ARG:HH22	8:R:76:THR:HG23	1.75	0.51
9:S:18:MET:HG2	9:S:21:TRP:H	1.75	0.51
11:V:17:ASP:N	11:V:17:ASP:OD1	2.43	0.51
1:A:216:GLN:HA	1:A:216:GLN:HE21	1.75	0.51
5:E:19:TYR:HB2	5:E:63:PHE:CE1	2.45	0.51
13:X:131:TYR:HB2	13:X:138:VAL:HG13	1.91	0.51
11:V:100:LEU:HB2	12:W:234:LEU:HB3	1.92	0.51
12:W:314:LEU:HD11	12:W:424:ILE:CD1	2.39	0.51
12:W:33:ASN:O	12:W:36:GLN:HG2	2.10	0.51
11:V:104:ILE:CG2	12:W:394:HIS:CE1	2.93	0.51
1:A:207:ASP:OD1	1:A:209:LYS:HG2	2.09	0.51
1:A:295:ARG:HB3	1:A:308:TYR:HB2	1.91	0.51
4:D:121:LEU:O	4:D:125:ILE:HG12	2.10	0.51
5:E:256:LYS:O	5:E:260:ILE:HG12	2.11	0.51
1:A:116:SER:HB3	7:G:111:GLY:C	2.30	0.51
13:X:173:VAL:HG21	13:X:182:MET:SD	2.50	0.51
5:E:246:MET:CE	5:E:253:PHE:HB3	2.39	0.51
4:D:100:ILE:HG22	5:E:291:LEU:HD12	1.91	0.51
5:E:29:GLU:HA	5:E:32:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:U:82:PHE:CE2	10:U:86:GLU:HA	2.45	0.51
3:C:14:ASP:N	3:C:14:ASP:OD1	2.43	0.51
4:D:9:GLN:O	4:D:12:ILE:HG12	2.10	0.51
10:U:40:LEU:HB3	12:W:105:LYS:HB2	1.92	0.51
12:W:208:LEU:HD23	12:W:227:LEU:HD12	1.92	0.51
12:W:288:GLN:CB	15:Z:93:VAL:HG21	2.39	0.51
1:A:23:PHE:HZ	1:A:61:THR:CG2	2.23	0.51
13:X:21:SER:C	13:X:199:PHE:HZ	2.14	0.51
12:W:397:PHE:HD1	12:W:397:PHE:C	2.14	0.51
1:A:489:LEU:CD1	1:A:505:LYS:HE3	2.41	0.51
1:A:533:ASN:HB3	1:A:539:LEU:HD11	1.92	0.51
8:R:78:LEU:HA	8:R:83:PHE:CD2	2.45	0.51
12:W:127:SER:O	12:W:137:SER:HB2	2.11	0.51
12:W:514:GLN:HG2	12:W:515:TYR:CD1	2.46	0.51
15:Z:18:ASN:HA	15:Z:21:ILE:HG22	1.91	0.51
1:A:173:GLU:HB2	1:A:220:VAL:HG12	1.93	0.51
13:X:206:ARG:HG3	13:X:207:LEU:HG	1.93	0.51
1:A:206:GLN:O	1:A:226:LEU:CB	2.52	0.50
1:A:567:ILE:O	1:A:571:ASN:ND2	2.43	0.50
7:G:149:THR:HG23	7:G:152:PHE:H	1.76	0.50
7:G:81:GLU:O	7:G:85:ILE:HG12	2.11	0.50
10:U:38:GLU:O	12:W:102:GLN:NE2	2.27	0.50
8:R:12:ASP:OD1	8:R:13:ASP:N	2.44	0.50
10:U:19:ARG:O	10:U:23:ILE:HG22	2.11	0.50
13:X:43:ASP:N	13:X:43:ASP:OD1	2.43	0.50
14:Y:89:LEU:HD12	14:Y:90:TRP:CE3	2.46	0.50
1:A:179:PHE:HE2	1:A:263:TYR:HB2	1.75	0.50
1:A:295:ARG:HD3	1:A:308:TYR:CD2	2.40	0.50
12:W:34:LEU:HA	12:W:37:ILE:HD12	1.94	0.50
14:Y:38:VAL:O	14:Y:58:GLN:HB3	2.11	0.50
10:U:41:SER:HB3	10:U:42:PRO:HD2	1.94	0.50
12:W:99:MET:N	12:W:99:MET:SD	2.85	0.50
1:A:215:PHE:HD1	1:A:215:PHE:N	2.09	0.50
4:D:93:ILE:CD1	5:E:284:ILE:HG12	2.42	0.50
2:B:109:GLU:HG2	5:E:247:ALA:HB1	1.93	0.50
7:G:146:MET:O	7:G:149:THR:HG22	2.11	0.50
9:S:34:LEU:HD21	9:S:80:ILE:HG13	1.94	0.50
14:Y:12:PRO:O	14:Y:15:ALA:CB	2.55	0.50
14:Y:67:CYS:HB2	14:Y:73:MET:HG2	1.93	0.50
15:Z:97:GLU:CD	15:Z:98:PRO:HD2	2.32	0.50
1:A:423:GLU:H	1:A:440:SER:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:GLY:C	4:D:31:ASP:HB3	2.32	0.50
4:D:30:HIS:CE1	4:D:32:PHE:HB2	2.47	0.50
11:V:79:LEU:HD21	15:Z:13:ARG:CZ	2.41	0.50
1:A:216:GLN:HE21	1:A:223:GLN:HG2	1.76	0.50
1:A:333:ASN:OD1	1:A:334:THR:N	2.45	0.50
4:D:69:PHE:CE2	5:E:236:MET:HB2	2.47	0.50
12:W:321:CYS:SG	12:W:326:VAL:HG21	2.52	0.50
1:A:222:PHE:CE1	1:A:258:ILE:HG23	2.46	0.50
1:A:429:ASN:OD1	1:A:432:THR:N	2.39	0.50
5:E:238:ASN:HD21	5:E:259:ASN:HD22	1.57	0.50
5:E:224:ARG:NH1	5:E:273:ASP:HB3	2.27	0.50
9:S:38:SER:HA	9:S:43:TYR:CD2	2.47	0.50
12:W:111:GLN:O	12:W:114:ILE:HG23	2.12	0.50
13:X:58:LEU:HB2	13:X:80:MET:HA	1.93	0.50
1:A:183:THR:HB	1:A:190:THR:CG2	2.41	0.49
8:R:97:ASN:O	8:R:100:ILE:HG23	2.11	0.49
9:S:67:ASN:O	9:S:71:LYS:HG2	2.12	0.49
14:Y:29:TYR:HE2	14:Y:149:LYS:HE2	1.77	0.49
1:A:224:PHE:CD1	1:A:224:PHE:N	2.80	0.49
1:A:268:LYS:HE3	1:A:356:PHE:CE2	2.47	0.49
4:D:118:LYS:HG2	5:E:308:MET:SD	2.52	0.49
12:W:288:GLN:HG3	15:Z:93:VAL:HG11	1.93	0.49
14:Y:141:PRO:O	14:Y:145:GLU:HB2	2.11	0.49
1:A:264:ASN:ND2	1:A:354:ASP:HB3	2.27	0.49
4:D:55:GLN:HA	4:D:58:GLN:HE21	1.75	0.49
5:E:251:GLU:OE2	5:E:251:GLU:N	2.40	0.49
10:U:20:ILE:HA	10:U:23:ILE:CG2	2.42	0.49
1:A:129:THR:CG2	8:R:69:PRO:HB2	2.43	0.49
1:A:298:TYR:HD1	1:A:299:ASP:N	2.10	0.49
12:W:292:SER:OG	12:W:295:LEU:HD13	2.12	0.49
14:Y:4:HIS:HB3	14:Y:129:THR:HG22	1.94	0.49
1:A:114:ARG:HD2	1:A:114:ARG:N	2.26	0.49
1:A:222:PHE:HE1	1:A:258:ILE:N	2.10	0.49
1:A:260:PRO:O	1:A:263:TYR:N	2.46	0.49
2:B:71:GLN:NE2	9:S:59:ASN:OD1	2.44	0.49
5:E:19:TYR:HE2	8:R:50:TYR:HH	1.59	0.49
6:F:87:LYS:NZ	7:G:68:ASP:OD1	2.45	0.49
9:S:128:ARG:NH1	12:W:118:GLU:OE2	2.45	0.49
12:W:133:PHE:CZ	12:W:156:PHE:HE1	2.31	0.49
12:W:272:ASN:HB3	12:W:278:ILE:HD11	1.94	0.49
13:X:90:ARG:CZ	13:X:93:LYS:HD3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:120:ALA:N	8:R:104:TRP:HH2	2.11	0.49
14:Y:152:LEU:HA	14:Y:155:ASN:ND2	2.28	0.49
15:Z:100:LEU:O	15:Z:103:VAL:N	2.45	0.49
1:A:215:PHE:O	1:A:218:ILE:HG22	2.12	0.49
1:A:224:PHE:HD1	1:A:224:PHE:N	2.11	0.49
2:B:88:ARG:NH2	3:C:41:ARG:HA	2.22	0.49
5:E:68:CYS:SG	5:E:69:LEU:N	2.85	0.49
1:A:338:SER:CB	1:A:341:GLU:HB2	2.43	0.49
1:A:423:GLU:HB2	1:A:440:SER:HB2	1.95	0.49
2:B:25:PHE:CE1	2:B:51:LEU:HD21	2.48	0.49
9:S:84:ARG:HG3	9:S:86:PRO:HD2	1.94	0.49
12:W:259:LEU:HD21	12:W:305:LEU:HB2	1.94	0.49
12:W:431:TYR:HD1	15:Z:111:GLN:NE2	2.10	0.49
13:X:200:CYS:SG	13:X:201:ASP:N	2.86	0.49
14:Y:67:CYS:HA	14:Y:73:MET:HA	1.95	0.49
15:Z:65:ARG:O	15:Z:69:GLN:HG3	2.13	0.49
1:A:116:SER:HB2	1:A:118:LEU:HD13	1.94	0.49
5:E:245:ILE:HD11	5:E:252:GLN:C	2.33	0.49
8:R:21:LEU:HD23	8:R:25:GLN:NE2	2.27	0.49
11:V:104:ILE:CD1	12:W:394:HIS:CE1	2.93	0.49
13:X:113:VAL:HG12	13:X:118:TYR:HB2	1.94	0.49
15:Z:13:ARG:HH11	15:Z:80:TYR:HE2	1.59	0.49
1:A:399:ARG:O	1:A:402:LEU:HB2	2.13	0.48
5:E:260:ILE:O	5:E:264:LEU:HD12	2.12	0.48
11:V:80:GLU:OE2	15:Z:11:VAL:HG12	2.12	0.48
14:Y:173:LEU:H	14:Y:173:LEU:CD2	2.24	0.48
14:Y:68:VAL:N	14:Y:72:THR:O	2.44	0.48
2:B:130:VAL:O	2:B:134:LEU:HD13	2.13	0.48
9:S:157:TYR:OH	10:U:43:TRP:N	2.46	0.48
9:S:88:LEU:HD21	10:U:83:PRO:HG3	1.95	0.48
12:W:321:CYS:O	12:W:326:VAL:HG22	2.13	0.48
14:Y:9:TYR:HB3	14:Y:14:MET:HG3	1.94	0.48
10:U:14:GLU:HA	12:W:130:LEU:HD11	1.95	0.48
11:V:97:SER:HB2	12:W:234:LEU:O	2.13	0.48
12:W:434:LEU:HD11	12:W:480:ILE:HD12	1.96	0.48
14:Y:148:LEU:O	14:Y:155:ASN:ND2	2.47	0.48
1:A:188:ARG:NH1	12:W:49:ARG:HA	2.29	0.48
3:C:38:LYS:O	3:C:49:ARG:NH2	2.46	0.48
7:G:150:LEU:HB2	8:R:19:ILE:HD11	1.96	0.48
1:A:265:ILE:HD11	9:S:206:LEU:HA	1.96	0.48
11:V:79:LEU:HB2	15:Z:81:TRP:HZ3	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:48:PHE:O	12:W:51:LEU:HG	2.13	0.48
1:A:105:ARG:O	1:A:108:LEU:HB3	2.13	0.48
5:E:63:PHE:HD2	5:E:64:LYS:HD3	1.78	0.48
13:X:114:GLU:HA	13:X:118:TYR:O	2.13	0.48
14:Y:54:GLU:HG2	14:Y:66:ALA:CB	2.44	0.48
2:B:102:ASN:HD22	4:D:35:LEU:HD11	1.79	0.48
8:R:12:ASP:HB3	8:R:15:SER:HB2	1.95	0.48
1:A:240:ILE:O	1:A:244:LEU:HB2	2.13	0.48
1:A:108:LEU:HD11	5:E:268:HIS:CD2	2.49	0.48
14:Y:75:ASP:OD1	14:Y:75:ASP:N	2.47	0.48
1:A:163:MET:O	1:A:167:ILE:HG12	2.14	0.48
1:A:16:LEU:HD12	2:B:65:VAL:HG11	1.96	0.48
1:A:244:LEU:O	1:A:248:ILE:HG22	2.14	0.48
2:B:50:THR:HA	2:B:53:ARG:HD3	1.95	0.48
4:D:25:TYR:CE1	4:D:29:HIS:HD2	2.31	0.48
9:S:119:PRO:HD2	10:U:95:LEU:CD2	2.44	0.48
14:Y:122:LYS:N	14:Y:122:LYS:HD3	2.28	0.48
14:Y:44:TYR:HB3	14:Y:92:PHE:O	2.13	0.48
1:A:229:PHE:CE1	1:A:240:ILE:HD11	2.49	0.48
9:S:83:GLU:OE2	9:S:89:TRP:NE1	2.39	0.48
10:U:85:LYS:NZ	10:U:88:GLU:HG2	2.28	0.48
12:W:269:SER:HA	12:W:279:GLY:O	2.14	0.48
13:X:26:LEU:HD11	13:X:138:VAL:HG11	1.95	0.48
1:A:179:PHE:CE2	1:A:263:TYR:HB2	2.49	0.48
1:A:25:HIS:HB3	3:C:82:ILE:HG21	1.95	0.48
4:D:92:LYS:O	4:D:96:LEU:HD12	2.13	0.48
4:D:9:GLN:HG3	5:E:271:ILE:HG21	1.95	0.48
8:R:44:ASP:OD2	8:R:46:ALA:HB3	2.14	0.48
12:W:168:ASP:O	12:W:171:LEU:HB3	2.14	0.48
13:X:12:SER:O	13:X:15:PHE:HB3	2.14	0.48
1:A:88:GLN:HG3	1:A:92:PHE:HE1	1.79	0.47
4:D:100:ILE:HG22	5:E:291:LEU:HB2	1.94	0.47
12:W:245:ARG:HH22	12:W:256:GLN:CD	2.17	0.47
12:W:168:ASP:OD2	15:Z:46:LYS:HD3	2.14	0.47
1:A:18:GLU:O	1:A:22:THR:HG23	2.14	0.47
1:A:378:ASP:HB3	1:A:381:HIS:CG	2.49	0.47
1:A:399:ARG:HB2	1:A:415:LEU:HD21	1.96	0.47
1:A:67:LEU:O	1:A:71:VAL:HG23	2.15	0.47
13:X:21:SER:C	13:X:199:PHE:CZ	2.87	0.47
15:Z:52:GLU:O	15:Z:56:ILE:HG12	2.14	0.47
1:A:153:GLN:O	1:A:157:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:HA	1:A:157:THR:CG2	2.42	0.47
2:B:37:ASP:OD1	2:B:37:ASP:N	2.47	0.47
2:B:65:VAL:HG12	2:B:66:ASN:N	2.29	0.47
5:E:25:ARG:HA	5:E:28:ILE:HD12	1.96	0.47
9:S:33:VAL:HG21	9:S:89:TRP:CD2	2.50	0.47
11:V:93:LYS:HE2	12:W:239:LEU:HB3	1.96	0.47
12:W:266:LEU:O	12:W:282:THR:HA	2.14	0.47
12:W:501:LEU:HB3	12:W:502:HIS:ND1	2.29	0.47
14:Y:96:PHE:CE2	14:Y:186:ILE:HG22	2.42	0.47
12:W:466:PHE:CE1	15:Z:100:LEU:HB2	2.49	0.47
15:Z:100:LEU:HD11	15:Z:104:LYS:HE3	1.95	0.47
1:A:168:ARG:HG3	1:A:223:GLN:OE1	2.14	0.47
1:A:441:ALA:O	1:A:442:SER:OG	2.23	0.47
4:D:89:GLN:HE22	5:E:281:GLU:HB3	1.78	0.47
10:U:139:GLN:O	10:U:143:ILE:HG23	2.13	0.47
10:U:150:ASN:O	10:U:160:ARG:NH2	2.47	0.47
14:Y:127:HIS:HD2	14:Y:173:LEU:HD13	1.79	0.47
1:A:155:LEU:HB2	12:W:56:LEU:HD21	1.97	0.47
1:A:171:LEU:HB3	1:A:217:TRP:CD1	2.48	0.47
4:D:6:THR:CB	5:E:275:ARG:HH22	2.18	0.47
13:X:90:ARG:HD2	13:X:94:CYS:O	2.14	0.47
14:Y:127:HIS:CD2	14:Y:173:LEU:HD13	2.50	0.47
1:A:149:LEU:HD22	12:W:44:GLU:CD	2.35	0.47
5:E:19:TYR:O	5:E:22:LEU:HB3	2.15	0.47
6:F:15:LEU:CD1	6:F:59:LYS:HB3	2.40	0.47
7:G:72:ASP:O	7:G:75:ILE:HG23	2.14	0.47
14:Y:112:ILE:HD11	14:Y:151:PHE:CE2	2.50	0.47
1:A:444:LEU:HG	12:W:429:ILE:HD11	1.97	0.47
9:S:120:ASN:HA	10:U:75:SER:HA	1.96	0.47
13:X:153:LYS:HD3	13:X:154:PRO:HD3	1.96	0.47
1:A:195:ASN:OD1	1:A:201:LEU:HB2	2.15	0.47
1:A:403:HIS:CD2	1:A:404:PRO:HD2	2.50	0.47
2:B:46:GLU:O	2:B:50:THR:HG23	2.14	0.47
5:E:25:ARG:O	5:E:29:GLU:HG2	2.15	0.47
6:F:80:LEU:O	6:F:83:ARG:HB2	2.15	0.47
7:G:144:ASP:HB3	7:G:148:LYS:HE3	1.96	0.47
4:D:122:ALA:HB2	7:G:86:TYR:CE2	2.50	0.47
14:Y:98:ILE:HG22	14:Y:113:ALA:HB1	1.97	0.47
11:V:84:VAL:HG13	15:Z:84:ASN:HB2	1.97	0.47
1:A:222:PHE:HA	1:A:222:PHE:HD1	1.57	0.47
1:A:222:PHE:CE1	1:A:258:ILE:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:CZ	8:R:100:ILE:HD13	2.44	0.47
12:W:129:LEU:O	12:W:132:LYS:HB3	2.14	0.47
13:X:14:ARG:NH1	13:X:200:CYS:HB2	2.11	0.47
1:A:516:TRP:HB3	1:A:563:LEU:HD11	1.97	0.47
1:A:567:ILE:HG12	1:A:567:ILE:H	1.45	0.47
4:D:79:LEU:HD11	5:E:274:TYR:CE2	2.50	0.47
8:R:28:SER:OG	8:R:71:CYS:HB3	2.14	0.47
9:S:115:ILE:HD12	9:S:115:ILE:O	2.14	0.47
10:U:183:ASN:OD1	10:U:184:ALA:N	2.48	0.47
12:W:187:LEU:HD11	15:Z:60:THR:HB	1.97	0.47
7:G:102:VAL:O	12:W:21:GLU:N	2.31	0.47
12:W:518:ASN:OD1	12:W:518:ASN:N	2.46	0.47
14:Y:25:LEU:HD11	14:Y:105:VAL:HG21	1.97	0.47
1:A:474:PHE:O	1:A:478:THR:HG23	2.16	0.46
1:A:102:GLN:HG2	4:D:20:TYR:CD2	2.50	0.46
4:D:30:HIS:HB2	4:D:48:PRO:CA	2.41	0.46
14:Y:51:LYS:CB	14:Y:69:ASP:HA	2.28	0.46
1:A:163:MET:SD	1:A:167:ILE:HD11	2.55	0.46
2:B:40:PRO:HG2	2:B:43:ALA:HB2	1.97	0.46
5:E:19:TYR:HB2	5:E:63:PHE:CZ	2.50	0.46
5:E:24:THR:N	5:E:27:ASN:OD1	2.47	0.46
7:G:152:PHE:CZ	7:G:156:THR:HG21	2.51	0.46
10:U:105:GLU:O	10:U:108:ALA:N	2.49	0.46
10:U:114:TYR:O	10:U:114:TYR:HD1	1.99	0.46
12:W:337:ILE:HA	12:W:337:ILE:HD12	1.58	0.46
14:Y:40:GLN:O	14:Y:55:PHE:HA	2.14	0.46
1:A:182:PHE:HB3	1:A:191:PHE:HE1	1.73	0.46
11:V:104:ILE:HG22	11:V:105:PHE:N	2.30	0.46
12:W:159:SER:OG	12:W:160:GLN:N	2.48	0.46
1:A:153:GLN:HG2	7:G:91:PRO:HB2	1.98	0.46
1:A:273:GLN:NE2	9:S:198:VAL:HG22	2.30	0.46
4:D:133:CYS:SG	4:D:134:VAL:N	2.88	0.46
4:D:96:LEU:O	4:D:100:ILE:HG23	2.15	0.46
6:F:84:ILE:HD12	7:G:67:GLN:HG3	1.98	0.46
9:S:37:PHE:HZ	9:S:108:TYR:CG	2.34	0.46
9:S:131:ASN:HB3	10:U:100:LEU:HD22	1.98	0.46
13:X:22:LEU:CA	13:X:199:PHE:HE2	2.27	0.46
14:Y:55:PHE:HE2	14:Y:178:LEU:HD23	1.81	0.46
15:Z:97:GLU:OE1	15:Z:98:PRO:HD2	2.16	0.46
2:B:18:LEU:O	2:B:22:THR:HG22	2.15	0.46
5:E:23:PHE:CZ	5:E:63:PHE:HE2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:9:SER:HG	7:G:40:HIS:HD1	1.34	0.46
7:G:92:LYS:H	7:G:92:LYS:HG3	1.57	0.46
9:S:94:GLN:HA	9:S:104:PRO:HA	1.97	0.46
10:U:81:GLU:HG2	12:W:151:PRO:O	2.15	0.46
1:A:125:LEU:HD13	7:G:102:VAL:HG22	1.98	0.46
1:A:59:ALA:HB1	3:C:69:LEU:HD21	1.97	0.46
2:B:75:GLU:OE2	3:C:75:LYS:NZ	2.42	0.46
4:D:76:ILE:HD13	5:E:228:LEU:HB3	1.98	0.46
5:E:241:GLU:OE2	5:E:256:LYS:HE3	2.16	0.46
5:E:27:ASN:O	5:E:31:VAL:HG23	2.15	0.46
12:W:519:GLN:H	12:W:519:GLN:HG2	1.57	0.46
1:A:199:VAL:HG21	1:A:231:SER:CA	2.43	0.46
1:A:232:THR:CG2	1:A:233:PRO:HD3	2.44	0.46
1:A:197:PHE:HE2	1:A:273:GLN:NE2	2.13	0.46
1:A:8:HIS:HA	1:A:82:ASP:OD1	2.15	0.46
2:B:98:ASN:C	2:B:98:ASN:HD22	2.19	0.46
3:C:19:ARG:HB3	3:C:20:PRO:CD	2.41	0.46
12:W:279:GLY:HA3	12:W:382:LEU:HD21	1.97	0.46
12:W:396:LEU:HD12	12:W:424:ILE:CB	2.46	0.46
13:X:35:PHE:N	13:X:62:ILE:HD11	2.31	0.46
13:X:66:ASP:OD1	13:X:152:ILE:HA	2.15	0.46
14:Y:45:ARG:HB2	14:Y:50:PRO:O	2.15	0.46
1:A:124:ILE:CD1	8:R:69:PRO:HB3	2.46	0.46
1:A:134:ALA:HA	1:A:140:LYS:CE	2.43	0.46
1:A:563:LEU:O	1:A:563:LEU:HD12	2.16	0.46
2:B:33:TYR:HD2	3:C:107:PHE:HE2	1.63	0.46
10:U:85:LYS:HE2	12:W:148:THR:HG22	1.98	0.46
12:W:398:LEU:HD22	12:W:402:ARG:HH12	1.81	0.46
13:X:123:GLU:OE2	13:X:149:GLN:HA	2.15	0.46
13:X:60:SER:HB3	13:X:78:TRP:HA	1.98	0.46
15:Z:21:ILE:O	15:Z:25:THR:HG23	2.15	0.46
1:A:150:SER:O	1:A:154:ILE:HG23	2.16	0.46
9:S:16:TRP:HB3	9:S:115:ILE:CD1	2.39	0.46
12:W:332:GLU:HG3	12:W:344:ARG:HG3	1.98	0.46
14:Y:96:PHE:HB3	14:Y:182:PHE:HE1	1.81	0.46
4:D:8:LEU:O	4:D:11:THR:OG1	2.27	0.45
5:E:57:GLU:HG3	5:E:57:GLU:H	1.41	0.45
1:A:340:PHE:HD2	6:F:76:ILE:HG21	1.81	0.45
9:S:38:SER:HA	9:S:43:TYR:CG	2.51	0.45
11:V:50:SER:HB3	11:V:53:ASP:HB2	1.97	0.45
12:W:334:LEU:HA	12:W:343:VAL:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:310:ILE:CA	12:W:397:PHE:CE2	2.91	0.45
14:Y:89:LEU:HG	14:Y:89:LEU:H	1.27	0.45
1:A:31:LEU:HD13	1:A:53:TRP:CZ3	2.52	0.45
6:F:64:GLU:N	6:F:64:GLU:OE2	2.43	0.45
9:S:28:LEU:HD23	9:S:32:ASN:OD1	2.17	0.45
9:S:56:SER:HB2	9:S:59:ASN:HD21	1.81	0.45
10:U:114:TYR:O	10:U:118:ILE:HG22	2.15	0.45
2:B:72:ASP:O	2:B:76:TYR:HD1	1.99	0.45
6:F:51:GLN:O	6:F:55:GLN:HG3	2.17	0.45
7:G:151:LEU:HB2	8:R:19:ILE:HG23	1.99	0.45
5:E:63:PHE:C	8:R:16:ARG:HH12	2.15	0.45
1:A:215:PHE:HD1	1:A:215:PHE:H	1.60	0.45
3:C:64:GLY:HA2	3:C:112:PHE:O	2.16	0.45
2:B:79:GLN:HG3	3:C:70:ARG:HD3	1.99	0.45
4:D:124:ARG:NH1	5:E:318:LEU:HB2	2.32	0.45
4:D:25:TYR:CZ	4:D:29:HIS:CD2	3.04	0.45
6:F:80:LEU:C	6:F:80:LEU:HD23	2.37	0.45
7:G:51:TYR:OH	7:G:55:ARG:NH1	2.48	0.45
10:U:17:ARG:NE	12:W:140:THR:OG1	2.45	0.45
12:W:208:LEU:CD2	12:W:227:LEU:HD12	2.47	0.45
14:Y:56:LEU:HD23	14:Y:56:LEU:HA	1.69	0.45
15:Z:13:ARG:HD3	15:Z:80:TYR:CE2	2.51	0.45
1:A:264:ASN:N	1:A:264:ASN:OD1	2.50	0.45
1:A:87:LEU:HD23	2:B:97:ASP:HB3	1.97	0.45
9:S:93:LYS:HB2	9:S:108:TYR:HE1	1.82	0.45
10:U:152:SER:HB3	10:U:160:ARG:NH1	2.31	0.45
11:V:86:VAL:HA	15:Z:13:ARG:NH1	2.31	0.45
1:A:552:SER:O	1:A:555:SER:OG	2.32	0.45
8:R:59:GLU:HG3	8:R:60:PRO:HD2	1.98	0.45
9:S:110:VAL:CG2	9:S:115:ILE:HG22	2.46	0.45
11:V:71:GLY:O	11:V:74:ARG:HB3	2.17	0.45
12:W:269:SER:HB3	12:W:280:SER:HB3	1.98	0.45
12:W:434:LEU:HD21	12:W:480:ILE:HD11	1.98	0.45
14:Y:89:LEU:HD12	14:Y:90:TRP:HE3	1.82	0.45
1:A:222:PHE:HD2	1:A:252:PHE:HA	1.81	0.45
1:A:30:GLU:OE2	1:A:56:ARG:NH2	2.49	0.45
2:B:25:PHE:CE1	2:B:51:LEU:HD11	2.52	0.45
2:B:139:VAL:HA	3:C:16:GLN:HE22	1.81	0.45
6:F:26:ARG:HD3	6:F:48:LEU:HD23	1.99	0.45
8:R:24:VAL:HG12	8:R:71:CYS:SG	2.56	0.45
13:X:152:ILE:HG13	13:X:155:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HA	1:A:294:LEU:HD23	1.79	0.45
1:A:564:GLU:HA	1:A:567:ILE:HD11	1.98	0.45
3:C:74:ILE:O	3:C:78:LEU:HD13	2.17	0.45
4:D:79:LEU:HD12	4:D:80:PRO:HD2	1.99	0.45
10:U:78:PRO:HG3	10:U:91:LEU:CD1	2.43	0.45
13:X:91:GLU:H	13:X:91:GLU:HG3	1.49	0.45
15:Z:90:PHE:O	15:Z:92:THR:HG23	2.17	0.45
4:D:30:HIS:CD2	4:D:48:PRO:HB3	2.51	0.45
7:G:19:ARG:HD2	7:G:19:ARG:HA	1.79	0.45
12:W:114:ILE:O	12:W:117:THR:HG22	2.17	0.45
13:X:5:TYR:CE1	13:X:95:GLY:HA3	2.52	0.45
1:A:229:PHE:CD1	1:A:240:ILE:HD11	2.52	0.45
1:A:90:GLN:O	1:A:93:CYS:HB2	2.16	0.45
3:C:79:THR:C	3:C:81:PRO:HD3	2.37	0.45
8:R:89:ARG:HB3	8:R:91:ASP:OD1	2.16	0.45
9:S:21:TRP:CZ3	9:S:32:ASN:ND2	2.85	0.45
10:U:20:ILE:HD12	10:U:23:ILE:HG23	1.99	0.45
13:X:44:VAL:N	13:X:45:PRO:HD3	2.32	0.45
2:B:82:ASN:HB2	3:C:54:SER:O	2.17	0.44
10:U:77:TYR:HE2	12:W:157:SER:HB2	1.83	0.44
11:V:104:ILE:CB	12:W:394:HIS:CE1	2.97	0.44
12:W:265:ALA:HA	12:W:307:GLU:HG3	1.99	0.44
11:V:104:ILE:CD1	12:W:394:HIS:HE1	2.29	0.44
1:A:307:LEU:HD12	1:A:307:LEU:N	2.33	0.44
1:A:391:ALA:HB1	1:A:428:VAL:CG2	2.47	0.44
1:A:508:TRP:CH2	1:A:563:LEU:HD23	2.52	0.44
1:A:63:ARG:NH2	3:C:69:LEU:HG	2.30	0.44
5:E:233:ARG:O	5:E:236:MET:HB3	2.17	0.44
5:E:69:LEU:HD12	5:E:70:THR:H	1.82	0.44
7:G:140:TRP:HB2	7:G:141:PRO:CD	2.47	0.44
10:U:187:MET:O	10:U:191:ILE:HG13	2.17	0.44
11:V:24:ILE:HD11	11:V:75:GLN:CG	2.47	0.44
14:Y:3:VAL:HA	14:Y:167:ASN:HA	1.99	0.44
1:A:330:ILE:HA	1:A:360:VAL:HG12	1.99	0.44
1:A:398:ILE:O	1:A:401:GLU:N	2.49	0.44
9:S:62:ASP:O	9:S:65:ASP:HB3	2.17	0.44
10:U:196:LYS:HA	13:X:57:ARG:NH2	2.32	0.44
10:U:31:LEU:HD12	10:U:31:LEU:HA	1.77	0.44
13:X:137:THR:HG22	13:X:138:VAL:H	1.83	0.44
14:Y:81:GLU:CG	14:Y:93:ARG:HH22	2.30	0.44
1:A:16:LEU:N	1:A:17:PRO:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:SER:HB2	1:A:341:GLU:HB2	1.99	0.44
2:B:16:SER:O	2:B:19:GLU:HG2	2.17	0.44
5:E:76:MET:HB3	7:G:145:GLN:NE2	2.32	0.44
7:G:3:TYR:H	7:G:3:TYR:HD1	1.65	0.44
13:X:170:TYR:HD1	13:X:170:TYR:HA	1.70	0.44
13:X:20:ASN:O	13:X:23:SER:HB3	2.17	0.44
14:Y:55:PHE:CE1	14:Y:175:SER:HB3	2.52	0.44
1:A:219:VAL:HG12	1:A:222:PHE:H	1.82	0.44
1:A:88:GLN:O	1:A:92:PHE:HD1	1.99	0.44
2:B:90:PHE:O	2:B:94:VAL:HG23	2.18	0.44
8:R:58:ARG:HG2	8:R:72:LEU:HD23	1.99	0.44
1:A:327:TYR:O	1:A:363:HIS:N	2.45	0.44
2:B:139:VAL:HG13	3:C:16:GLN:OE1	2.18	0.44
3:C:72:ASN:HB3	3:C:75:LYS:HE3	2.00	0.44
5:E:245:ILE:HD13	5:E:245:ILE:HG21	1.71	0.44
8:R:25:GLN:HE21	8:R:25:GLN:H	1.66	0.44
9:S:56:SER:HB2	9:S:59:ASN:ND2	2.32	0.44
10:U:138:ASP:O	10:U:142:ILE:HG12	2.17	0.44
12:W:283:TRP:CZ3	12:W:394:HIS:CB	2.94	0.44
1:A:177:THR:N	1:A:178:PRO:HD2	2.33	0.44
1:A:461:THR:HG23	1:A:462:GLN:HE21	1.82	0.44
2:B:35:LEU:HD12	2:B:35:LEU:HA	1.75	0.44
2:B:88:ARG:NH1	3:C:51:MET:SD	2.91	0.44
12:W:207:GLU:HG3	12:W:253:PHE:CD2	2.52	0.44
12:W:291:ASN:N	12:W:291:ASN:OD1	2.45	0.44
1:A:325:GLY:HA2	1:A:365:ASP:OD1	2.17	0.44
1:A:516:TRP:CD2	1:A:567:ILE:HG23	2.52	0.44
1:A:521:ASN:ND2	1:A:524:SER:OG	2.51	0.44
4:D:25:TYR:CZ	4:D:29:HIS:HD2	2.36	0.44
4:D:54:LEU:O	4:D:58:GLN:HG2	2.17	0.44
5:E:250:PRO:O	5:E:253:PHE:HD2	2.00	0.44
4:D:104:GLN:NE2	5:E:294:GLU:OE1	2.37	0.44
5:E:29:GLU:HA	5:E:32:ILE:CG2	2.48	0.44
7:G:27:GLN:O	7:G:31:ILE:HG22	2.18	0.44
10:U:110:THR:HG21	12:W:175:TRP:NE1	2.32	0.44
10:U:80:LEU:HD11	12:W:155:GLN:HG3	1.99	0.44
13:X:134:PHE:O	13:X:136:THR:HG22	2.18	0.44
14:Y:39:VAL:CG2	14:Y:98:ILE:HB	2.48	0.44
1:A:180:GLN:CD	4:D:137:GLN:HB3	2.38	0.43
5:E:28:ILE:O	5:E:32:ILE:HG22	2.18	0.43
5:E:324:LYS:HB2	5:E:324:LYS:HE3	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:56:GLU:HG3	7:G:57:LEU:N	2.31	0.43
9:S:42:PHE:HB3	9:S:108:TYR:CE2	2.52	0.43
9:S:16:TRP:O	9:S:115:ILE:HG13	2.18	0.43
11:V:27:LEU:HD23	11:V:72:LEU:HD13	1.99	0.43
12:W:160:GLN:HG2	12:W:161:PRO:HD2	1.99	0.43
11:V:29:ALA:HA	12:W:198:VAL:HG11	2.00	0.43
10:U:144:PHE:HE2	15:Z:33:GLN:HG2	1.83	0.43
15:Z:45:ASP:O	15:Z:48:THR:N	2.50	0.43
11:V:20:GLN:HB3	15:Z:81:TRP:CD1	2.53	0.43
11:V:79:LEU:CB	15:Z:81:TRP:CH2	3.01	0.43
1:A:235:LYS:HG3	1:A:236:TYR:HD1	1.82	0.43
1:A:403:HIS:CD2	1:A:405:ASN:HD22	2.36	0.43
1:A:88:GLN:HA	1:A:91:LYS:HD2	2.01	0.43
3:C:83:ARG:H	3:C:83:ARG:HG3	1.41	0.43
7:G:71:LEU:O	7:G:75:ILE:HG22	2.18	0.43
8:R:86:ASP:O	8:R:89:ARG:HB2	2.18	0.43
11:V:72:LEU:HB3	15:Z:21:ILE:CD1	2.47	0.43
11:V:111:LEU:HD22	12:W:387:ASP:HB3	2.00	0.43
15:Z:13:ARG:HD3	15:Z:80:TYR:HE2	1.82	0.43
15:Z:93:VAL:O	15:Z:93:VAL:CG1	2.64	0.43
1:A:351:CYS:HA	1:A:353:TYR:HE1	1.84	0.43
2:B:65:VAL:HG12	2:B:67:ASN:H	1.83	0.43
4:D:35:LEU:HB3	4:D:36:PRO:CD	2.48	0.43
8:R:84:ARG:O	8:R:87:ILE:HG12	2.18	0.43
11:V:79:LEU:HB2	15:Z:81:TRP:HH2	1.82	0.43
10:U:72:GLN:HB2	12:W:161:PRO:HB3	1.99	0.43
1:A:403:HIS:HB3	1:A:406:ILE:CG2	2.48	0.43
5:E:260:ILE:HG22	5:E:264:LEU:CD1	2.48	0.43
6:F:20:PHE:CE1	7:G:45:HIS:HB2	2.54	0.43
10:U:49:ASN:HA	10:U:52:ILE:CG2	2.48	0.43
11:V:94:ARG:HH11	12:W:403:LYS:HB2	1.84	0.43
13:X:48:LEU:H	13:X:49:PRO:HD2	1.83	0.43
14:Y:178:LEU:HA	14:Y:178:LEU:HD12	1.83	0.43
14:Y:43:LEU:HD23	14:Y:53:LEU:HB3	2.00	0.43
12:W:176:LYS:NZ	15:Z:38:ILE:O	2.34	0.43
1:A:169:LEU:HD12	1:A:169:LEU:HA	1.77	0.43
4:D:5:CYS:HB2	5:E:275:ARG:NH1	2.33	0.43
9:S:86:PRO:HB2	9:S:87:PHE:CD2	2.53	0.43
12:W:497:HIS:NE2	12:W:499:PRO:HG3	2.34	0.43
1:A:112:ARG:NH2	4:D:10:ASP:OD1	2.52	0.43
4:D:136:PHE:HE2	6:F:87:LYS:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:11:THR:O	4:D:15:VAL:HG23	2.18	0.43
5:E:17:PRO:HB3	5:E:19:TYR:CE1	2.53	0.43
5:E:60:ALA:O	5:E:63:PHE:HB3	2.18	0.43
12:W:288:GLN:N	12:W:288:GLN:OE1	2.51	0.43
14:Y:120:VAL:HG12	14:Y:121:TRP:N	2.32	0.43
15:Z:12:GLN:OE1	15:Z:16:THR:OG1	2.36	0.43
1:A:179:PHE:HE1	1:A:191:PHE:HB3	1.84	0.43
1:A:397:GLN:O	1:A:401:GLU:HG3	2.19	0.43
2:B:139:VAL:HA	3:C:16:GLN:NE2	2.34	0.43
7:G:3:TYR:CD2	7:G:47:LEU:HD21	2.53	0.43
7:G:110:TYR:CD1	8:R:64:LYS:HA	2.54	0.43
5:E:59:LEU:HB3	8:R:9:LYS:HD2	2.01	0.43
10:U:140:ALA:HB1	11:V:54:PHE:CZ	2.54	0.43
11:V:98:THR:OG1	11:V:99:PRO:HD3	2.19	0.43
11:V:95:TYR:HE2	12:W:233:CYS:HA	1.84	0.43
14:Y:185:ARG:NE	14:Y:185:ARG:HA	2.34	0.43
15:Z:17:LEU:HD22	15:Z:77:ILE:HD11	2.01	0.43
1:A:127:THR:CG2	8:R:58:ARG:HB3	2.49	0.43
11:V:24:ILE:HD11	11:V:75:GLN:HG2	2.01	0.43
10:U:31:LEU:HD13	12:W:112:ILE:CG1	2.49	0.43
12:W:261:TYR:CD1	12:W:349:THR:HB	2.54	0.43
1:A:216:GLN:HB3	1:A:223:GLN:CG	2.49	0.43
2:B:36:GLU:O	2:B:39:THR:OG1	2.31	0.43
2:B:71:GLN:HG3	2:B:72:ASP:OD1	2.19	0.43
5:E:275:ARG:N	5:E:276:PRO:HD2	2.34	0.43
7:G:110:TYR:CE2	7:G:114:LEU:HD12	2.53	0.43
8:R:12:ASP:O	8:R:16:ARG:HG2	2.19	0.43
9:S:194:GLU:O	9:S:198:VAL:HG23	2.19	0.43
12:W:279:GLY:HA3	12:W:382:LEU:CD2	2.49	0.43
12:W:326:VAL:HG12	12:W:335:VAL:CG2	2.45	0.43
13:X:121:SER:HB3	13:X:122:HIS:ND1	2.33	0.43
13:X:142:GLN:NE2	13:X:163:GLN:HB3	2.32	0.43
1:A:185:ALA:N	1:A:188:ARG:O	2.52	0.43
1:A:489:LEU:HD12	1:A:505:LYS:HE3	2.00	0.43
3:C:74:ILE:HD12	3:C:75:LYS:N	2.34	0.43
8:R:80:ASN:O	8:R:83:PHE:HB3	2.18	0.43
9:S:145:LYS:HD2	9:S:145:LYS:HA	1.91	0.43
10:U:180:GLU:OE2	13:X:13:ARG:NH1	2.49	0.43
14:Y:110:VAL:HA	14:Y:127:HIS:O	2.19	0.43
1:A:114:ARG:HG2	7:G:115:SER:OG	2.18	0.42
1:A:195:ASN:HB2	1:A:201:LEU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:GLU:HG3	4:D:66:VAL:HG11	2.00	0.42
1:A:39:PRO:HG3	3:C:96:VAL:HG22	2.01	0.42
4:D:30:HIS:CB	4:D:49:ILE:H	2.31	0.42
7:G:32:GLU:HA	7:G:35:THR:HG22	2.00	0.42
9:S:18:MET:N	9:S:36:TYR:OH	2.42	0.42
9:S:52:LEU:HD22	9:S:69:GLN:HE22	1.83	0.42
12:W:260:LEU:HD12	12:W:260:LEU:H	1.84	0.42
13:X:39:TYR:HD1	13:X:119:GLU:C	2.23	0.42
13:X:6:LEU:HD21	13:X:193:LYS:HD2	2.00	0.42
1:A:309:TYR:CZ	1:A:326:HIS:HD2	2.37	0.42
1:A:392:GLN:HA	1:A:395:LEU:HD22	2.01	0.42
2:B:25:PHE:HD1	2:B:51:LEU:HD11	1.83	0.42
3:C:19:ARG:HA	3:C:19:ARG:HD3	1.74	0.42
4:D:43:ASP:N	4:D:43:ASP:OD1	2.51	0.42
8:R:32:TYR:O	8:R:36:LEU:HB2	2.19	0.42
10:U:103:VAL:O	10:U:107:GLU:HG3	2.19	0.42
12:W:335:VAL:HB	12:W:343:VAL:HG23	2.00	0.42
15:Z:56:ILE:O	15:Z:60:THR:HG23	2.18	0.42
1:A:197:PHE:HE2	1:A:273:GLN:HE21	1.66	0.42
1:A:209:LYS:HE2	1:A:212:GLY:N	2.35	0.42
1:A:284:GLN:O	1:A:288:GLU:HG2	2.20	0.42
1:A:313:LEU:HD22	1:A:313:LEU:H	1.85	0.42
1:A:446:PRO:HD2	1:A:451:ARG:NH1	2.33	0.42
1:A:63:ARG:NH2	3:C:69:LEU:O	2.40	0.42
11:V:24:ILE:HA	11:V:24:ILE:HD13	1.76	0.42
14:Y:52:THR:CG2	14:Y:90:TRP:HE1	2.31	0.42
1:A:101:LEU:HA	1:A:104:ILE:HD11	2.01	0.42
1:A:204:ASN:HB2	1:A:228:ASP:HB2	2.00	0.42
1:A:237:ARG:O	1:A:241:GLU:HG3	2.18	0.42
1:A:399:ARG:HB2	1:A:415:LEU:HD11	2.02	0.42
1:A:403:HIS:HB2	1:A:469:ASN:ND2	2.35	0.42
1:A:516:TRP:CE2	1:A:567:ILE:CG2	3.02	0.42
1:A:546:THR:HG21	1:A:559:LEU:CD1	2.48	0.42
9:S:140:LEU:HB2	10:U:50:PHE:CE1	2.54	0.42
10:U:92:THR:O	10:U:96:ARG:HB3	2.20	0.42
12:W:179:SER:HB2	15:Z:53:VAL:HG22	2.00	0.42
12:W:244:ILE:HD13	12:W:294:LEU:HD21	2.02	0.42
12:W:337:ILE:CG2	12:W:341:HIS:HB2	2.45	0.42
14:Y:41:TYR:OH	14:Y:53:LEU:HD13	2.19	0.42
1:A:12:GLY:O	2:B:71:GLN:HG2	2.19	0.42
1:A:367:ILE:HD13	1:A:368:VAL:N	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:169:LEU:HD23	7:G:169:LEU:C	2.40	0.42
9:S:128:ARG:HD2	12:W:122:ALA:HB2	2.01	0.42
10:U:115:GLU:HA	10:U:118:ILE:CG2	2.50	0.42
11:V:45:ILE:HB	11:V:54:PHE:HB2	2.02	0.42
12:W:245:ARG:HB3	12:W:245:ARG:NH2	2.34	0.42
12:W:317:GLU:HG2	12:W:425:LEU:HB2	2.01	0.42
12:W:60:LEU:HD12	12:W:60:LEU:HA	1.76	0.42
13:X:152:ILE:HG13	13:X:155:PRO:CD	2.50	0.42
11:V:99:PRO:HG3	15:Z:92:THR:HG22	2.02	0.42
1:A:31:LEU:HA	1:A:31:LEU:HD12	1.75	0.42
1:A:415:LEU:HD12	1:A:415:LEU:HA	1.86	0.42
9:S:17:ARG:HG2	9:S:114:ASN:OD1	2.19	0.42
9:S:33:VAL:HG21	9:S:89:TRP:CG	2.55	0.42
9:S:63:LEU:O	9:S:66:LEU:N	2.51	0.42
13:X:29:PRO:HB3	13:X:131:TYR:CZ	2.54	0.42
14:Y:140:ARG:NE	14:Y:165:PHE:CE1	2.84	0.42
14:Y:39:VAL:CG1	14:Y:57:LYS:HG3	2.49	0.42
11:V:35:LEU:HD13	15:Z:67:VAL:HG21	2.01	0.42
2:B:125:GLU:CD	2:B:125:GLU:H	2.22	0.42
5:E:287:LEU:HD12	5:E:287:LEU:HA	1.85	0.42
9:S:35:GLU:O	9:S:38:SER:HB3	2.19	0.42
10:U:178:ALA:O	10:U:182:GLN:HG3	2.20	0.42
11:V:101:SER:HA	12:W:398:LEU:HD11	2.02	0.42
12:W:165:LYS:HB2	12:W:168:ASP:HB3	2.01	0.42
12:W:487:SER:HB2	12:W:490:GLU:HG3	2.01	0.42
14:Y:37:TRP:HB2	14:Y:102:ILE:CD1	2.50	0.42
14:Y:53:LEU:N	14:Y:53:LEU:HD23	2.35	0.42
1:A:209:LYS:O	1:A:209:LYS:HG3	2.20	0.42
1:A:229:PHE:CE1	1:A:231:SER:HB2	2.54	0.42
1:A:58:ARG:HA	2:B:25:PHE:HD2	1.85	0.42
3:C:13:VAL:HG22	5:E:256:LYS:NZ	2.34	0.42
5:E:331:GLN:H	5:E:331:GLN:HG2	1.68	0.42
11:V:111:LEU:HD23	11:V:111:LEU:HA	1.89	0.42
12:W:128:LEU:HD11	12:W:153:SER:H	1.84	0.42
10:U:17:ARG:NH1	12:W:136:ASN:O	2.53	0.42
13:X:8:GLY:O	13:X:166:ILE:HD12	2.20	0.42
13:X:196:LEU:HA	13:X:196:LEU:HD23	1.48	0.42
14:Y:140:ARG:NE	14:Y:165:PHE:HE1	2.10	0.42
14:Y:57:LYS:HZ2	14:Y:173:LEU:HG	1.84	0.42
14:Y:30:PHE:CD1	14:Y:30:PHE:N	2.86	0.42
14:Y:74:ILE:HG22	14:Y:75:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:TYR:HD2	1:A:502:THR:CG2	2.27	0.42
1:A:564:GLU:HA	1:A:567:ILE:CG1	2.50	0.42
2:B:106:TYR:O	2:B:109:GLU:HB2	2.20	0.42
5:E:252:GLN:C	5:E:254:PRO:HD2	2.40	0.42
9:S:133:THR:OG1	10:U:57:ILE:HD11	2.20	0.42
9:S:32:ASN:C	9:S:32:ASN:ND2	2.72	0.42
12:W:127:SER:O	12:W:131:SER:HB3	2.19	0.42
13:X:145:ILE:HG23	13:X:157:HIS:HB3	2.02	0.42
14:Y:39:VAL:HA	14:Y:56:LEU:O	2.20	0.42
15:Z:4:ASP:N	15:Z:4:ASP:OD1	2.50	0.42
1:A:136:ALA:HB1	8:R:99:GLU:CD	2.40	0.42
1:A:158:LEU:HD21	1:A:187:GLY:N	2.35	0.42
1:A:173:GLU:OE2	1:A:220:VAL:HB	2.20	0.42
1:A:388:GLN:O	1:A:392:GLN:HG2	2.20	0.42
2:B:102:ASN:HD22	4:D:35:LEU:CD1	2.32	0.42
7:G:163:SER:O	7:G:167:SER:OG	2.28	0.42
8:R:51:LEU:CD1	8:R:78:LEU:HD21	2.50	0.42
12:W:393:ALA:O	12:W:424:ILE:HD12	2.20	0.42
13:X:113:VAL:O	13:X:116:MET:HB2	2.19	0.42
4:D:136:PHE:HZ	6:F:87:LYS:CA	2.24	0.41
8:R:20:GLU:O	8:R:24:VAL:HG23	2.20	0.41
12:W:217:PRO:HG2	12:W:230:GLN:HB3	2.01	0.41
12:W:497:HIS:CD2	12:W:499:PRO:HD3	2.55	0.41
15:Z:18:ASN:O	15:Z:19:SER:C	2.58	0.41
2:B:74:LEU:HA	2:B:74:LEU:HD12	1.73	0.41
3:C:7:TYR:O	3:C:10:VAL:HG12	2.20	0.41
1:A:62:MET:HE1	3:C:66:ASN:HB3	2.01	0.41
5:E:28:ILE:HD11	8:R:49:GLN:HG2	2.02	0.41
5:E:73:THR:HG21	8:R:14:LYS:CE	2.50	0.41
6:F:15:LEU:HD11	6:F:59:LYS:CB	2.41	0.41
9:S:48:ASN:H	9:S:48:ASN:HD22	1.67	0.41
14:Y:3:VAL:HG21	14:Y:139:ALA:HB3	2.00	0.41
14:Y:127:HIS:CD2	14:Y:173:LEU:HD22	2.55	0.41
1:A:562:LEU:O	1:A:566:GLN:HG3	2.19	0.41
1:A:565:VAL:O	1:A:568:LEU:HB2	2.20	0.41
4:D:128:PHE:CD1	4:D:128:PHE:C	2.94	0.41
6:F:60:VAL:HA	6:F:63:MET:HG3	2.01	0.41
9:S:71:LYS:H	9:S:71:LYS:HG2	1.58	0.41
10:U:156:PHE:HE2	15:Z:18:ASN:HD21	1.68	0.41
13:X:118:TYR:OH	14:Y:89:LEU:HD11	2.21	0.41
15:Z:84:ASN:OD1	15:Z:86:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:86:VAL:HG11	15:Z:9:GLN:HB3	2.01	0.41
1:A:179:PHE:CE1	1:A:191:PHE:HB3	2.55	0.41
1:A:212:GLY:O	1:A:213:ILE:C	2.58	0.41
10:U:137:TRP:CZ3	11:V:45:ILE:HD12	2.54	0.41
11:V:34:ILE:HD13	11:V:65:VAL:HG22	2.02	0.41
12:W:262:SER:O	12:W:263:GLN:NE2	2.52	0.41
12:W:493:ILE:HD11	12:W:529:TYR:HE1	1.86	0.41
13:X:27:ASP:HB3	13:X:132:PHE:HB2	2.02	0.41
13:X:112:PHE:HD2	14:Y:74:ILE:HG13	1.83	0.41
12:W:171:LEU:CD2	15:Z:46:LYS:HD2	2.50	0.41
1:A:262:ILE:HA	1:A:265:ILE:HG22	2.02	0.41
1:A:64:LEU:HB3	2:B:18:LEU:HD21	2.02	0.41
7:G:109:ASP:OD1	7:G:109:ASP:N	2.53	0.41
1:A:138:THR:HG23	8:R:99:GLU:OE2	2.20	0.41
14:Y:100:GLY:HA3	14:Y:113:ALA:HA	2.02	0.41
1:A:234:ALA:O	1:A:237:ARG:HB3	2.21	0.41
1:A:342:ARG:HG3	1:A:351:CYS:SG	2.60	0.41
2:B:60:ASP:HA	2:B:63:ARG:HD3	2.02	0.41
3:C:24:GLN:O	3:C:26:LEU:HD12	2.20	0.41
3:C:92:PHE:CE2	3:C:96:VAL:HG21	2.55	0.41
9:S:18:MET:SD	9:S:21:TRP:HB2	2.61	0.41
9:S:92:GLN:OE1	9:S:94:GLN:HB3	2.21	0.41
10:U:100:LEU:HA	10:U:100:LEU:HD12	1.84	0.41
12:W:428:LEU:HA	12:W:428:LEU:HD12	1.80	0.41
1:A:188:ARG:NH1	12:W:48:PHE:HD1	2.18	0.41
6:F:76:ILE:O	6:F:80:LEU:HB3	2.21	0.41
7:G:44:LEU:HD23	7:G:44:LEU:C	2.41	0.41
8:R:23:PHE:HA	8:R:26:MET:HG3	2.03	0.41
12:W:307:GLU:O	12:W:310:ILE:HG22	2.20	0.41
12:W:62:LYS:HA	12:W:65:ILE:HD12	2.03	0.41
14:Y:127:HIS:NE2	14:Y:173:LEU:HB3	2.36	0.41
14:Y:81:GLU:OE1	14:Y:93:ARG:NH1	2.54	0.41
1:A:406:ILE:HD13	1:A:406:ILE:HG21	1.70	0.41
4:D:22:SER:HA	4:D:61:LEU:HD21	2.01	0.41
7:G:159:VAL:HG12	7:G:160:PRO:O	2.21	0.41
1:A:81:ILE:HD13	7:G:202:PRO:HB3	2.02	0.41
7:G:24:LYS:HG2	7:G:25:VAL:H	1.85	0.41
7:G:58:GLN:O	7:G:61:ILE:HB	2.21	0.41
8:R:26:MET:H	8:R:26:MET:HG2	1.55	0.41
1:A:127:THR:HG21	8:R:58:ARG:HB3	2.02	0.41
13:X:145:ILE:O	13:X:157:HIS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:86:SER:HB3	13:X:207:LEU:HA	2.02	0.41
14:Y:181:LEU:O	14:Y:185:ARG:HB2	2.21	0.41
1:A:195:ASN:CG	1:A:201:LEU:HB2	2.40	0.41
5:E:256:LYS:HD2	5:E:256:LYS:HA	1.71	0.41
5:E:14:PRO:HB3	7:G:152:PHE:HB2	2.03	0.41
12:W:216:TRP:CE2	15:Z:91:PRO:CG	3.03	0.41
12:W:272:ASN:OD1	12:W:275:ARG:N	2.53	0.41
14:Y:174:ASP:OD1	14:Y:175:SER:N	2.53	0.41
14:Y:53:LEU:HD21	14:Y:183:LYS:HZ2	1.85	0.41
15:Z:31:ARG:HA	15:Z:31:ARG:NE	2.35	0.41
5:E:260:ILE:HG12	5:E:260:ILE:H	1.62	0.41
6:F:27:LEU:HA	6:F:27:LEU:HD23	1.80	0.41
13:X:153:LYS:HD3	13:X:154:PRO:CD	2.51	0.41
13:X:189:LEU:HA	13:X:189:LEU:HD22	1.59	0.41
14:Y:18:LEU:HD21	14:Y:22:GLN:OE1	2.21	0.41
14:Y:53:LEU:HD21	14:Y:183:LYS:NZ	2.36	0.41
1:A:122:LEU:O	1:A:125:LEU:HB3	2.21	0.41
6:F:50:ARG:HA	6:F:53:ILE:CG2	2.51	0.41
5:E:23:PHE:O	8:R:46:ALA:HB2	2.21	0.41
10:U:159:ARG:HG3	10:U:159:ARG:H	1.44	0.41
10:U:196:LYS:NZ	13:X:85:ASN:HB3	2.36	0.41
12:W:231:TYR:HD2	12:W:302:GLN:HA	1.86	0.41
13:X:109:VAL:O	13:X:113:VAL:HG23	2.20	0.41
1:A:23:PHE:CZ	1:A:61:THR:HG22	2.54	0.40
3:C:56:LYS:HA	3:C:59:ILE:HG12	2.02	0.40
9:S:69:GLN:HG2	9:S:69:GLN:O	2.21	0.40
12:W:483:ARG:HA	12:W:494:PHE:HB3	2.03	0.40
15:Z:60:THR:O	15:Z:64:VAL:HG23	2.22	0.40
5:E:238:ASN:HB3	5:E:260:ILE:HD13	2.04	0.40
4:D:124:ARG:CZ	5:E:318:LEU:HD13	2.51	0.40
7:G:79:MET:O	7:G:83:THR:HG22	2.20	0.40
9:S:48:ASN:N	9:S:48:ASN:ND2	2.70	0.40
12:W:429:ILE:HD13	12:W:429:ILE:HG21	1.83	0.40
11:V:72:LEU:HD23	15:Z:21:ILE:HD11	2.04	0.40
1:A:392:GLN:HE22	1:A:413:GLY:C	2.23	0.40
1:A:498:PHE:C	1:A:498:PHE:CD1	2.94	0.40
4:D:114:ASN:ND2	4:D:118:LYS:HE3	2.36	0.40
6:F:80:LEU:HD23	6:F:81:LYS:N	2.36	0.40
1:A:132:ARG:CZ	8:R:100:ILE:HB	2.49	0.40
7:G:171:SER:HG	9:S:16:TRP:HD1	1.67	0.40
9:S:84:ARG:HD3	10:U:83:PRO:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:W:394:HIS:HB3	12:W:395:ILE:H	1.55	0.40
12:W:460:TRP:CE2	15:Z:107:LEU:HB3	2.56	0.40
1:A:191:PHE:O	1:A:202:THR:HA	2.22	0.40
1:A:209:LYS:HD3	1:A:216:GLN:NE2	2.33	0.40
4:D:41:VAL:HB	4:D:46:VAL:HG21	2.04	0.40
8:R:12:ASP:OD2	8:R:15:SER:OG	2.28	0.40
1:A:132:ARG:CZ	8:R:70:THR:OG1	2.70	0.40
11:V:36:SER:HB2	12:W:191:LYS:HG3	2.04	0.40
12:W:38:PHE:CE1	12:W:48:PHE:CE2	3.10	0.40
13:X:58:LEU:HD11	13:X:109:VAL:HG11	2.04	0.40
14:Y:34:LEU:HD12	14:Y:34:LEU:N	2.37	0.40
1:A:265:ILE:O	9:S:205:SER:OG	2.30	0.40
4:D:130:ARG:NE	5:E:322:MET:SD	2.95	0.40
5:E:312:LEU:HD22	5:E:316:LYS:HG3	2.03	0.40
5:E:73:THR:HG21	8:R:14:LYS:HE3	2.04	0.40
9:S:109:PHE:HB2	9:S:118:ALA:HB2	2.03	0.40
11:V:35:LEU:HD21	15:Z:64:VAL:HG13	2.03	0.40
12:W:138:ILE:HG13	12:W:138:ILE:H	1.65	0.40
12:W:231:TYR:HB2	12:W:302:GLN:HB2	2.03	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)
2:B:37:ASP:OD2	14:Y:130:TYR:OH[2_554]	2.03	0.17
1:A:497:SER:OG	3:C:33:THR:OG1[3_654]	2.14	0.06

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	562/591 (95%)	517 (92%)	36 (6%)	9 (2%)	11 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	131/144 (91%)	126 (96%)	4 (3%)	1 (1%)	22	62
3	C	109/138 (79%)	101 (93%)	8 (7%)	0	100	100
4	D	133/138 (96%)	125 (94%)	6 (4%)	2 (2%)	12	49
5	E	195/376 (52%)	184 (94%)	9 (5%)	2 (1%)	18	59
6	F	75/121 (62%)	73 (97%)	2 (3%)	0	100	100
7	G	155/239 (65%)	150 (97%)	5 (3%)	0	100	100
8	R	97/139 (70%)	94 (97%)	3 (3%)	0	100	100
9	S	167/216 (77%)	159 (95%)	8 (5%)	0	100	100
10	U	196/200 (98%)	187 (95%)	7 (4%)	2 (1%)	18	59
11	V	97/112 (87%)	91 (94%)	5 (5%)	1 (1%)	18	59
12	W	451/545 (83%)	436 (97%)	13 (3%)	2 (0%)	38	75
13	X	205/210 (98%)	190 (93%)	12 (6%)	3 (2%)	12	49
14	Y	183/193 (95%)	166 (91%)	16 (9%)	1 (0%)	32	71
15	Z	117/136 (86%)	110 (94%)	7 (6%)	0	100	100
All	All	2873/3498 (82%)	2709 (94%)	141 (5%)	23 (1%)	22	62

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	TRP
1	A	301	LYS
4	D	35	LEU
5	E	67	SER
1	A	213	ILE
10	U	80	LEU
12	W	394	HIS
14	Y	69	ASP
1	A	391	ALA
11	V	96	ALA
1	A	208	PRO
1	A	260	PRO
1	A	288	GLU
1	A	411	VAL
4	D	43	ASP
12	W	515	TYR
13	X	48	LEU
13	X	155	PRO

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Mol	Chain	Res	Type
2	B	65	VAL
10	U	198	GLY
5	E	66	PRO
1	A	227	PRO
13	X	138	VAL

### 5.3.2 Protein sidechains ⓘ

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	518/538 (96%)	407 (79%)	111 (21%)	1	5
2	B	120/131 (92%)	104 (87%)	16 (13%)	4	23
3	C	100/124 (81%)	85 (85%)	15 (15%)	3	18
4	D	126/128 (98%)	113 (90%)	13 (10%)	8	35
5	E	157/350 (45%)	129 (82%)	28 (18%)	2	11
6	F	71/110 (64%)	59 (83%)	12 (17%)	2	13
7	G	154/220 (70%)	125 (81%)	29 (19%)	2	9
8	R	96/131 (73%)	72 (75%)	24 (25%)	1	3
9	S	158/198 (80%)	132 (84%)	26 (16%)	2	14
10	U	183/185 (99%)	158 (86%)	25 (14%)	4	22
11	V	91/104 (88%)	81 (89%)	10 (11%)	7	31
12	W	415/509 (82%)	336 (81%)	79 (19%)	2	8
13	X	191/193 (99%)	158 (83%)	33 (17%)	2	12
14	Y	170/178 (96%)	131 (77%)	39 (23%)	1	4
15	Z	114/129 (88%)	100 (88%)	14 (12%)	5	26
All	All	2664/3228 (82%)	2190 (82%)	474 (18%)	2	11

All (474) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU

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Mol	Chain	Res	Type
1	A	6	ILE
1	A	16	LEU
1	A	25	HIS
1	A	28	LEU
1	A	29	GLN
1	A	38	LEU
1	A	40	SER
1	A	42	SER
1	A	44	VAL
1	A	54	LEU
1	A	76	SER
1	A	88	GLN
1	A	98	VAL
1	A	104	ILE
1	A	105	ARG
1	A	110	PHE
1	A	112	ARG
1	A	113	LEU
1	A	114	ARG
1	A	116	SER
1	A	118	LEU
1	A	125	LEU
1	A	133	LEU
1	A	144	LEU
1	A	150	SER
1	A	156	GLN
1	A	163	MET
1	A	168	ARG
1	A	169	LEU
1	A	172	TYR
1	A	180	GLN
1	A	195	ASN
1	A	196	GLU
1	A	197	PHE
1	A	199	VAL
1	A	200	SER
1	A	207	ASP
1	A	208	PRO
1	A	211	THR
1	A	213	ILE
1	A	215	PHE
1	A	216	GLN

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Mol	Chain	Res	Type
1	A	220	VAL
1	A	222	PHE
1	A	223	GLN
1	A	224	PHE
1	A	226	LEU
1	A	229	PHE
1	A	230	SER
1	A	231	SER
1	A	237	ARG
1	A	240	ILE
1	A	243	HIS
1	A	244	LEU
1	A	247	GLU
1	A	248	ILE
1	A	254	LEU
1	A	255	GLN
1	A	258	ILE
1	A	259	LEU
1	A	264	ASN
1	A	294	LEU
1	A	298	TYR
1	A	301	LYS
1	A	305	LEU
1	A	307	LEU
1	A	309	TYR
1	A	328	ILE
1	A	330	ILE
1	A	331	PHE
1	A	332	VAL
1	A	337	ILE
1	A	338	SER
1	A	340	PHE
1	A	341	GLU
1	A	346	SER
1	A	353	TYR
1	A	356	PHE
1	A	357	LEU
1	A	359	LEU
1	A	367	ILE
1	A	375	ASP
1	A	380	GLN
1	A	387	THR

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Mol	Chain	Res	Type
1	A	394	ILE
1	A	395	LEU
1	A	398	ILE
1	A	402	LEU
1	A	406	ILE
1	A	411	VAL
1	A	430	SER
1	A	444	LEU
1	A	475	CYS
1	A	485	GLN
1	A	500	TYR
1	A	501	LEU
1	A	515	LEU
1	A	517	VAL
1	A	518	LEU
1	A	530	ARG
1	A	531	LEU
1	A	532	LEU
1	A	540	TYR
1	A	550	THR
1	A	551	LEU
1	A	557	SER
1	A	560	SER
1	A	561	TYR
1	A	562	LEU
1	A	567	ILE
2	B	8	THR
2	B	9	ASP
2	B	17	ARG
2	B	22	THR
2	B	34	ASN
2	B	44	ILE
2	B	51	LEU
2	B	55	LEU
2	B	58	LEU
2	B	68	LEU
2	B	72	ASP
2	B	77	ILE
2	B	88	ARG
2	B	90	PHE
2	B	98	ASN
2	B	136	GLU

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Mol	Chain	Res	Type
3	C	8	HIS
3	C	14	ASP
3	C	19	ARG
3	C	58	TYR
3	C	59	ILE
3	C	60	GLN
3	C	61	ASP
3	C	69	LEU
3	C	71	ASP
3	C	72	ASN
3	C	83	ARG
3	C	90	ILE
3	C	99	VAL
3	C	103	ILE
3	C	104	ILE
4	D	4	ARG
4	D	6	THR
4	D	8	LEU
4	D	12	ILE
4	D	35	LEU
4	D	61	LEU
4	D	82	ILE
4	D	83	SER
4	D	96	LEU
4	D	110	LEU
4	D	113	GLU
4	D	124	ARG
4	D	133	CYS
5	E	13	PHE
5	E	20	TYR
5	E	22	LEU
5	E	32	ILE
5	E	34	ASN
5	E	35	MET
5	E	57	GLU
5	E	59	LEU
5	E	67	SER
5	E	68	CYS
5	E	73	THR
5	E	228	LEU
5	E	232	SER
5	E	238	ASN

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Mol	Chain	Res	Type
5	E	240	LEU
5	E	245	ILE
5	E	271	ILE
5	E	273	ASP
5	E	275	ARG
5	E	281	GLU
5	E	286	LEU
5	E	302	ARG
5	E	305	ASN
5	E	308	MET
5	E	309	THR
5	E	312	LEU
5	E	329	ILE
5	E	333	LYS
6	F	14	LEU
6	F	15	LEU
6	F	17	GLN
6	F	19	ASP
6	F	24	GLN
6	F	44	LYS
6	F	53	ILE
6	F	58	GLU
6	F	63	MET
6	F	64	GLU
6	F	68	MET
6	F	93	MET
7	G	9	SER
7	G	20	LEU
7	G	26	ASP
7	G	32	GLU
7	G	46	SER
7	G	56	GLU
7	G	61	ILE
7	G	64	LEU
7	G	71	LEU
7	G	75	ILE
7	G	78	CYS
7	G	90	LEU
7	G	102	VAL
7	G	106	THR
7	G	108	LEU
7	G	109	ASP

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Mol	Chain	Res	Type
7	G	114	LEU
7	G	142	SER
7	G	145	GLN
7	G	147	ARG
7	G	151	LEU
7	G	158	MET
7	G	165	THR
7	G	168	GLN
7	G	169	LEU
7	G	170	PHE
7	G	173	GLN
7	G	199	MET
7	G	200	ASN
8	R	6	LEU
8	R	16	ARG
8	R	19	ILE
8	R	25	GLN
8	R	28	SER
8	R	31	TRP
8	R	35	PHE
8	R	43	GLU
8	R	47	PHE
8	R	49	GLN
8	R	51	LEU
8	R	52	GLU
8	R	54	MET
8	R	56	TYR
8	R	57	TRP
8	R	61	GLU
8	R	65	PHE
8	R	76	THR
8	R	78	LEU
8	R	91	ASP
8	R	100	ILE
8	R	101	TYR
8	R	103	GLU
8	R	104	TRP
9	S	11	LEU
9	S	17	ARG
9	S	24	SER
9	S	32	ASN
9	S	33	VAL

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Mol	Chain	Res	Type
9	S	35	GLU
9	S	36	TYR
9	S	40	SER
9	S	48	ASN
9	S	55	GLN
9	S	59	ASN
9	S	62	ASP
9	S	69	GLN
9	S	70	LEU
9	S	71	LYS
9	S	88	LEU
9	S	92	GLN
9	S	102	VAL
9	S	111	CYS
9	S	125	LEU
9	S	127	THR
9	S	142	LYS
9	S	192	SER
9	S	195	ASP
9	S	202	PHE
9	S	203	MET
10	U	7	GLU
10	U	13	LEU
10	U	16	ILE
10	U	17	ARG
10	U	23	ILE
10	U	40	LEU
10	U	46	ILE
10	U	49	ASN
10	U	52	ILE
10	U	70	THR
10	U	80	LEU
10	U	95	LEU
10	U	96	ARG
10	U	100	LEU
10	U	102	GLU
10	U	105	GLU
10	U	114	TYR
10	U	118	ILE
10	U	126	GLU
10	U	156	PHE
10	U	157	VAL

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Mol	Chain	Res	Type
10	U	160	ARG
10	U	190	ASP
10	U	192	LEU
10	U	197	SER
11	V	17	ASP
11	V	18	THR
11	V	35	LEU
11	V	41	CYS
11	V	43	GLU
11	V	45	ILE
11	V	72	LEU
11	V	86	VAL
11	V	88	SER
11	V	108	SER
12	W	33	ASN
12	W	34	LEU
12	W	35	GLN
12	W	49	ARG
12	W	50	ASP
12	W	60	LEU
12	W	99	MET
12	W	109	ILE
12	W	112	ILE
12	W	114	ILE
12	W	117	THR
12	W	121	LEU
12	W	125	MET
12	W	135	GLU
12	W	137	SER
12	W	144	PHE
12	W	154	LEU
12	W	155	GLN
12	W	168	ASP
12	W	174	CYS
12	W	179	SER
12	W	180	LEU
12	W	183	SER
12	W	184	CYS
12	W	196	SER
12	W	199	GLU
12	W	218	LEU
12	W	219	PHE

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Mol	Chain	Res	Type
12	W	224	SER
12	W	232	SER
12	W	233	CYS
12	W	239	LEU
12	W	241	LEU
12	W	260	LEU
12	W	263	GLN
12	W	268	ILE
12	W	283	TRP
12	W	287	SER
12	W	289	ASN
12	W	290	CYS
12	W	310	ILE
12	W	317	GLU
12	W	320	SER
12	W	334	LEU
12	W	337	ILE
12	W	338	SER
12	W	346	THR
12	W	352	LYS
12	W	378	GLU
12	W	381	LEU
12	W	388	THR
12	W	397	PHE
12	W	405	ASP
12	W	414	TYR
12	W	415	MET
12	W	417	ILE
12	W	420	ASN
12	W	424	ILE
12	W	425	LEU
12	W	427	PRO
12	W	436	GLN
12	W	441	PHE
12	W	476	ASN
12	W	477	ARG
12	W	478	LEU
12	W	481	SER
12	W	484	ILE
12	W	485	MET
12	W	486	VAL
12	W	488	ASN

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Mol	Chain	Res	Type
12	W	494	PHE
12	W	501	LEU
12	W	506	LYS
12	W	508	VAL
12	W	510	ARG
12	W	518	ASN
12	W	519	GLN
12	W	529	TYR
12	W	533	HIS
13	X	5	TYR
13	X	7	LEU
13	X	13	ARG
13	X	14	ARG
13	X	20	ASN
13	X	21	SER
13	X	26	LEU
13	X	32	ILE
13	X	43	ASP
13	X	51	GLN
13	X	53	ASP
13	X	54	SER
13	X	55	TRP
13	X	56	LEU
13	X	58	LEU
13	X	62	ILE
13	X	63	GLU
13	X	70	THR
13	X	71	GLU
13	X	85	ASN
13	X	86	SER
13	X	91	GLU
13	X	92	ASP
13	X	105	THR
13	X	109	VAL
13	X	119	GLU
13	X	122	HIS
13	X	138	VAL
13	X	161	GLU
13	X	170	TYR
13	X	189	LEU
13	X	199	PHE
13	X	200	CYS

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Mol	Chain	Res	Type
14	Y	4	HIS
14	Y	10	SER
14	Y	28	THR
14	Y	32	GLN
14	Y	35	LYS
14	Y	40	GLN
14	Y	43	LEU
14	Y	44	TYR
14	Y	45	ARG
14	Y	46	ASN
14	Y	53	LEU
14	Y	55	PHE
14	Y	56	LEU
14	Y	58	GLN
14	Y	69	ASP
14	Y	73	MET
14	Y	75	ASP
14	Y	79	GLU
14	Y	81	GLU
14	Y	89	LEU
14	Y	93	ARG
14	Y	94	GLN
14	Y	97	THR
14	Y	99	GLU
14	Y	101	SER
14	Y	108	PHE
14	Y	110	VAL
14	Y	116	LEU
14	Y	121	TRP
14	Y	122	LYS
14	Y	131	ASP
14	Y	137	ASP
14	Y	146	PHE
14	Y	152	LEU
14	Y	158	VAL
14	Y	161	VAL
14	Y	165	PHE
14	Y	166	PHE
14	Y	185	ARG
15	Z	22	ASP
15	Z	33	GLN
15	Z	34	ASP

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Mol	Chain	Res	Type
15	Z	36	LEU
15	Z	41	ASN
15	Z	61	VAL
15	Z	70	LEU
15	Z	75	ARG
15	Z	81	TRP
15	Z	84	ASN
15	Z	97	GLU
15	Z	100	LEU
15	Z	114	LEU
15	Z	115	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	206	GLN
1	A	245	ASN
1	A	276	ASN
1	A	355	HIS
1	A	521	ASN
2	B	71	GLN
4	D	29	HIS
4	D	114	ASN
5	E	238	ASN
5	E	305	ASN
7	G	15	ASN
7	G	17	GLN
7	G	145	GLN
7	G	173	GLN
9	S	59	ASN
10	U	109	ASN
11	V	75	GLN
12	W	225	ASN
12	W	256	GLN
12	W	263	GLN
12	W	394	HIS
12	W	436	GLN
12	W	514	GLN
13	X	51	GLN
13	X	142	GLN
14	Y	22	GLN

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Mol	Chain	Res	Type
14	Y	58	GLN
14	Y	127	HIS
14	Y	155	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	566/591 (95%)	0.50	29 (5%) 29 26	88, 132, 207, 337	0
2	B	133/144 (92%)	0.33	3 (2%) 61 56	91, 128, 188, 241	0
3	C	111/138 (80%)	0.19	2 (1%) 69 64	93, 137, 190, 276	0
4	D	135/138 (97%)	0.10	2 (1%) 74 69	120, 174, 212, 295	0
5	E	201/376 (53%)	0.03	2 (0%) 82 78	112, 185, 256, 300	0
6	F	79/121 (65%)	0.04	3 (3%) 41 37	131, 183, 232, 264	0
7	G	163/239 (68%)	0.21	3 (1%) 69 64	104, 178, 237, 269	0
8	R	99/139 (71%)	0.52	12 (12%) 5 5	133, 172, 214, 246	0
9	S	171/216 (79%)	0.32	7 (4%) 38 34	118, 192, 242, 315	0
10	U	198/200 (99%)	0.15	10 (5%) 29 26	117, 170, 240, 327	0
11	V	99/112 (88%)	0.36	0 100 100	105, 126, 165, 211	0
12	W	463/545 (84%)	0.21	10 (2%) 62 57	93, 142, 230, 288	0
13	X	207/210 (98%)	0.15	6 (2%) 52 48	109, 160, 244, 299	0
14	Y	185/193 (95%)	0.27	3 (1%) 72 67	103, 149, 202, 237	0
15	Z	119/136 (87%)	0.36	3 (2%) 58 53	111, 130, 199, 225	0
All	All	2929/3498 (83%)	0.27	95 (3%) 48 45	88, 155, 231, 337	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	ARG	5.9
1	A	173	GLU	5.4
10	U	156	PHE	4.8
9	S	49	ASN	4.4
1	A	216	GLN	4.3
1	A	118	LEU	4.2
4	D	135	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	207	ASP	3.9
10	U	84	VAL	3.8
15	Z	47	TYR	3.7
8	R	54	MET	3.6
8	R	69	PRO	3.5
10	U	157	VAL	3.5
1	A	206	GLN	3.5
1	A	147	SER	3.4
13	X	144	LEU	3.4
1	A	135	ASN	3.3
12	W	415	MET	3.3
9	S	78	PHE	3.2
8	R	66	ILE	3.2
12	W	244	ILE	3.2
13	X	80	MET	3.1
9	S	135	CYS	2.9
12	W	130	LEU	2.9
14	Y	14	MET	2.9
2	B	97	ASP	2.9
10	U	41	SER	2.9
3	C	59	ILE	2.9
10	U	78	PRO	2.8
9	S	102	VAL	2.8
1	A	124	ILE	2.8
7	G	34	TRP	2.7
8	R	65	PHE	2.7
1	A	133	LEU	2.6
1	A	244	LEU	2.6
6	F	90	PHE	2.6
6	F	27	LEU	2.6
8	R	27	LEU	2.6
15	Z	85	SER	2.5
9	S	91	ILE	2.5
8	R	73	HIS	2.5
8	R	70	THR	2.5
8	R	87	ILE	2.5
1	A	203	THR	2.5
1	A	145	SER	2.4
12	W	414	TYR	2.4
14	Y	93	ARG	2.4
1	A	130	SER	2.3
6	F	46	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	157	THR	2.3
10	U	81	GLU	2.3
1	A	417	ILE	2.3
9	S	42	PHE	2.3
8	R	50	TYR	2.3
1	A	205	SER	2.3
13	X	56	LEU	2.3
9	S	125	LEU	2.2
10	U	200	ARG	2.2
8	R	23	PHE	2.2
10	U	53	LEU	2.2
12	W	249	GLU	2.2
1	A	143	MET	2.2
1	A	503	PHE	2.2
1	A	211	THR	2.2
12	W	394	HIS	2.2
1	A	424	ILE	2.2
13	X	189	LEU	2.2
10	U	188	LEU	2.1
1	A	213	ILE	2.1
10	U	30	PHE	2.1
7	G	41	LEU	2.1
14	Y	80	LEU	2.1
7	G	85	ILE	2.1
1	A	23	PHE	2.1
12	W	41	ILE	2.1
8	R	77	LEU	2.1
2	B	58	LEU	2.1
1	A	518	LEU	2.1
5	E	286	LEU	2.1
1	A	517	VAL	2.0
4	D	26	LEU	2.0
13	X	9	VAL	2.0
8	R	33	LEU	2.0
12	W	51	LEU	2.0
12	W	393	ALA	2.0
15	Z	56	ILE	2.0
12	W	454	PHE	2.0
1	A	19	ILE	2.0
1	A	240	ILE	2.0
2	B	77	ILE	2.0
3	C	97	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
5	E	323	GLU	2.0
13	X	67	GLU	2.0
1	A	64	LEU	2.0
1	A	219	VAL	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.