



## wwPDB EM Map/Model Validation Report ⓘ

May 26, 2016 – 04:46 PM EDT

PDB ID : 5FZ5  
EMDB ID: : 3383  
Title : Transcription initiation complex structures elucidate DNA opening (CC)  
Authors : Plaschka, C.; Hantsche, M.; Dienemann, C.; Burzinski, C.; Plitzko, J.; Cramer, P.  
Deposited on : 2016-03-10  
Resolution : 8.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027674

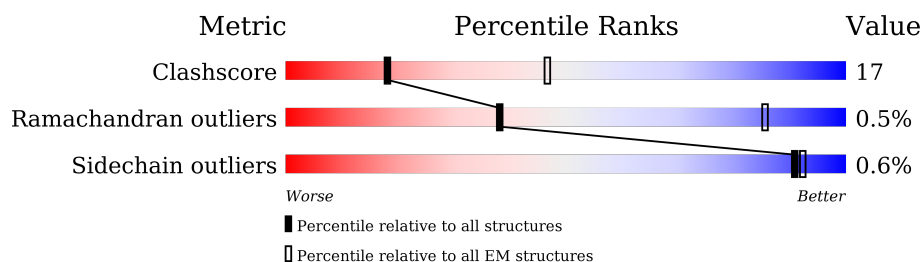
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.80 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	

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Mol	Chain	Length	Quality of chain
10	J	70	
11	K	120	
12	L	70	
13	M	345	
14	N	56	
15	O	240	
16	Q	735	
17	R	400	
18	T	85	
19	U	286	
20	V	122	
21	W	482	
22	X	328	

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 42144 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1398	Total	C	N	O	S	0	0
			10997	6931	1927	2078	61		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9200	5819	1613	1713	55		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	262	Total	C	N	O	S	0	0
			2061	1299	343	406	13		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	157	Total	C	N	O	S	0	0
			1253	779	220	252	2		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	213	Total	C	N	O	S	0	0
			1744	1107	308	318	11		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			670	428	114	125	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	136	Total	C	N	O	S	0	0
			1089	686	184	215	4		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	116	Total	C	N	O	S	0	0
			944	581	172	181	10		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	112	Total	C	N	O	S	0	0
			904	580	154	168	2		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	45	Total	C	N	O	S	0	0
			358	221	71	62	4		

- Molecule 13 is a protein called TRANSCRIPTION INITIATION FACTOR IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	231	Total	C	N	O	S	0	0
			1785	1145	299	326	15		

- Molecule 14 is a DNA chain called SYNTHETIC CLOSED PROMOTER DNA CONSTRUCT.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	56	Total	C	N	O	P	0	0
			1134	548	208	322	56		

- Molecule 15 is a protein called TATA-BOX-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 16 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O	S	0	0
			1141	731	195	212	3		

- Molecule 17 is a protein called TRANSCRIPTION INITIATION FACTOR IIF SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	199	Total	C	N	O	S	0	0
			1347	838	247	255	7		

- Molecule 18 is a DNA chain called SYNTHETIC CLOSED PROMOTER DNA CONSTRUCT.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	56	Total	C	N	O	P	0	0
			1134	548	208	322	56		

- Molecule 19 is a protein called TRANSCRIPTION INITIATION FACTOR IIA LARGE SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	92	Total	C	N	O	S	0	0
			757	474	130	150	3		

- Molecule 20 is a protein called TRANSCRIPTION INITIATION FACTOR IIA SUBUNIT

2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	100	Total	C	N	O	S	0	0
			782	492	130	156	4		

- Molecule 21 is a protein called TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	168	Total	C	N	O		0	0
			835	499	168	168			

- Molecule 22 is a protein called TRANSCRIPTION INITIATION FACTOR IIE SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	143	Total	C	N	O		0	0
			710	424	143	143			

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
23	J	1	Total	Zn	0
			1	1	
23	B	1	Total	Zn	0
			1	1	
23	I	2	Total	Zn	0
			2	2	
23	C	1	Total	Zn	0
			1	1	
23	W	1	Total	Zn	0
			1	1	
23	A	2	Total	Zn	0
			2	2	
23	L	1	Total	Zn	0
			1	1	
23	M	1	Total	Zn	0
			1	1	

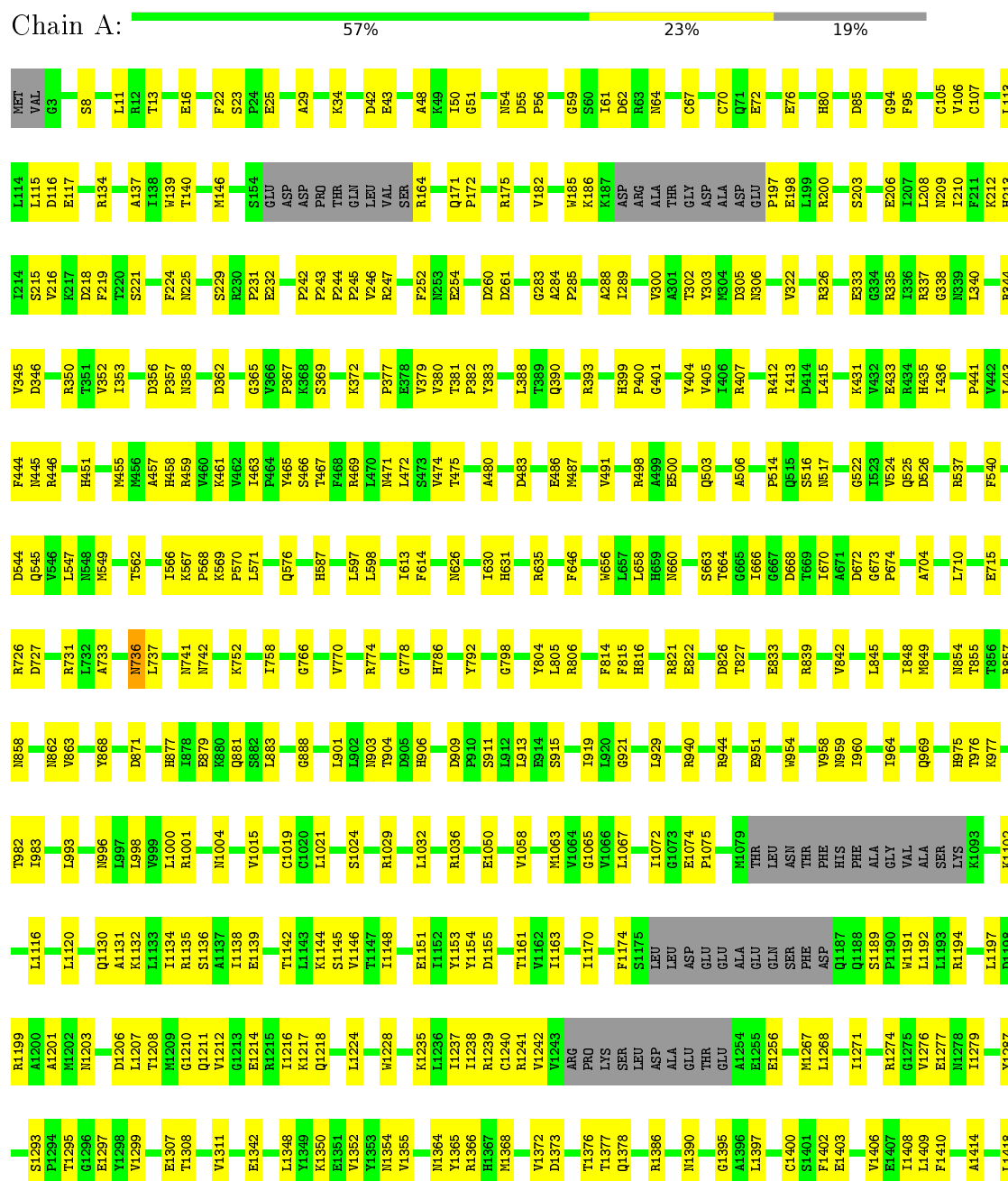
- Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Mg	0
			1	1	

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

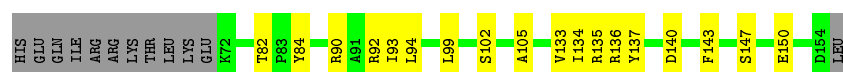
- Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1





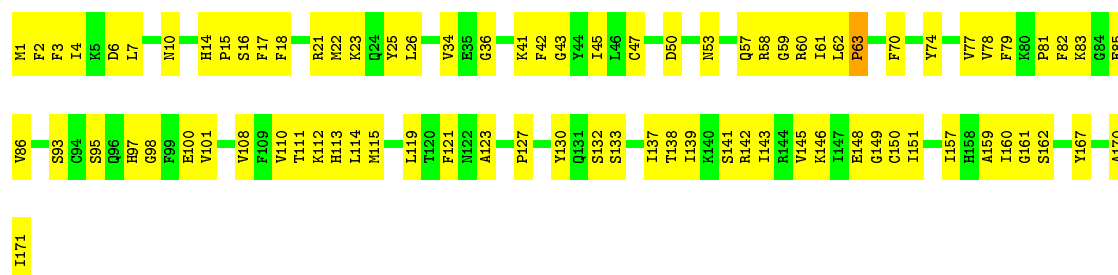






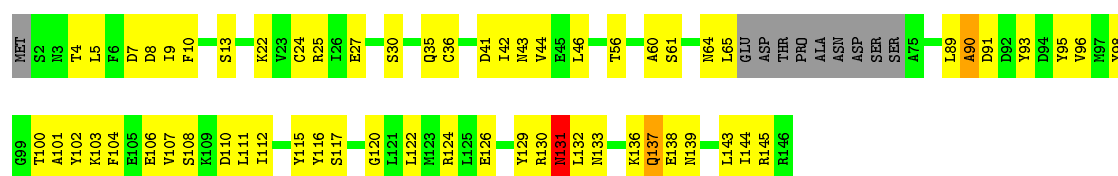
• Molecule 7: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

Chain G: 51% 48%



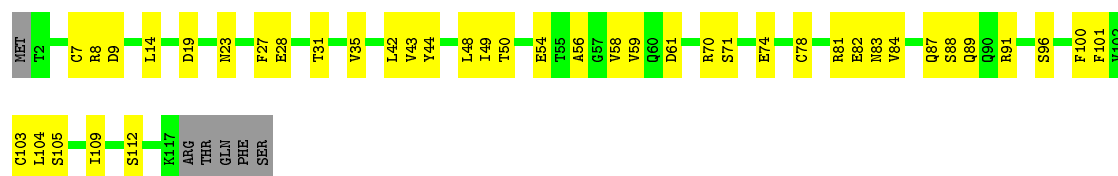
• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H: 51% 40% 7%



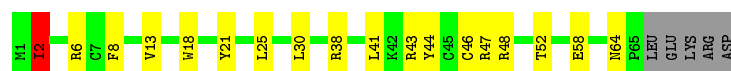
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I: 61% 34% 5%



• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J: 67% 24% 7%



• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K: 71% 23% 7%



• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4









## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	37000	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.46	0/11192	0.55	1/15128 (0.0%)
10	J	0.53	0/541	0.57	0/727
11	K	0.43	0/922	0.53	0/1244
12	L	0.40	0/360	0.60	0/478
13	M	0.40	0/1809	0.60	0/2435
14	N	1.00	20/1273 (1.6%)	1.23	2/1942 (0.1%)
15	O	0.59	0/1443	0.78	1/1942 (0.1%)
16	Q	0.53	0/1165	0.68	1/1576 (0.1%)
17	R	0.43	0/1354	0.68	1/1832 (0.1%)
18	T	1.21	26/1273 (2.0%)	1.46	18/1942 (0.9%)
19	U	0.40	0/766	0.61	0/1032
2	B	0.51	0/9378	0.59	1/12646 (0.0%)
20	V	0.38	0/789	0.62	1/1066 (0.1%)
21	W	0.35	1/832 (0.1%)	0.47	0/1157
22	X	0.26	0/706	0.47	0/979
3	C	0.52	0/2099	0.57	0/2845
4	D	0.25	0/1262	0.44	0/1693
5	E	0.40	0/1780	0.49	0/2395
6	F	0.47	0/682	0.52	0/922
7	G	0.31	0/1368	0.50	0/1844
8	H	0.60	1/1107 (0.1%)	0.97	6/1499 (0.4%)
9	I	0.40	0/962	0.50	0/1295
All	All	0.53	48/43063 (0.1%)	0.67	32/58619 (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
10	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	M	0	1
18	T	0	2
2	B	0	1
8	H	0	2
All	All	0	7

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	131	ASN	C-N	-13.03	1.04	1.34
18	T	66	DA	P-O5'	-11.67	1.48	1.59
18	T	60	DA	C1'-N9	-10.36	1.32	1.47
18	T	44	DA	O3'-P	7.31	1.70	1.61
18	T	69	DG	C1'-N9	-6.83	1.37	1.47
18	T	55	DC	C1'-N1	6.26	1.57	1.49
18	T	77	DC	C1'-N1	6.19	1.57	1.49
18	T	43	DA	C1'-N9	-6.16	1.38	1.47
18	T	50	DC	C1'-N1	6.16	1.57	1.49
18	T	74	DC	C1'-N1	6.14	1.57	1.49
18	T	30	DC	C1'-N1	6.11	1.57	1.49
18	T	27	DC	C1'-N1	6.09	1.57	1.49
18	T	49	DC	C1'-N1	6.08	1.57	1.49
18	T	59	DT	C4'-C3'	-5.60	1.47	1.52
14	N	44	DC	C1'-N1	5.55	1.56	1.49
21	W	76	PRO	C-N	5.34	1.44	1.34
14	N	15	DC	C1'-N1	5.29	1.56	1.49
14	N	32	DC	C1'-N1	5.25	1.56	1.49
14	N	33	DT	C1'-N1	5.22	1.56	1.49
14	N	35	DT	C1'-N1	5.21	1.56	1.49
18	T	40	DT	C1'-N1	5.21	1.56	1.49
18	T	48	DT	C1'-N1	5.20	1.56	1.49
18	T	81	DT	C1'-N1	5.20	1.56	1.49
14	N	40	DC	C1'-N1	5.20	1.56	1.49
18	T	29	DT	C1'-N1	5.19	1.55	1.49
18	T	78	DT	C1'-N1	5.19	1.55	1.49
14	N	49	DC	C1'-N1	5.19	1.55	1.49
14	N	10	DT	C1'-N1	5.18	1.55	1.49
18	T	75	DT	C1'-N1	5.18	1.55	1.49
18	T	47	DT	C1'-N1	5.18	1.55	1.49
14	N	54	DC	C1'-N1	5.17	1.55	1.49
14	N	53	DT	C1'-N1	5.16	1.55	1.49
14	N	58	DT	C1'-N1	5.16	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	51	DC	C1'-N1	5.15	1.55	1.49
14	N	60	DT	C1'-N1	5.15	1.55	1.49
18	T	52	DT	C1'-N1	5.15	1.55	1.49
14	N	52	DC	C1'-N1	5.15	1.55	1.49
14	N	48	DT	C1'-N1	5.15	1.55	1.49
14	N	13	DC	C1'-N1	5.15	1.55	1.49
18	T	80	DT	C1'-N1	5.15	1.55	1.49
14	N	55	DC	C1'-N1	5.14	1.55	1.49
18	T	36	DT	C1'-N1	5.13	1.55	1.49
18	T	70	DC	C1'-N1	5.13	1.55	1.49
18	T	56	DT	C1'-N1	5.12	1.55	1.49
14	N	7	DC	C1'-N1	5.12	1.55	1.49
18	T	72	DT	C1'-N1	5.11	1.55	1.49
14	N	47	DT	C1'-N1	5.10	1.55	1.49
14	N	17	DC	C1'-N1	5.04	1.55	1.49

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	131	ASN	N-CA-C	16.18	154.70	111.00
8	H	131	ASN	O-C-N	-15.87	97.31	122.70
8	H	131	ASN	C-N-CA	15.69	160.92	121.70
18	T	59	DT	O4'-C4'-C3'	-11.78	98.93	106.00
17	R	336	VAL	CB-CA-C	-10.95	90.59	111.40
18	T	44	DA	N9-C1'-C2'	10.59	132.71	112.60
8	H	131	ASN	CA-C-N	9.74	138.63	117.20
14	N	26	DT	O4'-C4'-C3'	-9.02	100.59	106.00
18	T	45	DC	C2'-C3'-O3'	-7.83	86.75	112.60
18	T	58	DT	O4'-C4'-C3'	-7.21	101.62	104.50
8	H	131	ASN	N-CA-CB	-6.97	98.05	110.60
18	T	65	DC	N1-C1'-C2'	6.65	125.23	112.60
18	T	64	DA	O5'-P-OP1	-6.62	99.74	105.70
8	H	131	ASN	CB-CA-C	-6.38	97.64	110.40
18	T	59	DT	O4'-C1'-C2'	-6.34	100.83	105.90
18	T	43	DA	O4'-C1'-N9	-6.29	103.60	108.00
18	T	44	DA	O4'-C1'-N9	6.11	112.28	108.00
18	T	44	DA	O4'-C1'-C2'	6.10	110.78	105.90
18	T	66	DA	N1-C6-N6	-6.08	114.95	118.60
18	T	59	DT	C4-C5-C6	5.84	121.50	118.00
1	A	658	LEU	CA-CB-CG	5.63	128.25	115.30
18	T	66	DA	P-O5'-C5'	5.49	129.68	120.90
15	O	175	LEU	CA-CB-CG	5.45	127.83	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	60	DA	O4'-C1'-N9	-5.44	104.19	108.00
20	V	9	LEU	CA-CB-CG	5.41	127.75	115.30
18	T	45	DC	O4'-C1'-C2'	5.34	110.17	105.90
14	N	26	DT	P-O3'-C3'	5.22	125.97	119.70
18	T	44	DA	C8-N9-C1'	5.22	137.10	127.70
18	T	44	DA	P-O3'-C3'	5.20	125.94	119.70
16	Q	376	LEU	CA-CB-CG	5.14	127.13	115.30
18	T	44	DA	C4-N9-C1'	-5.08	117.16	126.30
2	B	218	SER	CB-CA-C	-5.01	100.57	110.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1175	LEU	Peptide
8	H	131	ASN	Mainchain,Peptide
10	J	2	ILE	Peptide
13	M	292	PRO	Peptide
18	T	43	DA	Sidechain
18	T	45	DC	Sidechain

## 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	10997	0	11082	294	0
2	B	9200	0	9194	376	0
3	C	2061	0	2029	70	0
4	D	1253	0	1273	61	0
5	E	1744	0	1772	31	0
6	F	670	0	690	15	0
7	G	1340	0	1356	96	0
8	H	1089	0	1061	40	0
9	I	944	0	899	30	0
10	J	532	0	543	19	0
11	K	904	0	911	21	0
12	L	358	0	380	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1785	0	1891	165	0
14	N	1134	0	633	57	0
15	O	1416	0	1493	103	0
16	Q	1141	0	1027	99	0
17	R	1347	0	1130	89	0
18	T	1134	0	633	124	0
19	U	757	0	747	21	0
20	V	782	0	790	17	0
21	W	835	0	348	12	0
22	X	710	0	287	5	0
23	A	2	0	0	0	0
23	B	1	0	0	0	0
23	C	1	0	0	0	0
23	I	2	0	0	0	0
23	J	1	0	0	0	0
23	L	1	0	0	0	0
23	M	1	0	0	0	0
23	W	1	0	0	0	0
24	A	1	0	0	0	0
All	All	42144	0	40169	1424	0

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 17.

All (1424) 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)
2:B:405:ARG:NH1	2:B:632:ARG:HG2	1.23	1.42
2:B:865:LYS:CE	13:M:145:ILE:HD11	1.46	1.42
1:A:197:PRO:HD3	18:T:35:DG:OP2	1.22	1.36
2:B:868:MET:HB2	13:M:149:CYS:SG	1.64	1.35
13:M:267:LYS:HE3	15:O:208:VAL:CG1	1.59	1.31
13:M:267:LYS:CE	15:O:208:VAL:CG1	2.16	1.24
2:B:199:MET:CE	2:B:491:THR:HG22	1.69	1.21
14:N:41:DG:C6	18:T:44:DA:C6	2.29	1.20
2:B:865:LYS:HE2	13:M:145:ILE:CD1	1.70	1.20
2:B:405:ARG:NH1	2:B:632:ARG:CG	2.04	1.18
14:N:41:DG:O6	18:T:44:DA:C6	1.96	1.17
13:M:267:LYS:HE3	15:O:208:VAL:HG13	1.25	1.16
15:O:99:PHE:CZ	18:T:58:DT:O2	2.00	1.15
15:O:91:ASN:OD1	20:V:69:TYR:CZ	1.98	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:24:DT:H2''	14:N:25:DA:H5'	1.25	1.13
13:M:267:LYS:NZ	15:O:169:PRO:HB3	1.64	1.12
13:M:270:ALA:HB2	15:O:208:VAL:HG11	1.26	1.12
2:B:865:LYS:CE	13:M:145:ILE:CD1	2.27	1.11
13:M:198:VAL:O	13:M:202:GLU:OE1	1.68	1.11
15:O:99:PHE:HB2	18:T:58:DT:H4'	1.33	1.11
14:N:41:DG:H2''	14:N:42:DT:H72	1.32	1.10
13:M:272:LYS:HB3	18:T:66:DA:OP1	1.49	1.09
12:L:47:ARG:NH1	13:M:250:MET:HE3	1.68	1.09
18:T:44:DA:H1'	18:T:45:DC:C5	1.85	1.09
2:B:199:MET:HE1	2:B:491:THR:CG2	1.82	1.08
14:N:41:DG:O6	18:T:44:DA:C5	2.07	1.08
18:T:42:DG:H1'	18:T:43:DA:H5'	1.35	1.08
2:B:199:MET:CE	2:B:491:THR:CG2	2.32	1.07
2:B:865:LYS:HE2	13:M:145:ILE:HD11	1.09	1.07
1:A:197:PRO:CD	18:T:35:DG:OP2	2.01	1.07
13:M:269:ILE:HG23	13:M:272:LYS:HE3	1.33	1.06
14:N:21:DG:H2''	14:N:22:DT:H5'	1.10	1.05
18:T:44:DA:H1'	18:T:45:DC:C4	1.92	1.05
4:D:29:LEU:HD22	7:G:82:PHE:CZ	1.93	1.04
2:B:868:MET:CB	13:M:149:CYS:SG	2.46	1.03
2:B:70:ILE:HD11	16:Q:333:LYS:HB2	1.42	1.02
15:O:91:ASN:ND2	19:U:285:TRP:CZ2	2.28	1.02
2:B:1041:GLU:O	16:Q:22:ILE:CB	2.09	1.01
2:B:865:LYS:HE3	13:M:145:ILE:HD11	1.41	1.00
19:U:2:SER:N	19:U:274:TYR:HH	1.59	1.00
2:B:475:SER:O	2:B:476:ARG:HG3	1.61	1.00
2:B:199:MET:HE1	2:B:491:THR:HG22	1.04	0.99
2:B:325:GLN:HB3	16:Q:401:TYR:OH	1.59	0.99
4:D:29:LEU:HD22	7:G:82:PHE:CE2	1.96	0.99
15:O:191:PRO:HG3	18:T:65:DC:C5'	1.92	0.99
14:N:21:DG:C2'	14:N:22:DT:H5'	1.92	0.99
13:M:274:PRO:HD2	15:O:188:GLU:CG	1.92	0.98
15:O:114:LEU:HD11	18:T:59:DT:O2	1.62	0.97
12:L:47:ARG:NH1	13:M:250:MET:CE	2.27	0.96
7:G:151:ILE:CD1	21:W:134:LEU:CB	2.43	0.96
2:B:44:VAL:HG11	2:B:495:LEU:HD13	1.47	0.96
16:Q:127:ILE:HG22	16:Q:129:PRO:HD3	1.47	0.96
15:O:105:ARG:NH2	18:T:60:DA:OP1	1.98	0.95
2:B:249:ARG:NH1	2:B:415:GLN:O	1.89	0.95
13:M:269:ILE:CG2	13:M:272:LYS:HG3	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:79:PHE:HE2	7:G:81:PRO:HG3	1.31	0.94
13:M:269:ILE:HG22	13:M:272:LYS:HG3	1.50	0.94
14:N:21:DG:H2"	14:N:22:DT:C5'	1.97	0.94
14:N:22:DT:H2"	14:N:23:DA:H5'	1.47	0.94
2:B:44:VAL:HG11	2:B:495:LEU:CD1	1.98	0.94
15:O:191:PRO:CB	18:T:65:DC:H5"	1.97	0.94
14:N:29:DT:H2"	14:N:30:DA:C8	2.03	0.93
22:X:225:GLU:HA	22:X:231:LEU:HA	1.49	0.93
13:M:269:ILE:HG23	13:M:272:LYS:CE	1.99	0.92
7:G:79:PHE:CE2	7:G:81:PRO:HG3	2.05	0.92
1:A:70:CYS:SG	1:A:80:HIS:NE2	2.41	0.92
2:B:405:ARG:HH12	2:B:632:ARG:HG2	1.17	0.92
12:L:47:ARG:HH12	13:M:250:MET:HE3	1.23	0.91
2:B:405:ARG:HH11	2:B:632:ARG:HG2	1.08	0.91
2:B:68:THR:HB	16:Q:335:LEU:CD1	2.00	0.91
15:O:99:PHE:CD1	18:T:58:DT:H1'	2.07	0.90
13:M:270:ALA:HB1	15:O:208:VAL:HG21	1.53	0.89
13:M:267:LYS:HE3	15:O:208:VAL:HG11	1.52	0.89
2:B:914:LYS:HB3	2:B:937:ALA:O	1.73	0.89
2:B:868:MET:HB2	13:M:149:CYS:HG	1.31	0.89
4:D:49:ALA:HA	7:G:3:PHE:CD1	2.08	0.89
13:M:267:LYS:CE	15:O:208:VAL:HG11	2.03	0.88
18:T:62:DA:C2'	18:T:63:DT:H5'	2.03	0.88
2:B:247:GLY:N	2:B:418:LYS:HZ1	1.73	0.87
12:L:47:ARG:HH12	13:M:250:MET:CE	1.84	0.87
13:M:274:PRO:HD2	15:O:188:GLU:HG3	1.55	0.87
2:B:405:ARG:HH11	2:B:632:ARG:CG	1.78	0.87
13:M:274:PRO:HD2	15:O:188:GLU:HG2	1.56	0.86
17:R:98:ASN:HB3	17:R:103:LYS:O	1.75	0.86
18:T:43:DA:H2"	18:T:44:DA:H5'	1.58	0.86
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.57	0.86
14:N:22:DT:H2"	14:N:23:DA:C5'	2.04	0.86
16:Q:336:ASP:OD1	16:Q:337:GLU:N	2.09	0.85
2:B:1042:GLY:HA2	16:Q:22:ILE:HA	1.57	0.85
2:B:199:MET:HE3	2:B:491:THR:CG2	2.05	0.85
2:B:247:GLY:HA2	2:B:418:LYS:NZ	1.92	0.84
4:D:32:GLU:HG3	7:G:42:PHE:CE1	2.11	0.84
18:T:42:DG:H1'	18:T:43:DA:C5'	2.06	0.84
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.57	0.84
16:Q:373:TYR:CD1	17:R:70:LEU:HD21	2.13	0.84
2:B:644:GLU:HG3	2:B:646:LEU:H	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:44:DA:H4'	18:T:45:DC:OP1	1.76	0.84
2:B:87:LYS:HB2	2:B:137:TYR:HB2	1.58	0.84
14:N:41:DG:C6	18:T:44:DA:N6	2.46	0.83
2:B:217:ARG:NH1	2:B:407:ASP:OD2	2.12	0.83
2:B:199:MET:HE3	2:B:491:THR:HG21	1.59	0.83
18:T:43:DA:OP2	18:T:43:DA:H3'	1.79	0.83
18:T:43:DA:C2'	18:T:44:DA:H5'	2.08	0.83
7:G:151:ILE:HD11	21:W:134:LEU:CB	2.08	0.83
16:Q:141:ARG:HA	16:Q:350:TRP:HA	1.58	0.83
18:T:43:DA:H2''	18:T:44:DA:C5'	2.09	0.82
16:Q:366:GLU:HB3	16:Q:392:VAL:HG13	1.61	0.82
14:N:28:DA:C2	15:O:99:PHE:HZ	1.97	0.82
2:B:247:GLY:N	2:B:418:LYS:NZ	2.28	0.82
13:M:274:PRO:HG2	15:O:188:GLU:OE2	1.80	0.81
14:N:24:DT:C2'	14:N:25:DA:H5'	2.09	0.81
15:O:91:ASN:ND2	19:U:285:TRP:HZ2	1.77	0.81
16:Q:104:ARG:HG2	17:R:92:LEU:HD22	1.62	0.81
15:O:103:ILE:HD13	18:T:59:DT:C5'	2.11	0.81
13:M:267:LYS:HE2	15:O:208:VAL:CG1	2.09	0.81
18:T:62:DA:H2''	18:T:63:DT:H5'	1.61	0.81
7:G:4:ILE:HG12	7:G:77:VAL:HG22	1.63	0.80
13:M:267:LYS:CE	15:O:208:VAL:HG12	2.09	0.80
2:B:68:THR:CB	16:Q:335:LEU:CD1	2.60	0.80
2:B:365:THR:HG21	2:B:370:PHE:CD2	2.16	0.80
2:B:220:GLY:O	2:B:221:ASN:HB2	1.80	0.80
13:M:267:LYS:HZ3	15:O:169:PRO:HB3	1.44	0.80
2:B:757:PRO:HD3	2:B:983:ARG:HE	1.46	0.80
18:T:42:DG:H2''	18:T:43:DA:OP2	1.80	0.80
15:O:103:ILE:HD13	18:T:59:DT:H5''	1.64	0.80
17:R:138:GLN:HB2	17:R:211:LYS:HB3	1.64	0.80
4:D:190:GLU:HA	7:G:167:TYR:CE2	2.16	0.79
15:O:91:ASN:OD1	20:V:69:TYR:CE2	2.35	0.79
2:B:71:LEU:HD21	2:B:436:VAL:HG11	1.64	0.79
14:N:41:DG:C5	18:T:44:DA:N6	2.51	0.79
14:N:42:DT:H2''	14:N:43:DT:O4'	1.82	0.79
15:O:98:ARG:O	18:T:58:DT:H5'	1.83	0.79
18:T:65:DC:P	18:T:65:DC:H3'	2.22	0.79
15:O:91:ASN:OD1	20:V:69:TYR:OH	2.01	0.79
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.65	0.79
18:T:44:DA:C1'	18:T:45:DC:C5	2.66	0.79
15:O:191:PRO:CG	18:T:65:DC:H5''	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:103:ILE:HD11	18:T:59:DT:H5'	1.64	0.78
8:H:89:LEU:HG	8:H:90:ALA:H	1.48	0.78
17:R:129:VAL:HG11	17:R:221:GLU:HG2	1.66	0.78
8:H:129:TYR:O	8:H:133:ASN:ND2	2.17	0.78
15:O:99:PHE:CE1	18:T:58:DT:C2	2.72	0.78
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.19	0.78
2:B:53:GLN:OE1	2:B:547:VAL:HG22	1.84	0.77
16:Q:121:PHE:HB2	17:R:131:ASN:HB3	1.67	0.77
15:O:103:ILE:CD1	18:T:59:DT:H5'	2.14	0.77
9:I:82:GLU:HG2	9:I:104:LEU:HD12	1.65	0.77
2:B:68:THR:OG1	16:Q:335:LEU:HD12	1.85	0.77
17:R:73:LEU:HD12	17:R:74:PRO:HD2	1.65	0.77
15:O:191:PRO:HG3	18:T:65:DC:H5''	1.66	0.77
16:Q:102:PRO:HA	17:R:94:LYS:HA	1.67	0.76
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.67	0.76
14:N:28:DA:N3	15:O:116:PHE:CZ	2.53	0.76
15:O:99:PHE:CD1	18:T:58:DT:C1'	2.68	0.76
2:B:247:GLY:H	2:B:418:LYS:NZ	1.83	0.76
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	1.68	0.76
13:M:269:ILE:CG2	13:M:272:LYS:HE3	2.13	0.76
2:B:247:GLY:CA	2:B:418:LYS:NZ	2.48	0.76
13:M:268:GLU:OE1	13:M:319:HIS:NE2	2.12	0.76
18:T:61:DT:H2'	18:T:62:DA:C8	2.21	0.75
16:Q:375:LEU:O	16:Q:386:MET:HA	1.87	0.75
3:C:149:LYS:HG3	3:C:150:GLY:H	1.51	0.75
14:N:28:DA:H1'	15:O:116:PHE:CZ	2.21	0.75
15:O:99:PHE:CE1	18:T:58:DT:O2	2.39	0.75
18:T:60:DA:N7	18:T:61:DT:O4	2.19	0.75
16:Q:376:LEU:HD23	16:Q:386:MET:HG2	1.68	0.75
7:G:1:MET:HE3	7:G:85:GLU:OE2	1.87	0.74
7:G:160:ILE:HD12	7:G:160:ILE:N	2.02	0.74
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.19	0.74
1:A:379:VAL:HG22	1:A:431:LYS:HG2	1.69	0.74
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.69	0.74
2:B:345:LYS:HA	2:B:348:ARG:HG2	1.70	0.74
18:T:65:DC:H1'	18:T:66:DA:H5'	1.69	0.74
14:N:41:DG:C6	18:T:44:DA:N1	2.56	0.74
13:M:272:LYS:CB	18:T:66:DA:OP1	2.33	0.73
4:D:56:ARG:NH1	4:D:122:GLU:OE2	2.21	0.73
13:M:238:TYR:HB3	13:M:242:PHE:HE2	1.54	0.73
2:B:369:GLY:HA3	16:Q:367:ALA:HB2	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ARG:NH2	2:B:294:ASP:OD1	2.20	0.73
1:A:1136:SER:O	1:A:1274:ARG:NH1	2.22	0.73
17:R:120:TYR:HD1	17:R:226:PRO:HA	1.54	0.73
1:A:362:ASP:OD2	1:A:459:ARG:NH1	2.21	0.73
13:M:166:LYS:HB3	13:M:170:SER:HB3	1.70	0.73
2:B:919:SER:HB2	2:B:922:GLU:HB2	1.72	0.72
5:E:56:LYS:NZ	5:E:84:ASP:OD2	2.22	0.72
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.22	0.72
13:M:274:PRO:CD	15:O:188:GLU:HG3	2.20	0.72
14:N:28:DA:N3	15:O:116:PHE:HZ	1.88	0.72
12:L:32:ALA:HB2	12:L:55:ILE:HB	1.70	0.72
7:G:130:TYR:HB2	7:G:137:ILE:HB	1.72	0.71
13:M:157:CYS:HB2	13:M:163:LEU:HD11	1.72	0.71
17:R:64:SER:HA	17:R:216:GLY:HA2	1.72	0.71
14:N:41:DG:H2''	14:N:42:DT:C7	2.17	0.71
18:T:44:DA:H2''	18:T:45:DC:H5	1.54	0.71
13:M:272:LYS:HB3	18:T:66:DA:P	2.30	0.71
9:I:31:THR:O	16:Q:401:TYR:HB2	1.89	0.71
17:R:73:LEU:HD11	17:R:77:LEU:HD23	1.72	0.71
2:B:220:GLY:O	2:B:221:ASN:CB	2.38	0.71
5:E:116:ILE:HB	5:E:121:MET:HE2	1.72	0.71
13:M:236:LEU:HD11	13:M:257:GLU:HG3	1.72	0.71
16:Q:139:LEU:HB3	17:R:212:THR:HG21	1.71	0.71
1:A:107:CYS:SG	1:A:171:GLN:NE2	2.63	0.71
1:A:405:VAL:HG23	1:A:415:LEU:HD11	1.71	0.71
4:D:54:GLU:HB2	4:D:160:VAL:HG11	1.73	0.71
13:M:267:LYS:NZ	15:O:169:PRO:CB	2.51	0.71
13:M:270:ALA:CB	15:O:208:VAL:HG11	2.13	0.71
13:M:267:LYS:NZ	15:O:239:LYS:HD2	2.06	0.71
1:A:871:ASP:OD2	1:A:1366:ARG:NH2	2.24	0.71
1:A:881:GLN:NE2	1:A:959:ASN:HA	2.06	0.71
2:B:1056:SER:OG	2:B:1067:ARG:NH1	2.24	0.71
4:D:24:ALA:HA	7:G:83:LYS:HB2	1.73	0.71
15:O:191:PRO:CG	18:T:65:DC:C5'	2.69	0.71
2:B:984:HIS:NE2	2:B:1028:GLU:OE1	2.24	0.71
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.72	0.71
7:G:79:PHE:CD2	7:G:81:PRO:HD3	2.26	0.71
17:R:67:GLN:HB3	17:R:219:CYS:HB2	1.73	0.71
2:B:475:SER:O	2:B:476:ARG:CG	2.38	0.70
7:G:111:THR:HB	7:G:114:LEU:HD13	1.73	0.70
7:G:159:ALA:C	7:G:160:ILE:HD12	2.11	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:59:DT:H2''	18:T:60:DA:O5'	1.91	0.70
13:M:270:ALA:CB	15:O:208:VAL:HG21	2.20	0.70
2:B:437:GLU:OE2	16:Q:330:ARG:O	2.09	0.70
1:A:61:ILE:HG22	1:A:62:ASP:H	1.55	0.70
13:M:270:ALA:HB2	15:O:208:VAL:CG1	2.14	0.70
15:O:191:PRO:HG3	18:T:65:DC:H5'	1.73	0.70
7:G:151:ILE:HG13	21:W:134:LEU:CB	2.21	0.70
17:R:104:ILE:HD11	17:R:122:LEU:HB3	1.73	0.70
15:O:103:ILE:CD1	18:T:59:DT:C5'	2.69	0.70
1:A:598:LEU:HD21	8:H:124:ARG:HB2	1.73	0.70
1:A:441:PRO:HA	1:A:458:HIS:O	1.92	0.70
1:A:626:ASN:O	1:A:631:HIS:ND1	2.23	0.69
2:B:549:THR:OG1	2:B:628:THR:OG1	2.09	0.69
2:B:73:GLN:HB3	2:B:86:ARG:HB3	1.73	0.69
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.73	0.69
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.75	0.69
1:A:1136:SER:HB3	1:A:1274:ARG:HH12	1.58	0.69
2:B:593:PRO:HB2	2:B:617:ARG:HE	1.56	0.69
4:D:39:ASN:HD21	4:D:43:GLU:HB2	1.58	0.69
12:L:28:LYS:HA	12:L:39:SER:HA	1.74	0.69
5:E:26:ARG:HH12	5:E:189:GLY:HA3	1.58	0.69
15:O:99:PHE:CE1	18:T:58:DT:H1'	2.26	0.69
17:R:106:LEU:O	17:R:119:GLU:HA	1.93	0.69
18:T:44:DA:C4	18:T:45:DC:C4	2.80	0.69
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.74	0.69
2:B:71:LEU:HD23	2:B:88:TYR:HD2	1.57	0.69
18:T:61:DT:H2'	18:T:62:DA:N7	2.08	0.69
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.56	0.69
4:D:192:LYS:NZ	4:D:204:ASP:OD1	2.23	0.69
14:N:29:DT:H4'	14:N:30:DA:H5'	1.73	0.69
18:T:43:DA:H2''	18:T:44:DA:O4'	1.93	0.69
18:T:44:DA:C1'	18:T:45:DC:C4	2.75	0.68
13:M:269:ILE:CG2	13:M:272:LYS:CG	2.72	0.68
2:B:463:THR:O	2:B:465:ASN:OD1	2.11	0.68
2:B:53:GLN:OE1	2:B:547:VAL:CG2	2.42	0.68
4:D:32:GLU:CG	7:G:41:LYS:HE2	2.24	0.68
16:Q:397:ALA:HB3	16:Q:400:LYS:HE3	1.76	0.68
18:T:64:DA:H2'	18:T:65:DC:C6	2.28	0.68
1:A:906:HIS:O	1:A:1029:ARG:NH2	2.26	0.67
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.59	0.67
3:C:66:ARG:NH2	3:C:143:LEU:O	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:190:GLU:HA	7:G:167:TYR:CD2	2.28	0.67
13:M:267:LYS:HG3	13:M:268:GLU:H	1.59	0.67
17:R:63:ARG:NH1	17:R:66:ARG:HH22	1.92	0.67
18:T:60:DA:C8	18:T:61:DT:O4	2.48	0.67
2:B:247:GLY:HA2	2:B:418:LYS:HZ3	1.58	0.67
1:A:524:VAL:HG12	1:A:525:GLN:HG2	1.77	0.67
2:B:369:GLY:HA3	16:Q:367:ALA:CB	2.25	0.67
17:R:105:THR:HA	17:R:120:TYR:O	1.95	0.67
1:A:888:GLY:O	1:A:940:ARG:NH2	2.27	0.67
4:D:66:ARG:NH2	7:G:47:CYS:SG	2.67	0.67
2:B:215:GLN:NE2	2:B:479:VAL:HG22	2.09	0.66
1:A:186:LYS:O	18:T:34:DG:OP2	2.12	0.66
16:Q:135:LEU:HB2	16:Q:136:PRO:HA	1.77	0.66
2:B:798:TYR:O	2:B:821:GLN:NE2	2.20	0.66
4:D:32:GLU:HG3	7:G:41:LYS:HE2	1.76	0.66
9:I:78:CYS:SG	9:I:105:SER:OG	2.54	0.66
13:M:136:LEU:HD13	13:M:196:ILE:HD11	1.78	0.66
1:A:115:LEU:O	1:A:164:ARG:NH1	2.29	0.66
3:C:75:MET:O	3:C:246:ARG:NH2	2.23	0.66
13:M:286:ILE:HG13	13:M:291:ILE:HG13	1.77	0.66
13:M:267:LYS:CE	15:O:208:VAL:HG13	2.02	0.66
2:B:629:ASP:OD1	2:B:630:ALA:N	2.29	0.66
8:H:8:ASP:OD1	8:H:9:ILE:N	2.29	0.66
13:M:267:LYS:HZ2	15:O:169:PRO:HB3	1.59	0.66
19:U:30:ILE:HG23	19:U:31:ASP:H	1.60	0.66
1:A:407:ARG:HH11	1:A:413:ILE:HD11	1.60	0.66
4:D:32:GLU:HG3	7:G:42:PHE:CZ	2.30	0.66
13:M:272:LYS:HE2	18:T:65:DC:OP1	1.95	0.66
16:Q:397:ALA:HB3	16:Q:400:LYS:CE	2.26	0.66
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.77	0.65
16:Q:101:PHE:N	17:R:95:ILE:O	2.24	0.65
2:B:68:THR:OG1	16:Q:335:LEU:CD1	2.44	0.65
2:B:309:GLN:OE1	2:B:392:ARG:NH2	2.28	0.65
2:B:92:PHE:HD2	2:B:130:VAL:HG11	1.61	0.65
15:O:99:PHE:CB	18:T:58:DT:H4'	2.20	0.65
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.29	0.65
1:A:362:ASP:O	1:A:458:HIS:ND1	2.28	0.65
13:M:245:HIS:CD2	17:R:264:SER:HB2	2.32	0.65
13:M:34:ILE:HG22	13:M:45:CYS:HA	1.79	0.65
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.30	0.65
2:B:68:THR:HB	16:Q:335:LEU:HD11	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:GLU:OE2	12:L:70:ARG:NH2	2.30	0.65
1:A:198:GLU:OE2	1:A:200:ARG:NH2	2.27	0.65
3:C:22:LEU:HD11	11:K:101:LEU:HD11	1.77	0.65
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.62	0.64
13:M:22:LEU:HB3	13:M:52:LEU:HD23	1.77	0.64
2:B:247:GLY:CA	2:B:418:LYS:HZ1	2.09	0.64
10:J:48:ARG:O	10:J:52:THR:OG1	2.10	0.64
1:A:821:ARG:HE	2:B:514:LEU:HB2	1.62	0.64
18:T:41:DC:H3'	21:W:79:SER:CB	2.27	0.64
1:A:326:ARG:HE	1:A:1406:VAL:HG21	1.62	0.64
13:M:188:THR:HG22	13:M:190:LYS:H	1.63	0.64
13:M:245:HIS:HA	17:R:264:SER:HB3	1.79	0.64
7:G:151:ILE:CG1	21:W:134:LEU:CB	2.75	0.64
16:Q:378:VAL:HG22	16:Q:384:PHE:HE1	1.61	0.64
18:T:44:DA:H2''	18:T:45:DC:C5	2.31	0.64
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.80	0.64
1:A:537:ARG:NH1	8:H:120:GLY:O	2.31	0.64
18:T:43:DA:C1'	18:T:44:DA:H5'	2.28	0.64
8:H:110:ASP:O	8:H:129:TYR:N	2.30	0.64
1:A:881:GLN:HE21	1:A:959:ASN:HA	1.62	0.63
1:A:134:ARG:NH1	1:A:221:SER:O	2.31	0.63
2:B:959:ASP:HB2	13:M:143:PRO:HB2	1.79	0.63
7:G:111:THR:HG22	7:G:113:HIS:H	1.61	0.63
13:M:200:THR:O	13:M:203:PHE:HB3	1.97	0.63
16:Q:373:TYR:HD1	17:R:70:LEU:HD21	1.59	0.63
2:B:44:VAL:HG11	2:B:495:LEU:HD12	1.80	0.63
16:Q:141:ARG:O	17:R:207:THR:OG1	2.13	0.63
2:B:247:GLY:CA	2:B:418:LYS:HZ3	2.10	0.63
9:I:9:ASP:OD2	16:Q:125:LYS:CE	2.47	0.63
2:B:41:LYS:O	2:B:45:SER:HB3	1.99	0.63
9:I:58:VAL:HG21	9:I:109:ILE:HD11	1.80	0.63
2:B:44:VAL:CG1	2:B:495:LEU:HD13	2.26	0.63
5:E:76:GLY:N	5:E:106:GLN:OE1	2.31	0.63
15:O:98:ARG:CZ	18:T:59:DT:P	2.87	0.63
2:B:901:PRO:HG2	12:L:60:ARG:HA	1.80	0.63
4:D:49:ALA:CB	7:G:3:PHE:CE1	2.82	0.63
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.80	0.62
17:R:98:ASN:HB3	17:R:103:LYS:HG3	1.79	0.62
1:A:806:ARG:HH22	2:B:729:ILE:HG13	1.63	0.62
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.81	0.62
2:B:278:GLN:HB2	2:B:337:ARG:HD2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:151:ILE:HD12	21:W:134:LEU:CB	2.29	0.62
15:O:98:ARG:HG2	18:T:58:DT:H5'	1.80	0.62
3:C:153:LEU:HD11	3:C:155:LEU:HD23	1.82	0.62
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.81	0.62
10:J:8:PHE:HB2	10:J:48:ARG:HH22	1.64	0.62
13:M:274:PRO:CD	15:O:188:GLU:CG	2.74	0.62
3:C:146:LYS:NZ	10:J:58:GLU:OE2	2.24	0.62
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.35	0.62
1:A:335:ARG:NH2	2:B:1114:LEU:HD21	2.14	0.62
2:B:865:LYS:HE2	13:M:145:ILE:HD12	1.76	0.62
2:B:865:LYS:NZ	13:M:145:ILE:CD1	2.63	0.62
3:C:179:GLU:OE1	3:C:206:ASN:ND2	2.32	0.62
9:I:14:LEU:HB3	9:I:27:PHE:HB3	1.81	0.62
1:A:544:ASP:OD1	1:A:545:GLN:N	2.33	0.61
3:C:56:THR:HG22	3:C:147:LEU:HD21	1.81	0.61
5:E:78:LEU:HD21	5:E:109:ILE:HD12	1.80	0.61
2:B:68:THR:CB	16:Q:335:LEU:HD12	2.30	0.61
2:B:119:LEU:HD22	2:B:953:LEU:HD21	1.82	0.61
2:B:870:ILE:HG23	2:B:917:PRO:HD2	1.83	0.61
7:G:1:MET:CE	7:G:85:GLU:OE2	2.49	0.61
18:T:65:DC:H2''	18:T:66:DA:H5'	1.82	0.61
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.82	0.61
13:M:281:SER:O	13:M:285:ASN:ND2	2.31	0.61
13:M:43:VAL:HG12	13:M:53:SER:HB3	1.82	0.61
1:A:352:VAL:HB	1:A:467:THR:HG22	1.81	0.61
3:C:254:LYS:HG2	11:K:42:LEU:HD12	1.82	0.61
5:E:55:ARG:HB2	5:E:84:ASP:OD1	1.99	0.61
16:Q:339:ALA:HB1	16:Q:343:ARG:HH12	1.65	0.61
1:A:587:HIS:CD2	1:A:969:GLN:HG3	2.35	0.61
2:B:868:MET:HG2	13:M:182:ARG:HG3	1.83	0.61
15:O:170:ILE:O	15:O:239:LYS:HE2	2.00	0.61
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.81	0.61
18:T:62:DA:H2'	18:T:63:DT:H5'	1.80	0.61
18:T:63:DT:H2''	18:T:64:DA:H5'	1.82	0.61
18:T:64:DA:C2'	18:T:65:DC:C6	2.83	0.61
15:O:191:PRO:HB3	18:T:65:DC:H5''	1.80	0.61
4:D:32:GLU:CG	7:G:42:PHE:CE1	2.84	0.61
2:B:465:ASN:OD1	2:B:465:ASN:N	2.33	0.61
1:A:1189:SER:N	1:A:1242:VAL:O	2.28	0.60
19:U:37:ASP:O	19:U:41:ILE:HG13	2.01	0.60
1:A:260:ASP:OD1	1:A:261:ASP:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:MET:SD	2:B:492:LEU:HD23	2.42	0.60
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.82	0.60
16:Q:378:VAL:HG22	16:Q:384:PHE:CE1	2.36	0.60
15:O:98:ARG:NH1	18:T:59:DT:OP1	2.34	0.60
18:T:44:DA:H1'	18:T:45:DC:N4	2.17	0.60
1:A:929:LEU:HD11	1:A:983:ILE:HG21	1.83	0.60
2:B:283:VAL:HG11	2:B:321:GLY:HA3	1.82	0.60
21:W:39:ALA:HA	21:W:85:VAL:O	2.01	0.60
3:C:115:SER:HB3	3:C:142:VAL:HB	1.83	0.60
19:U:242:ASN:HA	19:U:268:THR:O	2.01	0.60
19:U:31:ASP:HB3	19:U:34:THR:OG1	2.02	0.60
1:A:1199:ARG:O	1:A:1203:ASN:ND2	2.35	0.60
2:B:71:LEU:HD12	16:Q:331:GLN:O	2.02	0.60
2:B:429:PHE:CZ	16:Q:332:LEU:HB2	2.37	0.60
1:A:993:LEU:HD11	1:A:1050:GLU:HB2	1.84	0.60
13:M:267:LYS:HD3	15:O:239:LYS:CD	2.31	0.60
2:B:325:GLN:NE2	16:Q:401:TYR:OH	2.28	0.60
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.83	0.59
4:D:148:LEU:O	4:D:152:SER:OG	2.15	0.59
4:D:57:LEU:O	4:D:61:GLU:N	2.32	0.59
7:G:138:THR:HG22	7:G:139:ILE:H	1.67	0.59
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.83	0.59
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.01	0.59
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.84	0.59
2:B:326:ASP:OD1	2:B:327:ARG:N	2.35	0.59
18:T:60:DA:H2'	18:T:61:DT:C5	2.38	0.59
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.84	0.59
1:A:568:PRO:HG2	8:H:46:LEU:HD23	1.84	0.59
18:T:42:DG:C1'	18:T:43:DA:H5'	2.23	0.59
2:B:62:ILE:O	2:B:65:GLU:HG2	2.01	0.59
4:D:54:GLU:HG2	4:D:58:VAL:HG23	1.84	0.59
8:H:104:PHE:HZ	8:H:137:GLN:H	1.48	0.59
1:A:95:PHE:HE1	1:A:1414:ALA:HB2	1.67	0.59
3:C:124:LEU:O	3:C:127:ARG:HG2	2.01	0.59
14:N:24:DT:H2''	14:N:25:DA:C5'	2.17	0.59
18:T:43:DA:H2''	18:T:44:DA:C4'	2.31	0.59
7:G:57:GLN:HG2	7:G:58:ARG:H	1.67	0.59
12:L:33:GLU:HG3	12:L:34:CYS:N	2.18	0.59
18:T:44:DA:N9	18:T:45:DC:N4	2.50	0.59
1:A:472:LEU:HD22	2:B:835:GLN:NE2	2.17	0.59
16:Q:119:LEU:O	17:R:132:GLU:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:148:GLU:H	7:G:161:GLY:HA2	1.67	0.58
2:B:1037:LEU:O	10:J:47:ARG:NH2	2.36	0.58
1:A:197:PRO:CG	18:T:35:DG:OP2	2.51	0.58
1:A:390:GLN:OE1	1:A:393:ARG:NH2	2.36	0.58
2:B:757:PRO:HG2	2:B:984:HIS:CE1	2.38	0.58
2:B:1065:GLN:OE1	2:B:1066:SER:N	2.37	0.58
2:B:186:GLU:HG2	2:B:190:TYR:HE2	1.67	0.58
12:L:47:ARG:NH1	13:M:250:MET:HE1	2.12	0.58
15:O:105:ARG:HD2	20:V:69:TYR:OH	2.03	0.58
18:T:44:DA:C2'	18:T:45:DC:C5	2.86	0.58
18:T:63:DT:H2'	18:T:64:DA:C8	2.38	0.58
1:A:1342:GLU:OE1	5:E:200:ARG:NH2	2.29	0.58
14:N:27:DA:H4'	15:O:73:THR:HG21	1.85	0.58
1:A:1116:LEU:HB2	1:A:1308:THR:HB	1.84	0.58
17:R:138:GLN:HB2	17:R:211:LYS:CB	2.31	0.58
18:T:61:DT:C2'	18:T:62:DA:C8	2.86	0.58
2:B:835:GLN:HA	2:B:1013:ASN:ND2	2.19	0.58
14:N:41:DG:N7	18:T:44:DA:N6	2.51	0.58
16:Q:373:TYR:OH	17:R:72:ARG:NH2	2.36	0.58
1:A:903:ASN:OD1	1:A:904:THR:N	2.37	0.58
2:B:43:LEU:HD11	2:B:812:LEU:HD23	1.84	0.58
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.39	0.58
2:B:209:GLU:OE2	2:B:788:ARG:NH2	2.37	0.58
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.86	0.58
4:D:153:ARG:NH1	4:D:183:LEU:O	2.37	0.58
14:N:22:DT:H2''	14:N:23:DA:O5'	2.04	0.58
1:A:503:GLN:OE1	6:F:90:ARG:NH1	2.32	0.57
2:B:1106:ARG:CZ	2:B:1118:PRO:HB3	2.34	0.57
2:B:676:VAL:O	2:B:677:GLU:HG2	2.04	0.57
2:B:956:THR:HG23	12:L:46:VAL:HB	1.86	0.57
5:E:65:THR:O	5:E:69:ILE:HD12	2.04	0.57
10:J:8:PHE:HB2	10:J:48:ARG:NH2	2.19	0.57
17:R:306:LEU:O	17:R:310:TYR:N	2.37	0.57
15:O:91:ASN:HD22	19:U:285:TRP:HZ2	1.51	0.57
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.38	0.57
2:B:259:TYR:HE2	2:B:270:LYS:HB2	1.69	0.57
16:Q:373:TYR:HD1	17:R:70:LEU:HD11	1.68	0.57
1:A:1138:ILE:O	1:A:1276:VAL:N	2.34	0.57
2:B:156:SER:O	2:B:163:GLY:N	2.37	0.57
5:E:43:LYS:O	5:E:47:CYS:HB2	2.05	0.57
3:C:148:ARG:NH2	10:J:64:ASN:HA	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ASN:OD1	1:A:472:LEU:N	2.37	0.57
2:B:109:THR:HG21	17:R:263:MET:HG3	1.86	0.57
8:H:7:ASP:OD1	8:H:8:ASP:N	2.37	0.57
12:L:33:GLU:HG3	12:L:34:CYS:H	1.68	0.57
12:L:47:ARG:HH11	13:M:250:MET:CE	2.17	0.57
16:Q:373:TYR:CE1	17:R:70:LEU:HD21	2.38	0.57
1:A:381:THR:HG23	1:A:383:TYR:H	1.69	0.57
3:C:149:LYS:HG3	3:C:150:GLY:N	2.19	0.57
1:A:752:LYS:HG3	2:B:1015:HIS:HB3	1.85	0.57
5:E:179:GLN:HA	5:E:215:MET:HG2	1.86	0.57
13:M:177:LEU:HD22	13:M:207:LEU:HD11	1.85	0.57
1:A:1146:VAL:HG23	1:A:1197:LEU:HD22	1.86	0.57
18:T:44:DA:C4	18:T:45:DC:N4	2.72	0.57
15:O:98:ARG:HG2	18:T:58:DT:C5'	2.34	0.57
1:A:367:PRO:HG2	1:A:466:SER:O	2.04	0.57
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.19	0.57
8:H:64:ASN:OD1	8:H:65:LEU:N	2.38	0.57
17:R:262:THR:O	17:R:266:THR:HG23	2.04	0.57
17:R:98:ASN:ND2	17:R:103:LYS:HE3	2.20	0.57
2:B:365:THR:HG21	2:B:370:PHE:CG	2.40	0.56
13:M:267:LYS:HE2	15:O:208:VAL:HG11	1.79	0.56
1:A:225:ASN:N	1:A:229:SER:OG	2.28	0.56
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.86	0.56
18:T:57:DA:H2"	18:T:58:DT:O5'	2.03	0.56
16:Q:100:GLU:HA	17:R:96:ARG:HA	1.86	0.56
1:A:1445:ILE:HB	7:G:61:ILE:HD11	1.87	0.56
1:A:34:LYS:NZ	1:A:85:ASP:OD2	2.38	0.56
1:A:29:ALA:HB1	2:B:1184:GLY:HA3	1.87	0.56
3:C:60:ASP:HB3	12:L:67:PHE:HE2	1.70	0.56
8:H:56:THR:O	8:H:144:ILE:HA	2.06	0.56
18:T:65:DC:P	18:T:65:DC:C3'	2.94	0.56
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.41	0.56
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.88	0.56
2:B:642:ASP:HA	2:B:649:LYS:HG2	1.86	0.56
3:C:6:PRO:HB3	3:C:25:VAL:CG2	2.35	0.56
7:G:101:VAL:N	7:G:108:VAL:O	2.36	0.56
2:B:108:VAL:HA	13:M:244:SER:OG	2.06	0.56
16:Q:339:ALA:HB1	16:Q:343:ARG:NH1	2.20	0.56
17:R:64:SER:O	17:R:217:THR:HG23	2.06	0.56
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.87	0.56
1:A:365:GLY:HA2	1:A:461:LYS:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:ARG:NH1	2:B:407:ASP:CG	2.58	0.56
2:B:211:VAL:O	2:B:480:SER:HA	2.06	0.56
9:I:31:THR:O	16:Q:401:TYR:CB	2.53	0.56
2:B:209:GLU:O	2:B:482:VAL:HA	2.05	0.56
1:A:1224:LEU:HD12	1:A:1241:ARG:O	2.05	0.56
1:A:1148:ILE:HA	9:I:49:ILE:HD12	1.87	0.56
21:W:39:ALA:O	21:W:41:ASP:N	2.28	0.56
1:A:940:ARG:HH21	1:A:944:ARG:NH2	2.03	0.56
7:G:79:PHE:CE2	7:G:81:PRO:CG	2.86	0.56
1:A:146:MET:O	1:A:171:GLN:N	2.38	0.56
1:A:203:SER:N	1:A:206:GLU:OE2	2.39	0.56
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.71	0.56
2:B:73:GLN:O	2:B:86:ARG:N	2.33	0.56
13:M:243:CYS:O	13:M:247:GLY:N	2.39	0.56
14:N:28:DA:C8	14:N:29:DT:H73	2.41	0.56
1:A:42:ASP:OD1	1:A:43:GLU:N	2.37	0.55
1:A:475:THR:OG1	1:A:480:ALA:O	2.21	0.55
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.39	0.55
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	1.87	0.55
13:M:267:LYS:HD3	15:O:239:LYS:HD3	1.87	0.55
17:R:127:LYS:HA	17:R:220:HIS:CE1	2.42	0.55
2:B:170:LEU:HD12	2:B:171:PRO:HD2	1.88	0.55
17:R:120:TYR:CD1	17:R:226:PRO:HA	2.39	0.55
17:R:341:LYS:CB	18:T:49:DC:OP1	2.53	0.55
18:T:45:DC:H2'	18:T:46:DG:C8	2.41	0.55
1:A:562:THR:O	1:A:576:GLN:NE2	2.37	0.55
2:B:296:GLU:HG2	2:B:300:HIS:NE2	2.22	0.55
2:B:46:GLN:HG2	2:B:408:LEU:HD21	1.88	0.55
2:B:557:PHE:CZ	2:B:603:LEU:HD11	2.41	0.55
7:G:50:ASP:OD2	7:G:53:ASN:HB2	2.07	0.55
14:N:22:DT:C2'	14:N:23:DA:O5'	2.54	0.55
17:R:122:LEU:HD21	17:R:222:CYS:HB3	1.89	0.55
2:B:29:ASP:OD2	2:B:658:ILE:HG13	2.06	0.55
13:M:180:CYS:SG	13:M:187:ARG:HG2	2.46	0.55
15:O:169:PRO:HG2	15:O:240:MET:SD	2.47	0.55
19:U:245:LEU:HB3	20:V:9:LEU:HD22	1.89	0.55
19:U:25:PHE:O	19:U:30:ILE:HG22	2.05	0.55
2:B:923:GLU:HB2	2:B:928:ARG:HD2	1.88	0.55
15:O:114:LEU:HD11	18:T:59:DT:C2	2.40	0.55
19:U:30:ILE:O	19:U:31:ASP:HB2	2.06	0.55
20:V:60:LEU:HD21	20:V:87:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:OD1	1:A:1365:TYR:N	2.40	0.55
1:A:1144:LYS:HE3	9:I:48:LEU:HD22	1.89	0.55
1:A:1386:ARG:O	1:A:1390:ASN:HB3	2.07	0.55
2:B:104:GLU:OE2	12:L:54:ARG:HD2	2.07	0.54
16:Q:366:GLU:CB	16:Q:392:VAL:HG13	2.36	0.54
3:C:46:ILE:HA	3:C:159:ALA:HA	1.89	0.54
15:O:99:PHE:CG	18:T:58:DT:H1'	2.41	0.54
1:A:441:PRO:HD2	1:A:498:ARG:NH1	2.22	0.54
1:A:833:GLU:OE2	1:A:1102:LYS:HD2	2.06	0.54
2:B:46:GLN:N	2:B:46:GLN:OE1	2.32	0.54
17:R:122:LEU:HD21	17:R:222:CYS:SG	2.47	0.54
1:A:977:LYS:O	1:A:1036:ARG:NH2	2.38	0.54
7:G:62:LEU:HD12	7:G:63:PRO:O	2.08	0.54
13:M:273:SER:HB2	15:O:188:GLU:HA	1.89	0.54
2:B:1073:TYR:CE1	2:B:1080:LYS:HG2	2.43	0.54
2:B:298:LEU:HD23	2:B:311:LEU:HD22	1.89	0.54
3:C:6:PRO:HB3	3:C:25:VAL:HG23	1.90	0.54
4:D:49:ALA:HB1	7:G:3:PHE:HE1	1.72	0.54
1:A:566:ILE:O	8:H:96:VAL:HB	2.07	0.54
13:M:43:VAL:O	13:M:52:LEU:N	2.39	0.54
16:Q:119:LEU:HD22	16:Q:395:PHE:CE2	2.41	0.54
1:A:436:ILE:HD11	1:A:491:VAL:HG21	1.89	0.54
4:D:134:THR:HG22	4:D:136:GLY:H	1.73	0.54
2:B:451:LYS:O	2:B:455:SER:OG	2.17	0.54
8:H:100:THR:OG1	8:H:139:ASN:OD1	2.20	0.54
1:A:284:ALA:HB1	1:A:289:ILE:HD11	1.90	0.54
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.43	0.54
1:A:821:ARG:HD2	2:B:514:LEU:H	1.73	0.54
3:C:136:ASP:OD1	3:C:137:LYS:N	2.41	0.54
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.88	0.54
13:M:201:LYS:HE3	14:N:23:DA:H3'	1.90	0.54
13:M:267:LYS:HE2	15:O:208:VAL:HG12	1.84	0.54
2:B:35:SER:OG	2:B:811:TYR:OH	2.18	0.54
2:B:368:GLU:OE2	16:Q:344:PHE:HD1	1.90	0.54
3:C:102:GLN:HG3	3:C:154:LYS:HG3	1.90	0.54
4:D:39:ASN:ND2	4:D:43:GLU:HB2	2.21	0.54
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.48	0.53
2:B:1094:ARG:NH2	2:B:1098:MET:SD	2.82	0.53
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.88	0.53
13:M:177:LEU:HD11	13:M:189:PHE:CD1	2.43	0.53
1:A:570:PRO:O	1:A:571:LEU:HD12	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ARG:HG3	2:B:137:TYR:O	2.08	0.53
3:C:254:LYS:O	3:C:257:SER:OG	2.21	0.53
4:D:49:ALA:HA	7:G:3:PHE:CE1	2.43	0.53
9:I:9:ASP:OD2	16:Q:125:LYS:HE3	2.07	0.53
16:Q:98:TYR:HA	17:R:97:ILE:O	2.08	0.53
2:B:129:PHE:HA	2:B:165:VAL:O	2.09	0.53
9:I:56:ALA:O	9:I:89:GLN:HG3	2.09	0.53
13:M:283:TYR:CZ	13:M:287:LEU:HD11	2.44	0.53
18:T:43:DA:P	18:T:43:DA:H3'	2.48	0.53
2:B:283:VAL:O	2:B:287:ARG:HG2	2.09	0.53
2:B:369:GLY:C	16:Q:367:ALA:HB3	2.29	0.53
5:E:26:ARG:NH2	5:E:133:GLU:OE1	2.42	0.53
1:A:13:THR:OG1	1:A:1432:GLN:OE1	2.27	0.53
4:D:64:VAL:HG13	4:D:67:ARG:HH22	1.74	0.53
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.90	0.53
2:B:296:GLU:OE2	16:Q:122:GLN:NE2	2.42	0.53
2:B:44:VAL:CG1	2:B:495:LEU:CD1	2.81	0.53
8:H:136:LYS:O	8:H:138:GLU:N	2.41	0.53
2:B:969:ARG:HH22	3:C:60:ASP:HB2	1.74	0.52
3:C:21:ILE:HG12	3:C:229:TYR:CD1	2.44	0.52
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.74	0.52
4:D:183:LEU:HD11	7:G:86:VAL:O	2.08	0.52
14:N:29:DT:C2'	14:N:30:DA:C8	2.85	0.52
13:M:267:LYS:HZ1	15:O:239:LYS:HD2	1.74	0.52
17:R:98:ASN:CB	17:R:103:LYS:O	2.53	0.52
1:A:208:LEU:HD21	1:A:212:LYS:HE3	1.90	0.52
2:B:756:ILE:HG12	2:B:770:GLN:HG2	1.89	0.52
13:M:174:ALA:O	13:M:178:ILE:HG12	2.10	0.52
1:A:285:PRO:HD2	1:A:288:ALA:HB3	1.89	0.52
8:H:130:ARG:O	8:H:133:ASN:ND2	2.41	0.52
1:A:839:ARG:NH2	1:A:1402:PHE:O	2.33	0.52
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.44	0.52
4:D:118:THR:HG21	4:D:121:LYS:HG2	1.91	0.52
9:I:19:ASP:O	9:I:23:ASN:HA	2.10	0.52
17:R:126:LYS:HD2	17:R:129:VAL:HG12	1.91	0.52
18:T:44:DA:N9	18:T:45:DC:C4	2.78	0.52
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.91	0.52
1:A:16:GLU:CG	1:A:1418:LEU:HD11	2.39	0.52
4:D:194:LEU:HD22	7:G:86:VAL:HG21	1.91	0.52
7:G:86:VAL:HA	7:G:146:LYS:HA	1.90	0.52
2:B:822:ASN:O	10:J:48:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:47:ARG:HH11	13:M:250:MET:HE1	1.73	0.52
16:Q:365:TYR:CZ	16:Q:367:ALA:HA	2.45	0.52
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.37	0.52
1:A:367:PRO:HA	1:A:463:ILE:O	2.09	0.52
1:A:522:GLY:O	1:A:524:VAL:HG23	2.10	0.52
1:A:806:ARG:NH2	2:B:729:ILE:HG13	2.24	0.52
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.92	0.52
2:B:841:MET:O	2:B:993:THR:HA	2.09	0.52
7:G:10:ASN:HA	7:G:70:PHE:O	2.10	0.52
7:G:160:ILE:CD1	7:G:160:ILE:N	2.73	0.52
13:M:154:TYR:CE1	13:M:171:ILE:HD13	2.45	0.52
17:R:63:ARG:HD2	17:R:66:ARG:CZ	2.39	0.52
2:B:499:ASN:OD1	2:B:500:THR:N	2.42	0.52
1:A:1350:LYS:O	1:A:1354:ASN:ND2	2.42	0.52
1:A:826:ASP:OD1	1:A:827:THR:N	2.43	0.52
2:B:99:LYS:HB3	2:B:180:TYR:CE1	2.45	0.52
16:Q:103:LEU:HD23	16:Q:384:PHE:HB2	1.92	0.52
16:Q:99:ASN:O	17:R:97:ILE:N	2.37	0.52
2:B:179:CYS:SG	2:B:180:TYR:N	2.82	0.52
5:E:122:LYS:O	5:E:125:PRO:HD2	2.10	0.52
7:G:95:SER:O	7:G:130:TYR:OH	2.27	0.52
13:M:177:LEU:O	13:M:181:ARG:HG2	2.09	0.52
13:M:272:LYS:CE	18:T:65:DC:OP1	2.58	0.52
2:B:776:GLN:HG3	2:B:1095:LEU:HD22	1.91	0.51
2:B:100:PRO:HD2	2:B:180:TYR:CZ	2.44	0.51
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.90	0.51
8:H:89:LEU:C	8:H:91:ASP:H	2.13	0.51
9:I:28:GLU:HA	9:I:35:VAL:HG22	1.92	0.51
14:N:21:DG:H2'	14:N:22:DT:H71	1.93	0.51
17:R:121:ASP:O	17:R:225:MET:HB2	2.10	0.51
1:A:1132:LYS:HG2	1:A:1135:ARG:HH22	1.75	0.51
4:D:70:PHE:HE2	4:D:133:THR:HA	1.75	0.51
4:D:49:ALA:HB1	7:G:3:PHE:CE1	2.45	0.51
15:O:191:PRO:HG3	18:T:65:DC:C4'	2.38	0.51
1:A:407:ARG:NH1	1:A:413:ILE:HD11	2.25	0.51
2:B:104:GLU:OE2	12:L:54:ARG:CD	2.55	0.51
2:B:281:PRO:HD2	2:B:284:ILE:HD12	1.93	0.51
7:G:21:ARG:HG3	7:G:25:TYR:HE1	1.75	0.51
8:H:107:VAL:HG13	8:H:108:SER:H	1.75	0.51
9:I:71:SER:OG	9:I:83:ASN:OD1	2.25	0.51
14:N:41:DG:O6	18:T:44:DA:N6	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:42:DT:H6	14:N:42:DT:H3'	1.75	0.51
15:O:99:PHE:CE1	18:T:58:DT:C1'	2.91	0.51
1:A:1151:GLU:OE2	9:I:42:LEU:HD13	2.10	0.51
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.91	0.51
2:B:840:ILE:O	2:B:1010:LEU:HD12	2.10	0.51
1:A:567:LYS:HZ2	8:H:91:ASP:HA	1.75	0.51
2:B:445:LYS:HZ3	17:R:268:MET:HA	1.75	0.51
2:B:757:PRO:HG3	2:B:983:ARG:HH21	1.75	0.51
6:F:147:SER:O	6:F:150:GLU:HG2	2.11	0.51
4:D:39:ASN:HA	7:G:6:ASP:OD2	2.10	0.51
1:A:23:SER:OG	1:A:25:GLU:OE1	2.28	0.51
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.92	0.51
2:B:1076:HIS:O	3:C:31:ASN:ND2	2.44	0.51
8:H:36:CYS:HA	8:H:126:GLU:O	2.11	0.51
19:U:259:LYS:HA	19:U:281:VAL:O	2.10	0.51
1:A:1402:PHE:CD2	1:A:1403:GLU:HG2	2.45	0.51
1:A:377:PRO:HB3	1:A:433:GLU:HG2	1.93	0.51
1:A:407:ARG:NH2	13:M:26:GLU:OE2	2.44	0.51
2:B:247:GLY:HA2	2:B:418:LYS:HZ1	1.73	0.51
13:M:325:ASP:HB3	13:M:326:PRO:HD3	1.92	0.51
1:A:209:ASN:OD1	1:A:213:HIS:NE2	2.44	0.51
3:C:40:GLU:OE1	3:C:254:LYS:HE3	2.10	0.51
16:Q:399:ASN:OD1	16:Q:402:ALA:HA	2.11	0.51
1:A:613:ILE:HG22	1:A:614:PHE:HD1	1.76	0.51
1:A:996:ASN:HB3	1:A:1050:GLU:OE2	2.11	0.51
13:M:306:GLU:O	13:M:309:ILE:HG12	2.11	0.51
2:B:868:MET:CG	13:M:149:CYS:SG	2.99	0.51
7:G:151:ILE:HG13	21:W:134:LEU:CA	2.41	0.51
10:J:6:ARG:HA	10:J:13:VAL:HA	1.92	0.51
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.93	0.51
13:M:191:GLU:HB3	17:R:268:MET:SD	2.51	0.51
2:B:311:LEU:HA	2:B:314:LEU:HD12	1.93	0.50
3:C:35:ARG:NE	11:K:41:THR:OG1	2.35	0.50
13:M:143:PRO:HG2	13:M:146:VAL:HG23	1.93	0.50
13:M:267:LYS:HZ2	15:O:239:LYS:HD2	1.76	0.50
1:A:1442:ASP:OD2	7:G:60:ARG:HD2	2.12	0.50
2:B:706:GLN:HB2	2:B:709:ASP:HB2	1.93	0.50
10:J:21:TYR:CZ	10:J:25:LEU:HD11	2.45	0.50
13:M:255:SER:OG	13:M:285:ASN:OD1	2.18	0.50
1:A:1138:ILE:HG13	1:A:1139:GLU:N	2.27	0.50
1:A:1402:PHE:CE2	1:A:1403:GLU:HG2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:SER:O	2:B:475:SER:HB3	2.11	0.50
1:A:909:ASP:OD2	1:A:911:SER:OG	2.21	0.50
2:B:405:ARG:HH12	2:B:632:ARG:CG	1.99	0.50
2:B:475:SER:O	2:B:476:ARG:CB	2.60	0.50
7:G:101:VAL:HG21	7:G:145:VAL:HG21	1.92	0.50
9:I:103:CYS:SG	9:I:105:SER:OG	2.62	0.50
14:N:23:DA:N6	18:T:64:DA:N6	2.60	0.50
2:B:87:LYS:HE3	2:B:147:LEU:HD11	1.92	0.50
2:B:187:SER:HA	2:B:190:TYR:HD2	1.76	0.50
2:B:69:LEU:O	2:B:69:LEU:HD12	2.12	0.50
4:D:32:GLU:HB3	7:G:42:PHE:HE1	1.77	0.50
1:A:381:THR:OG1	1:A:382:PRO:HD2	2.11	0.50
2:B:486:TYR:HA	2:B:1096:ARG:HH21	1.76	0.50
15:O:99:PHE:CZ	18:T:58:DT:C2	2.87	0.50
16:Q:100:GLU:HG2	17:R:96:ARG:HB2	1.94	0.50
1:A:1155:ASP:OD2	1:A:1161:THR:HA	2.12	0.50
1:A:1116:LEU:HD12	1:A:1311:VAL:HG22	1.93	0.50
1:A:901:LEU:HB3	1:A:921:GLY:H	1.77	0.50
2:B:496:ARG:NH2	2:B:540:SER:O	2.45	0.50
3:C:52:GLU:HG2	3:C:53:THR:HG23	1.94	0.50
13:M:134:THR:HG23	13:M:147:LYS:NZ	2.26	0.50
2:B:368:GLU:OE2	16:Q:344:PHE:CD1	2.65	0.50
1:A:733:ALA:O	1:A:737:LEU:HG	2.11	0.50
2:B:861:ASP:OD1	2:B:862:GLN:N	2.38	0.50
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.93	0.50
5:E:202:SER:HB3	5:E:206:GLY:H	1.77	0.50
13:M:30:TYR:CD1	13:M:31:PRO:HD2	2.47	0.50
1:A:350:ARG:NE	1:A:486:GLU:OE1	2.44	0.50
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.27	0.50
7:G:83:LYS:HE3	7:G:150:CYS:HB2	1.94	0.50
9:I:88:SER:O	9:I:91:ARG:NH1	2.45	0.50
5:E:16:PHE:CZ	5:E:20:LYS:HE3	2.46	0.49
1:A:597:LEU:HD13	8:H:103:LYS:HD3	1.93	0.49
14:N:29:DT:H5''	14:N:30:DA:OP1	2.12	0.49
1:A:137:ALA:O	1:A:140:THR:OG1	2.19	0.49
2:B:22:SER:O	2:B:654:ARG:NH1	2.44	0.49
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.94	0.49
9:I:59:VAL:HG12	9:I:61:ASP:H	1.76	0.49
21:W:43:LEU:O	21:W:47:LEU:N	2.44	0.49
2:B:548:GLY:HA3	2:B:630:ALA:HB2	1.94	0.49
7:G:115:MET:HB3	7:G:119:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:35:GLN:HB3	8:H:111:LEU:HD21	1.94	0.49
2:B:55:VAL:O	17:R:252:ILE:HD12	2.12	0.49
2:B:778:MET:HA	2:B:1096:ARG:HH12	1.76	0.49
2:B:601:ARG:HD3	2:B:605:ARG:NH2	2.28	0.49
18:T:43:DA:H2"	18:T:44:DA:OP2	2.13	0.49
20:V:25:THR:O	20:V:29:ASP:HB3	2.13	0.49
1:A:821:ARG:HD2	2:B:514:LEU:N	2.27	0.49
2:B:106:ASP:OD1	2:B:108:VAL:HG12	2.12	0.49
3:C:125:MET:HB2	3:C:127:ARG:NH1	2.26	0.49
5:E:48:ASP:OD1	5:E:51:GLY:N	2.45	0.49
7:G:114:LEU:HD23	7:G:162:SER:HB3	1.94	0.49
8:H:101:ALA:HB2	8:H:116:TYR:CE1	2.47	0.49
1:A:51:GLY:H	1:A:55:ASP:HB3	1.78	0.49
1:A:64:ASN:HA	13:M:20:ILE:HB	1.95	0.49
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.13	0.49
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.95	0.49
14:N:28:DA:C2	15:O:99:PHE:CZ	2.89	0.49
15:O:169:PRO:HB2	15:O:239:LYS:HB2	1.93	0.49
18:T:57:DA:C2'	18:T:58:DT:O5'	2.60	0.49
1:A:445:ASN:OD1	1:A:446:ARG:N	2.46	0.49
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.47	0.49
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.45	0.49
3:C:25:VAL:HG12	3:C:26:ASP:O	2.13	0.49
5:E:191:LYS:N	5:E:194:GLU:OE1	2.39	0.49
4:D:33:PHE:HZ	7:G:42:PHE:HA	1.77	0.49
8:H:89:LEU:O	8:H:91:ASP:N	2.46	0.49
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.94	0.49
13:M:277:ILE:HA	13:M:280:VAL:HG22	1.94	0.49
16:Q:139:LEU:HD12	16:Q:351:VAL:O	2.13	0.49
1:A:663:SER:OG	1:A:664:THR:N	2.44	0.49
1:A:848:ILE:HG12	1:A:858:ASN:HB3	1.94	0.49
1:A:8:SER:OG	2:B:1178:ASN:ND2	2.45	0.49
7:G:138:THR:O	7:G:141:SER:OG	2.23	0.49
2:B:619:ILE:O	9:I:59:VAL:HG21	2.12	0.49
13:M:157:CYS:HB3	13:M:210:MET:SD	2.52	0.49
16:Q:100:GLU:OE2	17:R:96:ARG:NH2	2.45	0.49
19:U:241:GLU:O	19:U:241:GLU:HG2	2.12	0.49
2:B:53:GLN:HG3	2:B:57:TYR:HD2	1.77	0.49
2:B:604:ARG:NH2	2:B:615:MET:HG2	2.28	0.49
2:B:807:ARG:HG2	2:B:1043:ASP:OD1	2.13	0.49
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:154:TYR:HE1	13:M:171:ILE:HD13	1.78	0.49
1:A:1444:MET:SD	6:F:135:ARG:NE	2.82	0.49
2:B:67:SER:HB2	2:B:92:PHE:HB2	1.94	0.49
2:B:856:PHE:CE1	2:B:969:ARG:HB3	2.48	0.49
4:D:52:LEU:HA	4:D:55:ALA:HB3	1.94	0.49
5:E:161:LYS:NZ	5:E:193:GLY:O	2.41	0.49
13:M:199:LYS:O	13:M:200:THR:HB	2.13	0.49
13:M:22:LEU:O	13:M:32:PRO:HB3	2.13	0.49
18:T:65:DC:H2''	18:T:66:DA:C5'	2.43	0.49
1:A:666:ILE:HD11	2:B:1030:LEU:HD22	1.94	0.48
2:B:210:LYS:NZ	2:B:462:ALA:HA	2.28	0.48
5:E:23:VAL:HG12	5:E:28:TYR:HB2	1.95	0.48
3:C:60:ASP:HB3	12:L:67:PHE:CE2	2.47	0.48
16:Q:133:PHE:HZ	16:Q:353:GLU:HA	1.77	0.48
18:T:42:DG:C1'	18:T:43:DA:C5'	2.85	0.48
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.95	0.48
7:G:83:LYS:HG2	7:G:149:GLY:HA2	1.94	0.48
13:M:238:TYR:HB3	13:M:242:PHE:CE2	2.40	0.48
14:N:24:DT:H3'	14:N:24:DT:H6	1.79	0.48
2:B:569:TYR:CE2	2:B:571:PRO:HG3	2.48	0.48
3:C:59:ALA:O	3:C:62:PHE:HB3	2.13	0.48
1:A:1438:THR:HG23	6:F:92:ARG:HB2	1.96	0.48
7:G:143:ILE:HG13	7:G:170:ALA:HA	1.94	0.48
8:H:93:TYR:CD1	8:H:143:LEU:HD23	2.48	0.48
16:Q:119:LEU:HD21	17:R:135:PHE:CE1	2.48	0.48
16:Q:121:PHE:HD1	16:Q:395:PHE:HB2	1.78	0.48
1:A:1373:ASP:O	1:A:1377:THR:HG23	2.14	0.48
4:D:194:LEU:HB3	7:G:86:VAL:HG21	1.96	0.48
7:G:97:HIS:O	7:G:112:LYS:N	2.43	0.48
16:Q:405:THR:CB	16:Q:409:ALA:HB2	2.44	0.48
15:O:98:ARG:CZ	18:T:59:DT:OP1	2.61	0.48
1:A:1130:GLN:O	1:A:1134:ILE:HD12	2.12	0.48
1:A:113:LEU:HD11	1:A:218:ASP:HA	1.96	0.48
2:B:1004:GLU:O	3:C:177:GLU:HG2	2.14	0.48
2:B:801:LYS:HG2	10:J:52:THR:O	2.13	0.48
2:B:856:PHE:CD1	2:B:969:ARG:HB3	2.48	0.48
3:C:80:LEU:HD12	3:C:94:LYS:O	2.13	0.48
13:M:147:LYS:HE2	13:M:151:LYS:HE3	1.95	0.48
13:M:140:ALA:HB2	13:M:195:LEU:HD11	1.95	0.48
16:Q:376:LEU:O	17:R:69:TRP:N	2.39	0.48
18:T:62:DA:C2'	18:T:63:DT:C5'	2.85	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:261:LYS:O	22:X:265:ASN:N	2.47	0.48
1:A:326:ARG:NE	1:A:1406:VAL:HG21	2.27	0.48
2:B:249:ARG:HH12	2:B:418:LYS:HB2	1.78	0.48
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.95	0.48
8:H:22:LYS:O	8:H:43:ASN:HA	2.13	0.48
13:M:155:LYS:O	13:M:158:HIS:HB2	2.13	0.48
13:M:272:LYS:O	13:M:273:SER:OG	2.24	0.48
16:Q:121:PHE:CD1	16:Q:395:PHE:HB2	2.49	0.48
16:Q:344:PHE:O	16:Q:347:PHE:HD2	1.97	0.48
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.96	0.48
1:A:380:VAL:HG22	1:A:388:LEU:HD13	1.96	0.48
1:A:471:ASN:O	1:A:474:VAL:HG12	2.13	0.48
1:A:337:ARG:HH12	1:A:839:ARG:NE	2.11	0.48
2:B:983:ARG:NH2	2:B:1028:GLU:OE2	2.46	0.48
4:D:49:ALA:HA	7:G:3:PHE:HD1	1.72	0.48
5:E:106:GLN:O	5:E:130:ALA:HA	2.14	0.48
5:E:79:TRP:HE1	5:E:81:GLU:HG3	1.79	0.48
19:U:2:SER:N	19:U:274:TYR:OH	2.36	0.48
1:A:630:ILE:HG12	1:A:646:PHE:HE1	1.78	0.48
2:B:167:ILE:O	2:B:450:ALA:HA	2.14	0.48
18:T:63:DT:H3'	18:T:63:DT:H6	1.79	0.48
2:B:642:ASP:HB3	2:B:649:LYS:NZ	2.29	0.48
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.95	0.48
2:B:865:LYS:HZ1	13:M:145:ILE:CD1	2.26	0.48
1:A:1072:ILE:O	1:A:1075:PRO:HD2	2.14	0.48
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.96	0.48
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.95	0.48
2:B:1089:PRO:HD3	10:J:44:TYR:HE2	1.78	0.48
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.96	0.48
3:C:214:ASN:ND2	3:C:217:ASP:OD2	2.46	0.48
4:D:64:VAL:HG12	4:D:68:ARG:NH1	2.29	0.48
8:H:13:SER:N	8:H:27:GLU:O	2.46	0.48
2:B:995:ARG:NH1	11:K:9:LEU:HD13	2.29	0.48
14:N:43:DT:H2'	14:N:44:DC:OP2	2.12	0.48
1:A:412:ARG:O	13:M:51:VAL:HG12	2.14	0.47
1:A:11:LEU:HD12	2:B:1193:GLN:O	2.14	0.47
2:B:336:ARG:HD2	2:B:348:ARG:NH1	2.29	0.47
2:B:300:HIS:CE1	2:B:376:PHE:HE1	2.31	0.47
13:M:267:LYS:HG3	13:M:268:GLU:N	2.27	0.47
14:N:42:DT:H2'	14:N:43:DT:C2	2.48	0.47
13:M:267:LYS:HD3	15:O:239:LYS:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ILE:HG21	16:Q:335:LEU:HD21	1.96	0.47
17:R:105:THR:CA	17:R:120:TYR:O	2.60	0.47
17:R:133:TYR:CE1	17:R:217:THR:HG22	2.49	0.47
1:A:283:GLY:O	1:A:285:PRO:HD3	2.13	0.47
1:A:597:LEU:O	8:H:102:TYR:OH	2.32	0.47
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.49	0.47
3:C:180:TYR:HB3	3:C:228:PHE:HD1	1.80	0.47
6:F:99:LEU:O	6:F:102:SER:OG	2.19	0.47
18:T:60:DA:C8	18:T:61:DT:C4	3.03	0.47
1:A:737:LEU:HD22	1:A:741:ASN:HD22	1.78	0.47
2:B:914:LYS:CB	2:B:937:ALA:O	2.53	0.47
13:M:137:CYS:SG	13:M:147:LYS:HB2	2.54	0.47
13:M:16:PRO:HB3	21:W:127:CYS:HA	1.95	0.47
14:N:41:DG:C2'	14:N:42:DT:H72	2.24	0.47
17:R:105:THR:OG1	17:R:120:TYR:O	2.18	0.47
16:Q:102:PRO:HB3	17:R:94:LYS:HG2	1.95	0.47
1:A:61:ILE:HG22	1:A:62:ASP:N	2.27	0.47
13:M:171:ILE:HD12	13:M:172:MET:HG3	1.96	0.47
1:A:670:ILE:HG12	1:A:805:LEU:HD21	1.96	0.47
2:B:213:ILE:HG21	2:B:499:ASN:HB2	1.95	0.47
2:B:923:GLU:HB3	2:B:925:LEU:HG	1.96	0.47
2:B:869:SER:HB3	13:M:152:GLU:OE2	2.14	0.47
15:O:170:ILE:HD13	15:O:234:LEU:HD22	1.96	0.47
15:O:171:ARG:HD3	15:O:238:ARG:O	2.14	0.47
19:U:277:GLN:HG2	20:V:56:THR:OG1	2.14	0.47
1:A:224:PHE:CE2	1:A:231:PRO:HG3	2.50	0.47
1:A:804:TYR:HH	1:A:816:HIS:CE1	2.32	0.47
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.96	0.47
5:E:64:PRO:HB2	5:E:69:ILE:HD11	1.95	0.47
1:A:567:LYS:NZ	8:H:91:ASP:HA	2.30	0.47
1:A:1032:LEU:O	1:A:1036:ARG:HD2	2.15	0.47
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.80	0.47
1:A:804:TYR:HH	1:A:816:HIS:HE2	1.59	0.47
2:B:713:ALA:HA	2:B:733:HIS:CD2	2.50	0.47
3:C:98:VAL:HB	3:C:122:SER:HB3	1.95	0.47
14:N:28:DA:H1'	15:O:116:PHE:CE1	2.49	0.47
17:R:133:TYR:CD1	17:R:217:THR:HA	2.50	0.47
1:A:1142:THR:O	1:A:1145:SER:OG	2.19	0.47
1:A:225:ASN:H	1:A:229:SER:HG	1.56	0.47
2:B:898:LEU:HD21	2:B:964:VAL:HG11	1.97	0.47
7:G:14:HIS:HB3	7:G:17:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:TYR:HE2	9:I:87:GLN:HE22	1.63	0.47
3:C:148:ARG:HH21	10:J:64:ASN:HA	1.79	0.47
14:N:28:DA:H1'	15:O:116:PHE:CE2	2.50	0.47
1:A:975:HIS:O	1:A:976:THR:OG1	2.24	0.47
2:B:642:ASP:HB3	2:B:649:LYS:HZ2	1.80	0.47
2:B:879:ARG:HG2	2:B:885:MET:SD	2.55	0.47
8:H:101:ALA:HA	8:H:115:TYR:O	2.15	0.47
16:Q:99:ASN:O	17:R:96:ARG:HA	2.15	0.47
1:A:446:ARG:HB2	1:A:487:MET:HG2	1.96	0.47
1:A:879:GLU:OE1	1:A:959:ASN:HB2	2.15	0.47
2:B:20:ASP:OD1	2:B:21:GLU:N	2.42	0.47
12:L:46:VAL:HG13	12:L:56:LEU:HD12	1.97	0.47
2:B:617:ARG:NH1	2:B:619:ILE:HG12	2.30	0.47
2:B:770:GLN:HG2	2:B:983:ARG:O	2.15	0.47
11:K:20:LYS:O	11:K:33:ILE:HA	2.15	0.47
13:M:246:LEU:HD22	13:M:293:ILE:HD13	1.96	0.47
16:Q:116:THR:O	16:Q:390:ASP:HB3	2.15	0.47
1:A:1208:THR:HB	1:A:1211:GLN:HG2	1.96	0.46
1:A:302:THR:HA	1:A:305:ASP:O	2.15	0.46
2:B:944:THR:HG21	2:B:1122:ARG:HH22	1.80	0.46
2:B:820:GLY:N	2:B:1091:TYR:OH	2.48	0.46
4:D:52:LEU:HD12	4:D:52:LEU:O	2.15	0.46
7:G:93:SER:OG	7:G:100:GLU:OE1	2.33	0.46
3:C:66:ARG:NH1	10:J:2:ILE:O	2.48	0.46
13:M:241:ARG:O	13:M:245:HIS:ND1	2.45	0.46
16:Q:117:HIS:HB2	17:R:135:PHE:CE1	2.50	0.46
16:Q:361:TRP:HA	16:Q:396:THR:O	2.15	0.46
17:R:108:LEU:HD11	17:R:120:TYR:HE2	1.80	0.46
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.81	0.46
16:Q:117:HIS:NE2	16:Q:390:ASP:OD2	2.49	0.46
18:T:63:DT:C2'	18:T:64:DA:H5'	2.46	0.46
1:A:444:PHE:HE2	1:A:487:MET:SD	2.37	0.46
2:B:460:ALA:O	2:B:464:GLY:N	2.38	0.46
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.46	0.46
1:A:465:TYR:CG	2:B:976:ILE:HD12	2.50	0.46
16:Q:140:HIS:O	16:Q:351:VAL:HG12	2.15	0.46
16:Q:375:LEU:HB2	16:Q:387:ILE:O	2.15	0.46
2:B:134:LYS:HD3	17:R:277:PHE:HB2	1.97	0.46
17:R:78:ALA:O	17:R:82:ARG:HG2	2.14	0.46
19:U:30:ILE:HD11	20:V:32:ILE:HG13	1.98	0.46
1:A:1120:LEU:HD21	1:A:1131:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASP:OD1	1:A:117:GLU:N	2.42	0.46
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.48	0.46
1:A:483:ASP:HA	2:B:989:THR:HG23	1.97	0.46
1:A:668:ASP:OD2	1:A:742:ASN:HB2	2.15	0.46
8:H:56:THR:HB	8:H:145:ARG:HG2	1.97	0.46
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.81	0.46
17:R:63:ARG:HD2	17:R:66:ARG:NH1	2.31	0.46
2:B:1042:GLY:HA2	16:Q:22:ILE:CA	2.36	0.46
2:B:604:ARG:NH2	2:B:615:MET:H	2.13	0.46
7:G:22:MET:HA	7:G:25:TYR:HD1	1.80	0.46
13:M:273:SER:CB	15:O:188:GLU:HA	2.46	0.46
18:T:44:DA:N3	18:T:45:DC:N3	2.64	0.46
1:A:216:VAL:HA	1:A:219:PHE:CE2	2.51	0.46
2:B:862:GLN:HA	2:B:963:PHE:HB2	1.98	0.46
20:V:32:ILE:HD12	20:V:32:ILE:N	2.30	0.46
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.80	0.46
2:B:839:MET:O	2:B:991:GLY:N	2.41	0.46
4:D:33:PHE:CZ	7:G:42:PHE:HA	2.50	0.46
13:M:267:LYS:HD3	15:O:239:LYS:CE	2.45	0.46
15:O:94:TYR:CZ	15:O:96:PRO:HG3	2.51	0.46
17:R:104:ILE:HD11	17:R:122:LEU:HD22	1.98	0.46
1:A:1170:ILE:HG23	1:A:1174:PHE:CE2	2.51	0.46
2:B:199:MET:CE	2:B:491:THR:HG21	2.21	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG22	1.96	0.46
3:C:241:ASP:OD1	3:C:242:GLN:N	2.48	0.46
7:G:101:VAL:O	7:G:108:VAL:N	2.43	0.46
13:M:267:LYS:NZ	15:O:208:VAL:CG1	2.78	0.46
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.98	0.46
2:B:300:HIS:CE1	2:B:376:PHE:CE1	3.04	0.46
2:B:71:LEU:HB3	2:B:88:TYR:HB2	1.97	0.46
3:C:21:ILE:HG12	3:C:229:TYR:HD1	1.79	0.46
4:D:208:GLU:HA	4:D:211:LEU:HB2	1.98	0.46
13:M:137:CYS:SG	13:M:142:LEU:HB2	2.56	0.46
2:B:286:PHE:CD2	2:B:297:ILE:HG23	2.51	0.45
2:B:923:GLU:HB2	2:B:928:ARG:CD	2.46	0.45
3:C:133:ILE:HD12	3:C:237:SER:HA	1.97	0.45
3:C:76:ASP:OD2	3:C:127:ARG:HB2	2.16	0.45
17:R:68:VAL:O	17:R:69:TRP:HD1	1.99	0.45
19:U:244:MET:HB2	19:U:267:VAL:HG13	1.99	0.45
1:A:1132:LYS:HG2	1:A:1135:ARG:HH12	1.80	0.45
1:A:1390:ASN:HD21	1:A:1408:ILE:HD11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:ASP:OD1	1:A:673:GLY:N	2.49	0.45
2:B:1163:CYS:HB3	2:B:1166:CYS:O	2.15	0.45
2:B:289:LEU:HD13	2:B:375:ALA:HA	1.96	0.45
9:I:70:ARG:HD3	9:I:84:VAL:HG22	1.97	0.45
13:M:198:VAL:HG11	13:M:203:PHE:HD1	1.82	0.45
13:M:269:ILE:C	13:M:271:GLY:H	2.17	0.45
16:Q:117:HIS:HD2	16:Q:391:LYS:HB2	1.80	0.45
2:B:336:ARG:HD2	2:B:348:ARG:HH11	1.81	0.45
2:B:432:MET:O	2:B:436:VAL:HG12	2.17	0.45
7:G:149:GLY:O	7:G:159:ALA:HB1	2.17	0.45
13:M:295:ALA:O	13:M:298:VAL:HG12	2.16	0.45
1:A:526:ASP:OD1	2:B:1015:HIS:ND1	2.49	0.45
1:A:660:ASN:OD1	2:B:1082:MET:HB3	2.16	0.45
1:A:871:ASP:CG	1:A:1366:ARG:HH21	2.18	0.45
6:F:82:THR:HG22	6:F:84:TYR:H	1.80	0.45
14:N:17:DC:H2'	14:N:18:DT:H71	1.98	0.45
17:R:263:MET:O	17:R:266:THR:OG1	2.19	0.45
20:V:34:ALA:O	20:V:35:SER:HB2	2.16	0.45
1:A:212:LYS:HA	1:A:232:GLU:OE2	2.16	0.45
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.16	0.45
2:B:280:ILE:HD13	2:B:334:ILE:HG13	1.97	0.45
2:B:776:GLN:O	2:B:1096:ARG:HG2	2.16	0.45
4:D:50:LEU:HB2	7:G:2:PHE:O	2.16	0.45
7:G:98:GLY:HA3	7:G:110:VAL:O	2.16	0.45
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.57	0.45
2:B:104:GLU:CD	12:L:54:ARG:NE	2.43	0.45
22:X:168:ARG:O	22:X:181:LEU:N	2.48	0.45
1:A:1277:GLU:O	1:A:1279:ILE:HD12	2.17	0.45
1:A:353:ILE:HG21	1:A:487:MET:SD	2.56	0.45
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.98	0.45
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.81	0.45
2:B:463:THR:C	2:B:465:ASN:OD1	2.55	0.45
2:B:569:TYR:CE1	2:B:589:VAL:HG11	2.51	0.45
2:B:601:ARG:HD3	2:B:605:ARG:CZ	2.47	0.45
2:B:69:LEU:HD23	2:B:425:THR:HG23	1.99	0.45
4:D:130:LEU:HD13	4:D:142:LYS:HG2	1.99	0.45
12:L:58:LYS:O	12:L:58:LYS:HG3	2.17	0.45
18:T:65:DC:C2'	18:T:66:DA:H5'	2.45	0.45
20:V:11:ARG:NH1	20:V:41:LEU:HD13	2.31	0.45
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.81	0.45
8:H:5:LEU:HD11	8:H:61:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:998:LEU:HD23	1:A:1001:ARG:HG2	1.98	0.45
1:A:1295:THR:HG23	1:A:1297:GLU:OE1	2.17	0.45
1:A:526:ASP:HB2	2:B:835:GLN:OE1	2.16	0.45
2:B:580:VAL:O	2:B:586:TRP:HD1	2.00	0.45
1:A:786:HIS:NE2	2:B:705:MET:SD	2.90	0.45
6:F:105:ALA:HA	7:G:16:SER:HA	1.98	0.45
13:M:134:THR:HA	13:M:147:LYS:HE3	1.99	0.45
18:T:56:DT:H2''	18:T:57:DA:C8	2.52	0.45
11:K:7:PHE:HB2	11:K:11:LEU:HD13	1.98	0.45
14:N:28:DA:H8	14:N:29:DT:H73	1.80	0.45
2:B:244:LEU:HD13	2:B:250:PHE:CE2	2.52	0.45
2:B:500:THR:OG1	2:B:537:LYS:NZ	2.48	0.45
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.56	0.45
4:D:56:ARG:HD3	4:D:149:THR:HA	1.99	0.45
8:H:25:ARG:NH2	8:H:41:ASP:OD2	2.50	0.45
3:C:6:PRO:O	11:K:104:ASN:ND2	2.49	0.45
17:R:257:GLU:OE1	17:R:257:GLU:N	2.48	0.45
1:A:372:LYS:HA	1:A:435:HIS:HD2	1.80	0.44
1:A:736:ASN:HD22	1:A:736:ASN:C	2.19	0.44
5:E:26:ARG:NH1	5:E:189:GLY:HA3	2.29	0.44
11:K:59:ALA:HA	11:K:74:ARG:O	2.17	0.44
13:M:199:LYS:O	13:M:199:LYS:HG3	2.17	0.44
14:N:25:DA:C8	14:N:25:DA:O5'	2.71	0.44
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.58	0.44
2:B:842:ASN:HB3	2:B:845:SER:HB2	1.99	0.44
14:N:24:DT:H2'	14:N:25:DA:C8	2.52	0.44
14:N:27:DA:H2'	14:N:28:DA:C8	2.52	0.44
2:B:445:LYS:NZ	17:R:268:MET:HA	2.31	0.44
16:Q:103:LEU:O	17:R:92:LEU:HB2	2.16	0.44
15:O:114:LEU:CD1	18:T:59:DT:O2	2.49	0.44
18:T:68:DA:H2''	18:T:69:DG:C8	2.52	0.44
20:V:34:ALA:C	20:V:36:LEU:H	2.21	0.44
3:C:67:LEU:HD13	3:C:157:CYS:SG	2.56	0.44
4:D:140:ASP:O	4:D:144:THR:N	2.46	0.44
4:D:53:SER:HB2	4:D:154:PHE:HB2	1.97	0.44
8:H:4:THR:HA	8:H:60:ALA:HA	1.99	0.44
14:N:15:DC:H1'	14:N:16:DG:H5'	1.99	0.44
14:N:29:DT:H2''	14:N:30:DA:N9	2.31	0.44
18:T:60:DA:C5	18:T:61:DT:O4	2.70	0.44
1:A:1352:VAL:O	1:A:1355:VAL:HG12	2.16	0.44
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:ASP:N	2:B:649:LYS:HZ2	2.14	0.44
1:A:1444:MET:HB2	6:F:133:VAL:HG13	2.00	0.44
7:G:15:PRO:HA	7:G:18:PHE:CZ	2.52	0.44
9:I:7:CYS:SG	9:I:8:ARG:N	2.90	0.44
13:M:177:LEU:HD11	13:M:189:PHE:CE1	2.53	0.44
13:M:269:ILE:HG22	13:M:272:LYS:CG	2.34	0.44
15:O:239:LYS:O	15:O:240:MET:HG3	2.16	0.44
1:A:849:MET:HB3	1:A:1063:MET:SD	2.58	0.44
2:B:68:THR:CB	16:Q:335:LEU:HD13	2.46	0.44
3:C:148:ARG:NH2	10:J:64:ASN:OD1	2.50	0.44
13:M:167:SER:O	13:M:168:MET:HB2	2.18	0.44
16:Q:374:VAL:HB	17:R:71:VAL:HB	1.98	0.44
16:Q:128:ASN:HB2	17:R:131:ASN:OD1	2.18	0.44
17:R:133:TYR:HD1	17:R:217:THR:HA	1.82	0.44
1:A:358:ASN:OD1	2:B:833:TYR:OH	2.24	0.44
2:B:1175:LEU:O	2:B:1175:LEU:HD12	2.16	0.44
2:B:446:LEU:HA	2:B:446:LEU:HD23	1.83	0.44
4:D:177:VAL:HA	4:D:180:LEU:HD12	2.00	0.44
4:D:194:LEU:HD22	7:G:86:VAL:HG11	1.99	0.44
4:D:65:GLU:HA	4:D:68:ARG:HH11	1.82	0.44
8:H:42:ILE:HG23	8:H:95:TYR:CZ	2.52	0.44
11:K:18:LYS:NZ	11:K:38:GLU:OE2	2.47	0.44
1:A:1207:LEU:HA	1:A:1211:GLN:NE2	2.33	0.44
1:A:1235:LYS:HG2	1:A:1237:ILE:HD11	1.99	0.44
3:C:4:GLU:O	3:C:24:ASN:ND2	2.51	0.44
7:G:7:LEU:HB2	7:G:74:TYR:CZ	2.53	0.44
7:G:79:PHE:CE2	7:G:81:PRO:HD3	2.53	0.44
14:N:43:DT:C6	14:N:43:DT:OP2	2.71	0.44
15:O:191:PRO:HB2	18:T:65:DC:H5"	1.94	0.44
8:H:10:PHE:CD1	8:H:30:SER:HA	2.53	0.44
10:J:30:LEU:HD13	10:J:38:ARG:NH1	2.32	0.44
13:M:285:ASN:O	13:M:288:LEU:HB3	2.18	0.44
17:R:69:TRP:CD1	17:R:219:CYS:HB3	2.53	0.44
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	2.00	0.44
2:B:195:CYS:SG	2:B:197:PHE:HD2	2.41	0.44
2:B:274:PRO:O	2:B:276:ILE:HD12	2.18	0.44
2:B:331:LEU:HA	2:B:334:ILE:HG22	1.98	0.44
2:B:785:TYR:HA	2:B:788:ARG:HG2	1.99	0.44
2:B:799:PRO:CB	2:B:818:PRO:HG2	2.48	0.44
7:G:160:ILE:HG22	7:G:161:GLY:N	2.33	0.44
16:Q:373:TYR:CD1	17:R:70:LEU:HD11	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1217:LYS:HE2	1:A:1228:TRP:HZ3	1.82	0.43
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	2.18	0.43
6:F:136:ARG:O	6:F:143:PHE:HA	2.18	0.43
11:K:46:ILE:O	11:K:49:GLU:N	2.51	0.43
18:T:44:DA:C8	18:T:45:DC:N4	2.86	0.43
2:B:996:ARG:HH22	3:C:175:ALA:HA	1.82	0.43
6:F:133:VAL:HG11	7:G:58:ARG:NH2	2.33	0.43
4:D:24:ALA:CA	7:G:83:LYS:HB2	2.45	0.43
19:U:21:VAL:HG12	19:U:25:PHE:CD1	2.54	0.43
1:A:252:PHE:C	1:A:254:GLU:H	2.20	0.43
1:A:857:ARG:HB2	1:A:862:ASN:O	2.17	0.43
1:A:915:SER:O	1:A:919:ILE:HG12	2.18	0.43
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.99	0.43
2:B:850:LEU:HG	2:B:851:PHE:CD2	2.54	0.43
2:B:918:ILE:HG12	2:B:933:SER:O	2.18	0.43
13:M:132:LYS:O	13:M:136:LEU:HG	2.18	0.43
1:A:710:LEU:HD23	9:I:96:SER:HA	2.00	0.43
1:A:770:VAL:HA	1:A:822:GLU:OE1	2.19	0.43
2:B:322:PHE:HA	2:B:325:GLN:OE1	2.18	0.43
2:B:365:THR:HG21	2:B:370:PHE:CB	2.48	0.43
2:B:457:LEU:HA	2:B:457:LEU:HD23	1.81	0.43
2:B:512:ARG:NH1	2:B:533:CYS:O	2.50	0.43
2:B:950:ASP:N	2:B:967:ARG:O	2.46	0.43
7:G:127:PRO:HG3	7:G:139:ILE:HD12	2.01	0.43
13:M:293:ILE:O	13:M:294:THR:OG1	2.28	0.43
1:A:197:PRO:HG3	18:T:35:DG:OP2	2.18	0.43
1:A:1208:THR:O	1:A:1211:GLN:HG2	2.18	0.43
2:B:839:MET:SD	2:B:1010:LEU:HD11	2.58	0.43
2:B:1022:THR:HG23	2:B:1022:THR:O	2.18	0.43
2:B:248:SER:HB3	2:B:250:PHE:CE2	2.54	0.43
2:B:273:LEU:HB2	2:B:276:ILE:HD13	2.00	0.43
12:L:38:LEU:HD21	12:L:48:CYS:HA	2.00	0.43
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.49	0.43
13:M:158:HIS:CG	13:M:159:ASP:N	2.87	0.43
13:M:39:SER:OG	13:M:40:GLU:OE1	2.37	0.43
19:U:9:VAL:HG13	20:V:51:THR:HG22	1.99	0.43
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.18	0.43
2:B:310:MET:O	2:B:314:LEU:HG	2.19	0.43
2:B:850:LEU:HG	2:B:851:PHE:HD2	1.83	0.43
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.00	0.43
5:E:43:LYS:HG3	5:E:47:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:122:LEU:HA	8:H:122:LEU:HD23	1.77	0.43
10:J:43:ARG:O	10:J:47:ARG:HG3	2.18	0.43
1:A:737:LEU:HD11	1:A:758:ILE:HG21	2.00	0.43
2:B:199:MET:CE	2:B:492:LEU:HD23	2.48	0.43
2:B:635:ARG:NH1	2:B:637:LEU:HD21	2.34	0.43
2:B:839:MET:HG2	2:B:989:THR:O	2.18	0.43
1:A:412:ARG:HB3	13:M:51:VAL:HG11	2.01	0.43
14:N:25:DA:H1'	15:O:159:ASN:ND2	2.33	0.43
16:Q:101:PHE:CD1	16:Q:382:GLY:HA3	2.54	0.43
16:Q:108:LYS:O	16:Q:112:GLU:HG3	2.19	0.43
17:R:129:VAL:HG21	17:R:218:VAL:HG12	2.01	0.43
19:U:262:LEU:HB2	19:U:279:ALA:HB3	2.01	0.43
1:A:1189:SER:OG	1:A:1256:GLU:OE2	2.22	0.43
2:B:217:ARG:HH12	2:B:407:ASP:CG	2.22	0.43
3:C:133:ILE:CD1	3:C:237:SER:HA	2.48	0.43
6:F:137:TYR:HD1	6:F:143:PHE:HB3	1.83	0.43
13:M:187:ARG:NH1	13:M:241:ARG:HE	2.16	0.43
17:R:63:ARG:C	17:R:65:ASN:H	2.21	0.43
1:A:105:CYS:SG	1:A:139:TRP:HD1	2.42	0.43
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.19	0.43
1:A:1210:GLY:HA2	1:A:1228:TRP:CE2	2.54	0.43
1:A:1421:CYS:HA	1:A:1426:GLU:OE1	2.18	0.43
1:A:982:THR:HG22	1:A:983:ILE:N	2.34	0.43
2:B:515:HIS:CE1	2:B:517:THR:HG23	2.54	0.43
2:B:924:GLU:HG3	2:B:929:THR:HB	2.00	0.43
9:I:54:GLU:HB3	9:I:100:PHE:HE2	1.84	0.43
13:M:237:THR:O	13:M:240:PRO:HD2	2.18	0.43
13:M:279:VAL:HG11	13:M:304:VAL:HG21	2.01	0.43
16:Q:130:VAL:O	16:Q:133:PHE:HB3	2.18	0.43
18:T:43:DA:C2'	18:T:44:DA:O4'	2.64	0.43
1:A:1144:LYS:HB2	1:A:1268:LEU:HB3	2.01	0.43
1:A:1395:GLY:HA3	1:A:1426:GLU:OE2	2.19	0.43
1:A:206:GLU:O	1:A:210:ILE:HG12	2.18	0.43
1:A:737:LEU:HD22	1:A:741:ASN:ND2	2.34	0.43
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.51	0.43
2:B:199:MET:HG3	2:B:200:GLY:O	2.18	0.43
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.47	0.43
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.83	0.43
11:K:19:LEU:HD22	11:K:35:PHE:CD1	2.54	0.43
1:A:1444:MET:SD	6:F:135:ARG:NH2	2.84	0.42
2:B:823:ALA:O	2:B:825:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:979:LYS:HA	2:B:989:THR:HA	2.01	0.42
13:M:140:ALA:HB1	13:M:142:LEU:HD13	2.01	0.42
13:M:16:PRO:O	13:M:18:LEU:HG	2.19	0.42
15:O:171:ARG:HG3	15:O:239:LYS:HG2	2.00	0.42
17:R:118:HIS:HB2	17:R:120:TYR:CE2	2.54	0.42
18:T:62:DA:H2'	18:T:63:DT:C5'	2.48	0.42
1:A:306:ASN:ND2	1:A:322:VAL:O	2.49	0.42
1:A:444:PHE:CE2	1:A:487:MET:SD	3.12	0.42
3:C:56:THR:HG22	3:C:147:LEU:CD2	2.47	0.42
13:M:44:VAL:HG22	13:M:51:VAL:HA	2.00	0.42
16:Q:121:PHE:HE1	16:Q:395:PHE:HD2	1.66	0.42
17:R:94:LYS:O	17:R:106:LEU:HD12	2.19	0.42
1:A:854:ASN:HB2	1:A:1000:LEU:HD21	2.01	0.42
1:A:1214:GLU:O	1:A:1218:GLN:HG2	2.19	0.42
1:A:404:TYR:OH	13:M:40:GLU:HG2	2.19	0.42
2:B:103:ASN:O	2:B:958:GLN:OE1	2.36	0.42
3:C:190:ASP:OD1	3:C:191:TYR:N	2.52	0.42
6:F:94:LEU:HA	6:F:94:LEU:HD23	1.66	0.42
9:I:27:PHE:O	9:I:35:VAL:HA	2.20	0.42
13:M:239:ILE:HB	13:M:240:PRO:HD3	2.01	0.42
17:R:251:ARG:HG3	17:R:252:ILE:N	2.34	0.42
17:R:70:LEU:HD12	17:R:71:VAL:H	1.84	0.42
1:A:1293:SER:HB3	1:A:1299:VAL:HG23	2.02	0.42
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.00	0.42
2:B:120:ARG:CG	12:L:55:ILE:HD11	2.50	0.42
2:B:213:ILE:CG2	2:B:499:ASN:HB2	2.49	0.42
2:B:59:LEU:O	2:B:63:ILE:HG12	2.19	0.42
3:C:12:GLU:HB2	3:C:19:ASP:HB3	2.01	0.42
17:R:68:VAL:HG21	17:R:134:VAL:HG21	2.01	0.42
18:T:44:DA:N3	18:T:45:DC:C4	2.87	0.42
1:A:1144:LYS:NZ	2:B:262:GLU:OE2	2.51	0.42
1:A:1267:MET:HA	1:A:1271:ILE:HD12	2.01	0.42
1:A:1376:THR:O	1:A:1378:GLN:N	2.52	0.42
2:B:1159:ARG:HD2	2:B:1193:GLN:OE1	2.19	0.42
2:B:435:THR:O	2:B:439:ALA:N	2.53	0.42
4:D:194:LEU:CB	7:G:86:VAL:HG21	2.50	0.42
2:B:1113:VAL:HG22	13:M:57:VAL:HB	2.02	0.42
17:R:135:PHE:HA	17:R:215:VAL:HG23	2.01	0.42
18:T:61:DT:H2'	18:T:62:DA:C5	2.54	0.42
1:A:455:MET:HB3	1:A:455:MET:HE2	1.84	0.42
4:D:214:LEU:O	4:D:218:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:363:GLY:HA2	16:Q:394:LYS:O	2.19	0.42
1:A:337:ARG:HH12	1:A:839:ARG:HE	1.67	0.42
1:A:353:ILE:HG13	1:A:353:ILE:H	1.66	0.42
1:A:469:ARG:HA	1:A:469:ARG:HD3	1.75	0.42
1:A:673:GLY:N	1:A:674:PRO:HD2	2.34	0.42
1:A:94:GLY:HA3	1:A:1410:PHE:CE2	2.54	0.42
1:A:951:GLU:O	1:A:954:TRP:NE1	2.52	0.42
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.50	0.42
3:C:167:HIS:HB3	3:C:170:TRP:CZ3	2.55	0.42
3:C:54:ASN:HD21	3:C:63:ILE:HD12	1.84	0.42
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.53	0.42
13:M:132:LYS:HB3	13:M:172:MET:HE3	2.02	0.42
13:M:200:THR:HG22	13:M:201:LYS:N	2.35	0.42
14:N:28:DA:H2'	14:N:29:DT:C6	2.54	0.42
18:T:41:DC:H2''	18:T:42:DG:O5'	2.20	0.42
1:A:106:VAL:HG22	1:A:107:CYS:H	1.84	0.42
1:A:300:VAL:O	1:A:303:TYR:HB3	2.20	0.42
1:A:48:ALA:HB3	1:A:56:PRO:HD3	2.01	0.42
2:B:309:GLN:HE22	9:I:50:THR:HG21	1.85	0.42
2:B:369:GLY:O	16:Q:367:ALA:HB3	2.19	0.42
2:B:44:VAL:HG11	2:B:199:MET:SD	2.59	0.42
3:C:83:SER:OG	3:C:160:LYS:HD3	2.20	0.42
7:G:43:GLY:HA2	7:G:157:ILE:HD11	2.02	0.42
12:L:31:CYS:SG	12:L:32:ALA:N	2.93	0.42
13:M:198:VAL:HG12	13:M:202:GLU:OE1	2.20	0.42
14:N:28:DA:C8	14:N:29:DT:C7	3.03	0.42
1:A:80:HIS:H	1:A:243:PRO:HB3	1.85	0.42
1:A:399:HIS:O	1:A:401:GLY:N	2.53	0.42
1:A:635:ARG:NH2	1:A:877:HIS:HA	2.35	0.42
2:B:53:GLN:HG3	2:B:57:TYR:CD2	2.54	0.42
2:B:642:ASP:OD1	2:B:643:ASP:N	2.52	0.42
2:B:755:ILE:HG22	2:B:983:ARG:HD2	2.00	0.42
4:D:192:LYS:HB3	4:D:199:ASN:OD1	2.20	0.42
5:E:153:HIS:CD2	5:E:184:VAL:HG11	2.55	0.42
5:E:180:ARG:HH21	5:E:192:ARG:HG3	1.85	0.42
7:G:138:THR:HG22	7:G:139:ILE:N	2.32	0.42
7:G:142:ARG:HB3	7:G:171:ILE:HD12	2.01	0.42
11:K:35:PHE:CD2	11:K:71:PHE:CZ	3.07	0.42
13:M:198:VAL:HG11	13:M:203:PHE:CD1	2.54	0.42
16:Q:115:ARG:HD3	16:Q:390:ASP:OD2	2.20	0.42
16:Q:405:THR:O	16:Q:409:ALA:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:141:ARG:HD3	17:R:210:LYS:HZ3	1.84	0.42
15:O:98:ARG:NH2	18:T:59:DT:P	2.93	0.42
1:A:242:PRO:HB2	1:A:246:VAL:HB	2.01	0.42
2:B:106:ASP:N	2:B:106:ASP:OD1	2.52	0.42
5:E:163:GLU:O	5:E:167:ARG:HG2	2.20	0.42
9:I:101:PHE:CZ	9:I:112:SER:HB3	2.55	0.42
13:M:201:LYS:HE3	14:N:23:DA:C3'	2.50	0.42
14:N:27:DA:H1'	15:O:122:VAL:CG2	2.50	0.42
15:O:227:PHE:HA	15:O:230:ILE:HG22	2.01	0.42
1:A:1154:TYR:HB2	1:A:1191:TRP:CZ3	2.55	0.41
2:B:238:ALA:HB3	2:B:256:VAL:HB	2.02	0.41
2:B:357:GLN:CD	2:B:368:GLU:HG2	2.40	0.41
9:I:42:LEU:HD12	9:I:43:VAL:N	2.34	0.41
10:J:41:LEU:HD22	10:J:46:CYS:HB3	2.01	0.41
16:Q:369:ASN:HB2	16:Q:392:VAL:HG11	2.02	0.41
20:V:38:MET:O	20:V:42:GLU:HG3	2.19	0.41
1:A:1212:VAL:O	1:A:1216:ILE:HD12	2.20	0.41
1:A:185:TRP:HB2	1:A:198:GLU:HB3	2.02	0.41
1:A:855:THR:HG21	1:A:863:VAL:HG22	2.01	0.41
2:B:1187:ASN:OD1	2:B:1189:ILE:N	2.48	0.41
2:B:120:ARG:HB2	2:B:122:LEU:HG	2.01	0.41
2:B:134:LYS:HG2	2:B:154:GLU:O	2.20	0.41
2:B:185:THR:O	2:B:188:ASP:HB3	2.19	0.41
2:B:977:GLY:HA3	2:B:1099:VAL:HB	2.03	0.41
13:M:171:ILE:CD1	13:M:172:MET:HG3	2.50	0.41
13:M:269:ILE:O	13:M:271:GLY:N	2.53	0.41
16:Q:129:PRO:HG2	16:Q:132:ASP:HB2	2.03	0.41
17:R:105:THR:HG1	17:R:106:LEU:H	1.68	0.41
17:R:277:PHE:CE2	17:R:278:LEU:HD13	2.56	0.41
1:A:333:GLU:HA	1:A:338:GLY:HA3	2.01	0.41
2:B:189:LEU:HA	2:B:189:LEU:HD23	1.89	0.41
2:B:529:GLU:OE1	2:B:529:GLU:N	2.53	0.41
7:G:151:ILE:HG13	21:W:134:LEU:HA	2.00	0.41
7:G:23:LYS:O	7:G:26:LEU:HB2	2.19	0.41
8:H:117:SER:HA	8:H:122:LEU:HD23	2.02	0.41
14:N:42:DT:C6	14:N:42:DT:C3'	3.04	0.41
13:M:274:PRO:CG	15:O:188:GLU:OE2	2.61	0.41
16:Q:379:GLU:HG2	16:Q:383:SER:O	2.20	0.41
1:A:1420:ASP:OD2	1:A:1422:ARG:NE	2.36	0.41
1:A:356:ASP:OD2	11:K:65:HIS:NE2	2.28	0.41
2:B:1094:ARG:HH21	2:B:1098:MET:HG2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.50	0.41
2:B:412:LEU:HD23	2:B:476:ARG:HH12	1.85	0.41
5:E:58:MET:HE1	5:E:82:PHE:HE2	1.86	0.41
7:G:150:CYS:SG	7:G:159:ALA:HB2	2.61	0.41
4:D:32:GLU:HG2	7:G:41:LYS:HE2	1.98	0.41
16:Q:119:LEU:HD23	16:Q:119:LEU:HA	1.77	0.41
1:A:516:SER:O	1:A:517:ASN:OD1	2.39	0.41
2:B:1069:PHE:HE2	3:C:192:TRP:CD2	2.38	0.41
9:I:74:GLU:HB3	9:I:81:ARG:HG2	2.01	0.41
10:J:2:ILE:O	10:J:2:ILE:HG23	2.21	0.41
1:A:1397:LEU:HA	1:A:1400:CYS:SG	2.60	0.41
1:A:960:ILE:O	1:A:964:ILE:HD12	2.21	0.41
2:B:342:GLY:C	2:B:344:LYS:H	2.24	0.41
3:C:174:ALA:N	3:C:233:GLU:O	2.52	0.41
4:D:155:ARG:HB3	4:D:219:THR:HG21	2.01	0.41
5:E:169:ARG:HD3	6:F:140:ASP:OD2	2.20	0.41
13:M:164:LYS:HG2	13:M:164:LYS:O	2.20	0.41
13:M:168:MET:HA	13:M:171:ILE:CG1	2.50	0.41
13:M:267:LYS:HZ1	15:O:169:PRO:HB3	1.73	0.41
20:V:119:LYS:N	20:V:119:LYS:HD3	2.36	0.41
1:A:175:ARG:O	1:A:182:VAL:HG12	2.20	0.41
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	2.01	0.41
2:B:70:ILE:HG22	2:B:89:GLU:HG3	2.02	0.41
3:C:101:LEU:HB2	3:C:118:LEU:HD23	2.02	0.41
7:G:121:PHE:CE2	7:G:123:ALA:HB2	2.56	0.41
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.46	0.41
13:M:251:GLN:HA	13:M:254:THR:HG22	2.02	0.41
17:R:61:LEU:HD21	17:R:63:ARG:O	2.20	0.41
2:B:676:VAL:C	2:B:678:GLU:H	2.23	0.41
13:M:162:THR:HG23	13:M:213:ILE:HD11	2.03	0.41
13:M:191:GLU:O	13:M:194:SER:OG	2.25	0.41
14:N:25:DA:H8	14:N:25:DA:O5'	2.03	0.41
16:Q:378:VAL:HA	16:Q:384:PHE:CD1	2.56	0.41
16:Q:115:ARG:O	17:R:136:THR:HA	2.20	0.41
1:A:1194:ARG:HA	1:A:1238:ILE:O	2.20	0.41
1:A:215:SER:O	1:A:218:ASP:HB2	2.20	0.41
1:A:540:PHE:CG	1:A:571:LEU:HD23	2.56	0.41
1:A:814:PHE:HB2	2:B:519:TRP:HZ3	1.86	0.41
2:B:290:GLY:HA2	2:B:327:ARG:HD2	2.03	0.41
4:D:30:GLY:O	4:D:34:GLN:N	2.54	0.41
22:X:225:GLU:CB	22:X:232:VAL:CB	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:225:GLU:CB	22:X:232:VAL:H	2.33	0.41
1:A:1021:LEU:O	1:A:1024:SER:OG	2.25	0.41
1:A:244:PRO:O	1:A:247:ARG:N	2.54	0.41
2:B:757:PRO:HD3	2:B:983:ARG:NE	2.26	0.41
2:B:914:LYS:O	2:B:937:ALA:O	2.39	0.41
1:A:544:ASP:HB2	11:K:47:ARG:HH12	1.85	0.41
1:A:1132:LYS:HA	1:A:1135:ARG:NH1	2.35	0.41
1:A:727:ASP:HB3	1:A:731:ARG:HH12	1.85	0.41
2:B:240:ILE:HG23	2:B:254:LEU:HB3	2.03	0.41
2:B:339:THR:HG21	2:B:351:TYR:OH	2.20	0.41
2:B:546:SER:OG	2:B:632:ARG:N	2.54	0.41
2:B:705:MET:H	2:B:710:LEU:HD12	1.86	0.41
2:B:796:LEU:HD11	2:B:851:PHE:HA	2.02	0.41
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.57	0.41
7:G:59:GLY:HA2	7:G:70:PHE:HD1	1.85	0.41
10:J:18:TRP:O	10:J:21:TYR:HB3	2.21	0.41
18:T:64:DA:N3	18:T:65:DC:C2	2.89	0.41
1:A:913:LEU:HD23	1:A:1032:LEU:HD13	2.03	0.40
2:B:760:ASP:N	2:B:760:ASP:OD1	2.53	0.40
8:H:98:TYR:OH	8:H:139:ASN:ND2	2.54	0.40
13:M:44:VAL:HG13	13:M:50:LEU:O	2.21	0.40
13:M:267:LYS:CD	15:O:239:LYS:HE3	2.52	0.40
13:M:267:LYS:CE	15:O:239:LYS:HE3	2.52	0.40
16:Q:361:TRP:CH2	16:Q:397:ALA:HB2	2.56	0.40
1:A:1368:MET:O	1:A:1372:VAL:HG23	2.21	0.40
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	2.03	0.40
2:B:1171:VAL:HG22	2:B:1182:CYS:HB2	2.02	0.40
2:B:171:PRO:O	2:B:172:ILE:HD13	2.21	0.40
2:B:416:LEU:HA	2:B:416:LEU:HD12	1.84	0.40
2:B:604:ARG:HH22	2:B:615:MET:H	1.69	0.40
2:B:826:ALA:HB2	2:B:1087:PHE:HD1	1.86	0.40
2:B:941:LEU:HD23	2:B:942:ARG:O	2.21	0.40
2:B:98:THR:OG1	2:B:127:GLY:N	2.54	0.40
4:D:194:LEU:CD2	7:G:86:VAL:HG21	2.51	0.40
8:H:106:GLU:HG2	8:H:112:ILE:HD13	2.04	0.40
11:K:35:PHE:O	11:K:70:ARG:HB2	2.21	0.40
13:M:162:THR:CG2	13:M:213:ILE:HD11	2.52	0.40
20:V:51:THR:HA	20:V:55:ASN:HD22	1.87	0.40
1:A:369:SER:HB3	11:K:2:ASN:OD1	2.20	0.40
2:B:88:TYR:CD1	2:B:136:THR:HG23	2.57	0.40
2:B:243:ALA:HA	2:B:250:PHE:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:GLU:HG3	2:B:771:SER:HB2	2.03	0.40
4:D:138:ASN:ND2	7:G:36:GLY:CA	2.84	0.40
7:G:132:SER:OG	7:G:133:SER:N	2.54	0.40
13:M:157:CYS:SG	13:M:158:HIS:N	2.93	0.40
15:O:99:PHE:CD1	18:T:58:DT:O4'	2.74	0.40
18:T:44:DA:C2'	18:T:44:DA:OP2	2.69	0.40
1:A:1287:TYR:OH	1:A:1307:GLU:OE2	2.37	0.40
2:B:724:ASP:OD1	2:B:725:PRO:HD2	2.21	0.40
2:B:979:LYS:HG2	2:B:980:PHE:N	2.37	0.40
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.52	0.40
15:O:171:ARG:HA	15:O:239:LYS:HZ3	1.87	0.40
19:U:5:GLU:O	19:U:9:VAL:HG23	2.21	0.40
1:A:1015:VAL:O	1:A:1015:VAL:HG12	2.22	0.40
9:I:43:VAL:HG23	9:I:44:TYR:H	1.86	0.40
17:R:118:HIS:HB2	17:R:120:TYR:CZ	2.57	0.40
17:R:98:ASN:O	17:R:102:SER:N	2.54	0.40

There are no symmetry-related clashes.

## 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 PDB entries followed by that with respect to all EM entries.

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	1386/1733 (80%)	1306 (94%)	77 (6%)	3 (0%)	52	86
2	B	1139/1224 (93%)	1085 (95%)	49 (4%)	5 (0%)	39	80
3	C	260/318 (82%)	246 (95%)	14 (5%)	0	100	100
4	D	153/221 (69%)	145 (95%)	8 (5%)	0	100	100
5	E	211/215 (98%)	209 (99%)	2 (1%)	0	100	100
6	F	81/155 (52%)	76 (94%)	5 (6%)	0	100	100
7	G	169/171 (99%)	160 (95%)	8 (5%)	1 (1%)	30	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	132/146 (90%)	114 (86%)	14 (11%)	4 (3%)	5	42
9	I	114/122 (93%)	105 (92%)	9 (8%)	0	100	100
10	J	63/70 (90%)	57 (90%)	5 (8%)	1 (2%)	12	56
11	K	110/120 (92%)	107 (97%)	3 (3%)	0	100	100
12	L	43/70 (61%)	37 (86%)	6 (14%)	0	100	100
13	M	225/345 (65%)	202 (90%)	20 (9%)	3 (1%)	15	60
15	O	178/240 (74%)	174 (98%)	4 (2%)	0	100	100
16	Q	140/735 (19%)	124 (89%)	13 (9%)	3 (2%)	9	50
17	R	181/400 (45%)	171 (94%)	9 (5%)	1 (1%)	30	74
19	U	88/286 (31%)	82 (93%)	3 (3%)	3 (3%)	5	40
20	V	96/122 (79%)	88 (92%)	7 (7%)	1 (1%)	19	65
21	W	162/482 (34%)	154 (95%)	7 (4%)	1 (1%)	30	74
22	X	135/328 (41%)	125 (93%)	9 (7%)	1 (1%)	26	71
All	All	5066/7503 (68%)	4767 (94%)	272 (5%)	27 (0%)	38	77

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	343	ILE
2	B	476	ARG
8	H	132	LEU
13	M	269	ILE
17	R	259	VAL
22	X	231	LEU
2	B	221	ASN
8	H	131	ASN
8	H	137	GLN
13	M	200	THR
19	U	31	ASP
19	U	264	ASP
20	V	6	TYR
21	W	40	GLU
2	B	364	ILE
7	G	63	PRO
8	H	90	ALA
16	Q	26	ARG
16	Q	406	ILE

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Mol	Chain	Res	Type
2	B	743	ILE
13	M	31	PRO
1	A	958	VAL
1	A	50	ILE
16	Q	127	ILE
19	U	30	ILE
10	J	2	ILE
1	A	569	LYS

### 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 PDB entries followed by that with respect to all EM entries.

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	1221/1520 (80%)	1219 (100%)	2 (0%)	95	97
2	B	999/1061 (94%)	998 (100%)	1 (0%)	95	97
3	C	230/274 (84%)	230 (100%)	0	100	100
4	D	139/200 (70%)	139 (100%)	0	100	100
5	E	195/197 (99%)	195 (100%)	0	100	100
6	F	73/137 (53%)	73 (100%)	0	100	100
7	G	152/152 (100%)	152 (100%)	0	100	100
8	H	119/128 (93%)	119 (100%)	0	100	100
9	I	110/116 (95%)	110 (100%)	0	100	100
10	J	60/65 (92%)	60 (100%)	0	100	100
11	K	97/102 (95%)	97 (100%)	0	100	100
12	L	40/57 (70%)	40 (100%)	0	100	100
13	M	201/299 (67%)	200 (100%)	1 (0%)	92	96
15	O	152/205 (74%)	141 (93%)	11 (7%)	18	55
16	Q	108/641 (17%)	108 (100%)	0	100	100
17	R	107/363 (30%)	107 (100%)	0	100	100
19	U	84/260 (32%)	79 (94%)	5 (6%)	24	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	V	90/108 (83%)	85 (94%)	5 (6%)	26 62
All	All	4177/5885 (71%)	4152 (99%)	25 (1%)	91 95

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	736	ASN
2	B	465	ASN
13	M	202	GLU
15	O	70	ILE
15	O	79	ARG
15	O	108	GLU
15	O	130	ASP
15	O	134	LEU
15	O	175	LEU
15	O	199	LYS
15	O	219	GLN
15	O	225	GLN
15	O	235	SER
15	O	240	MET
19	U	25	PHE
19	U	241	GLU
19	U	253	ARG
19	U	267	VAL
19	U	277	GLN
20	V	9	LEU
20	V	33	GLU
20	V	39	ARG
20	V	57	GLN
20	V	108	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	60	GLN
2	B	215	GLN
2	B	325	GLN
4	D	143	ASN
4	D	173	HIS
13	M	197	HIS

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Mol	Chain	Res	Type
15	O	95	ASN
15	O	158	GLN
15	O	219	GLN
16	Q	122	GLN
19	U	280	GLN
20	V	55	ASN
20	V	57	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.